



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:39 pm BST

PDB ID : 4XSY
Title : Crystal structure of CBR 9379 bound to Escherichia coli RNA polymerase holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-22
Resolution : 4.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

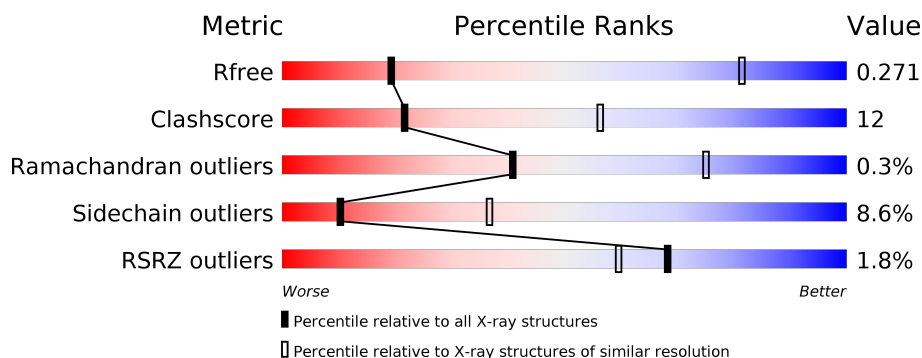
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.01 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 ≥ 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	239	<div> <div>63%</div> <div>29%</div> <div>6%</div> </div>
1	B	239	<div>4%</div> <div>60%</div> <div>30%</div> <div>8%</div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div><div>%</div><div><div></div><div>54%</div><div>25%</div><div>•</div><div>17%</div></div></div></div>
3	J	1407	<div><div><div>%</div><div><div></div><div>57%</div><div>27%</div><div>•</div><div>12%</div></div></div></div>
4	E	91	<div><div><div></div><div><div>78%</div><div>16%</div><div>• •</div></div></div></div>
4	K	91	<div><div><div></div><div><div>62%</div><div>23%</div><div>•</div><div>13%</div></div></div></div>
5	F	522	<div><div><div>3%</div><div><div></div><div>64%</div><div>23%</div><div>•</div><div>10%</div></div></div></div>
5	L	522	<div><div><div>2%</div><div><div></div><div>63%</div><div>23%</div><div>•</div><div>10%</div></div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55746 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	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP A7ZSI4
A	236	VAL	-	expression tag	UNP A7ZSI4
A	237	LEU	-	expression tag	UNP A7ZSI4
A	238	PHE	-	expression tag	UNP A7ZSI4
A	239	GLN	-	expression tag	UNP A7ZSI4
B	235	GLU	-	expression tag	UNP A7ZSI4
B	236	VAL	-	expression tag	UNP A7ZSI4
B	237	LEU	-	expression tag	UNP A7ZSI4
B	238	PHE	-	expression tag	UNP A7ZSI4
B	239	GLN	-	expression tag	UNP A7ZSI4
G	235	GLU	-	expression tag	UNP A7ZSI4
G	236	VAL	-	expression tag	UNP A7ZSI4
G	237	LEU	-	expression tag	UNP A7ZSI4
G	238	PHE	-	expression tag	UNP A7ZSI4
G	239	GLN	-	expression tag	UNP A7ZSI4
H	235	GLU	-	expression tag	UNP A7ZSI4
H	236	VAL	-	expression tag	UNP A7ZSI4
H	237	LEU	-	expression tag	UNP A7ZSI4
H	238	PHE	-	expression tag	UNP A7ZSI4
H	239	GLN	-	expression tag	UNP A7ZSI4

- 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	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1236	Total	C	N	O	S	0	0	0
			9638	6058	1726	1807	47			

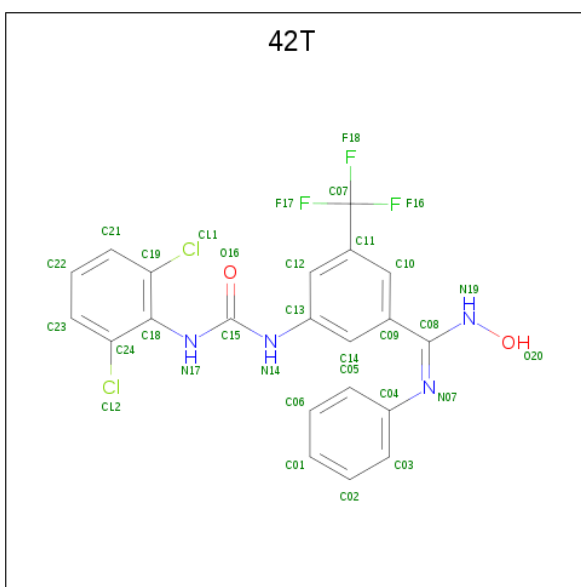
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is 3-([(2,6-dichlorophenyl)carbamoyl]amino)-N-hydroxy-N'-phenyl-5-(trifluoromethyl)benzenecarboximidamide (three-letter code: 42T) (formula: C₂₁H₁₅Cl₂F₃N₄O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	Cl	F	N	O	0	0
			32	21	2	3	4	2		
6	J	1	Total	C	Cl	F	N	O	0	0
			32	21	2	3	4	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		

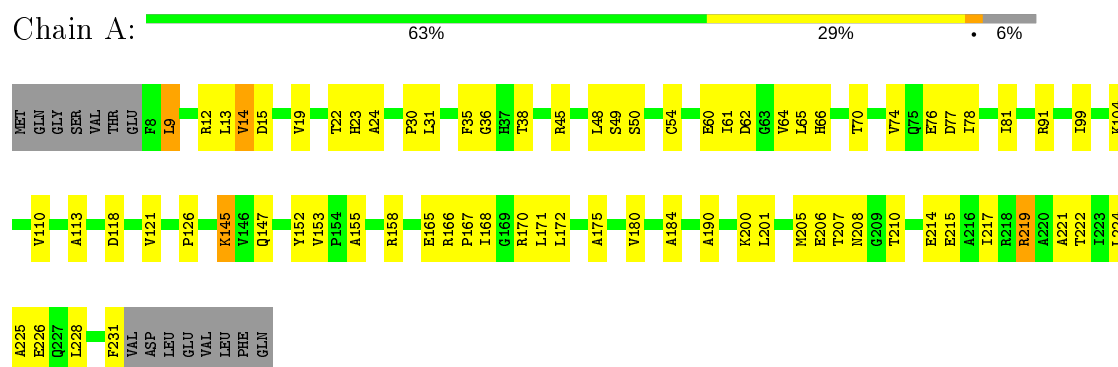
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

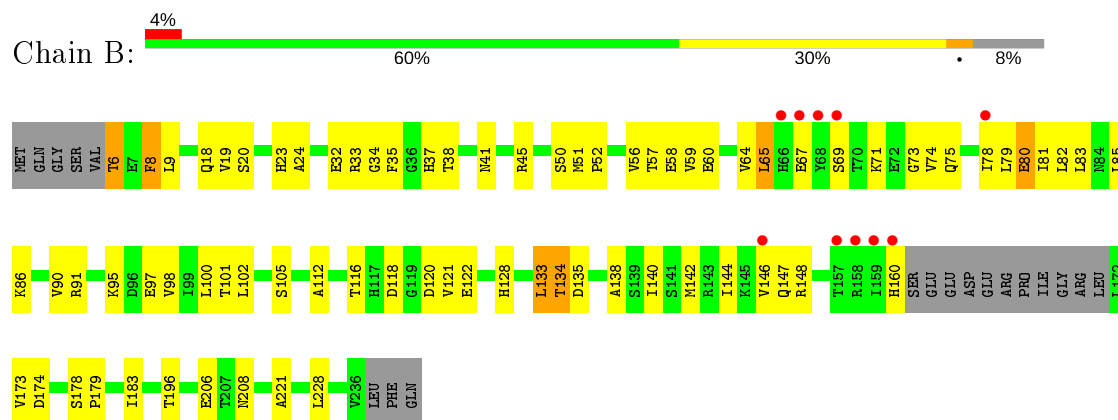
3 Residue-property plots

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

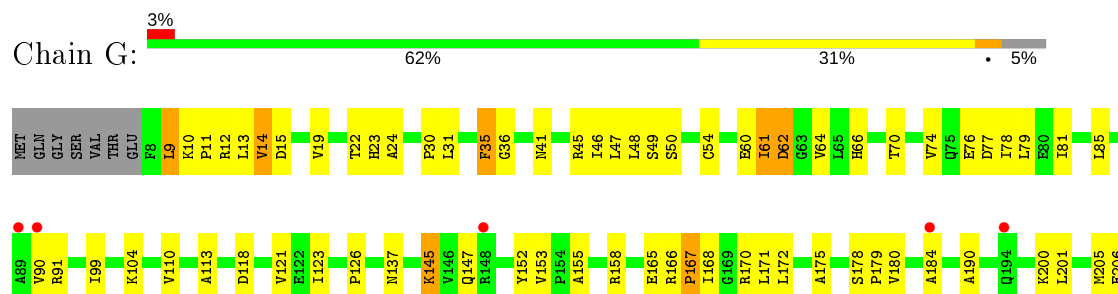
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

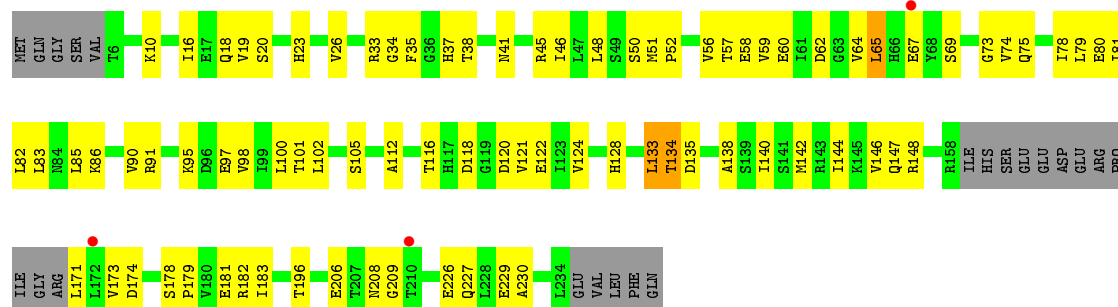


• Molecule 1: DNA-directed RNA polymerase subunit alpha

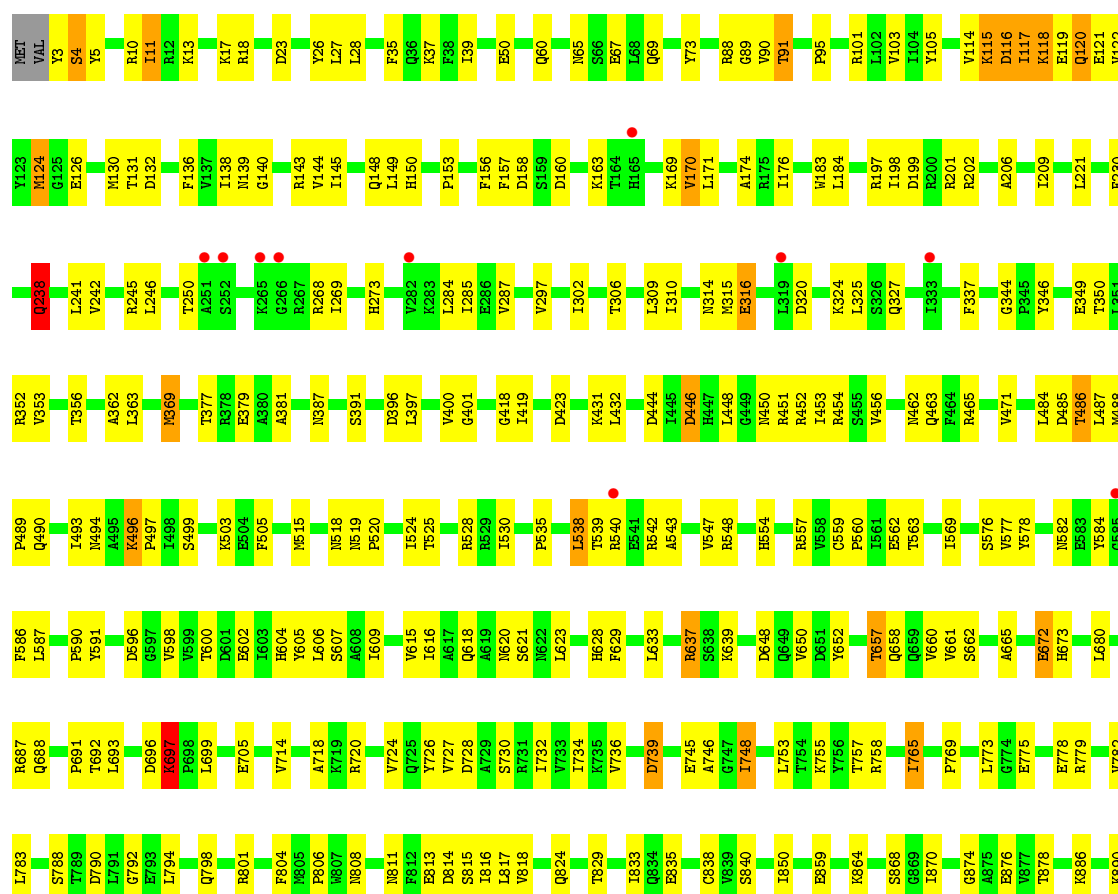


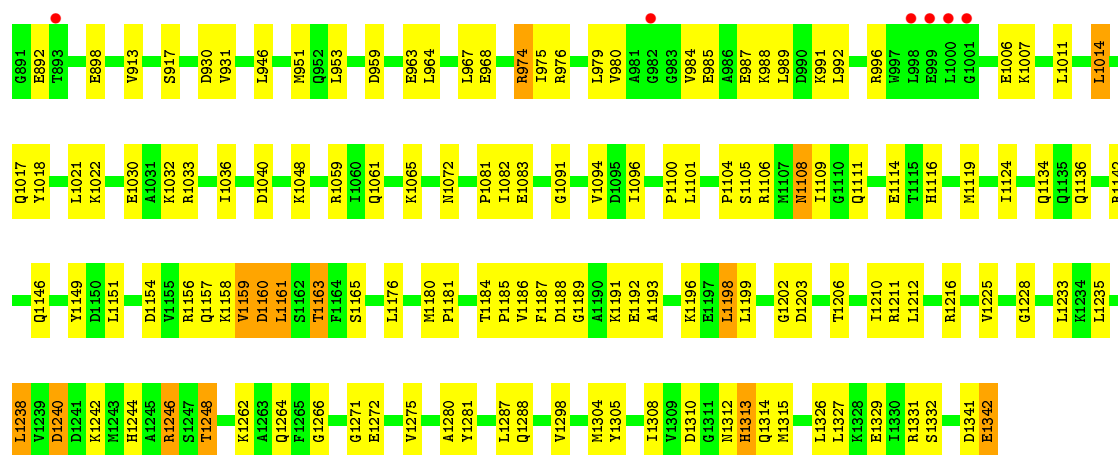


• Molecule 1: DNA-directed RNA polymerase subunit alpha

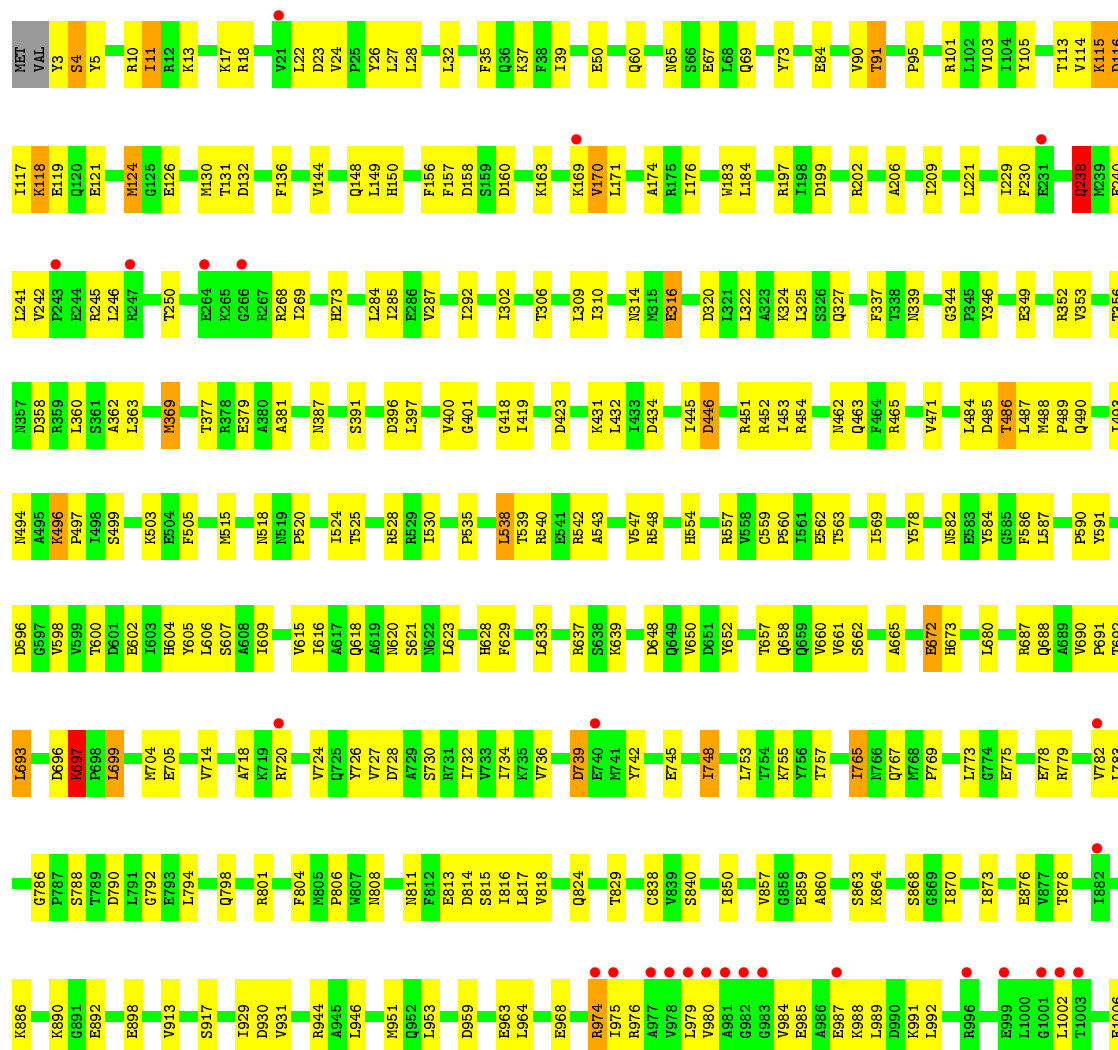


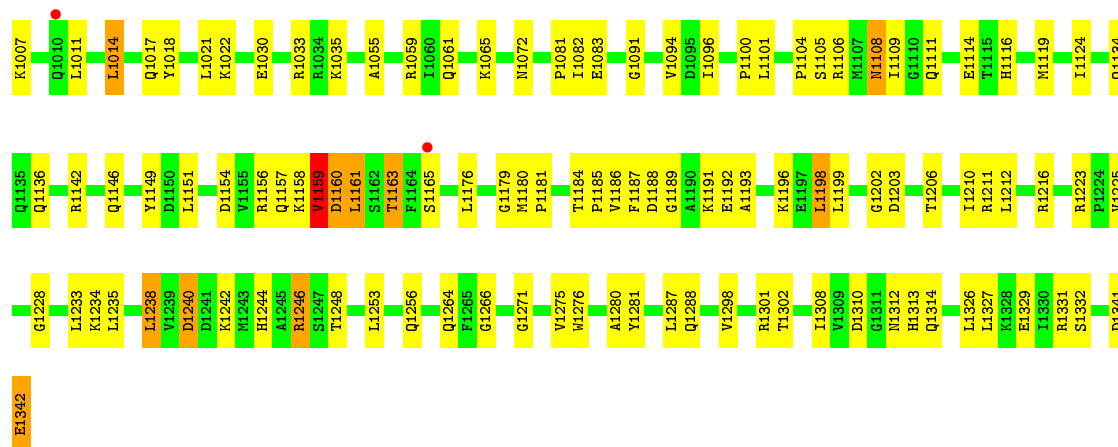
• Molecule 2: DNA-directed RNA polymerase subunit beta



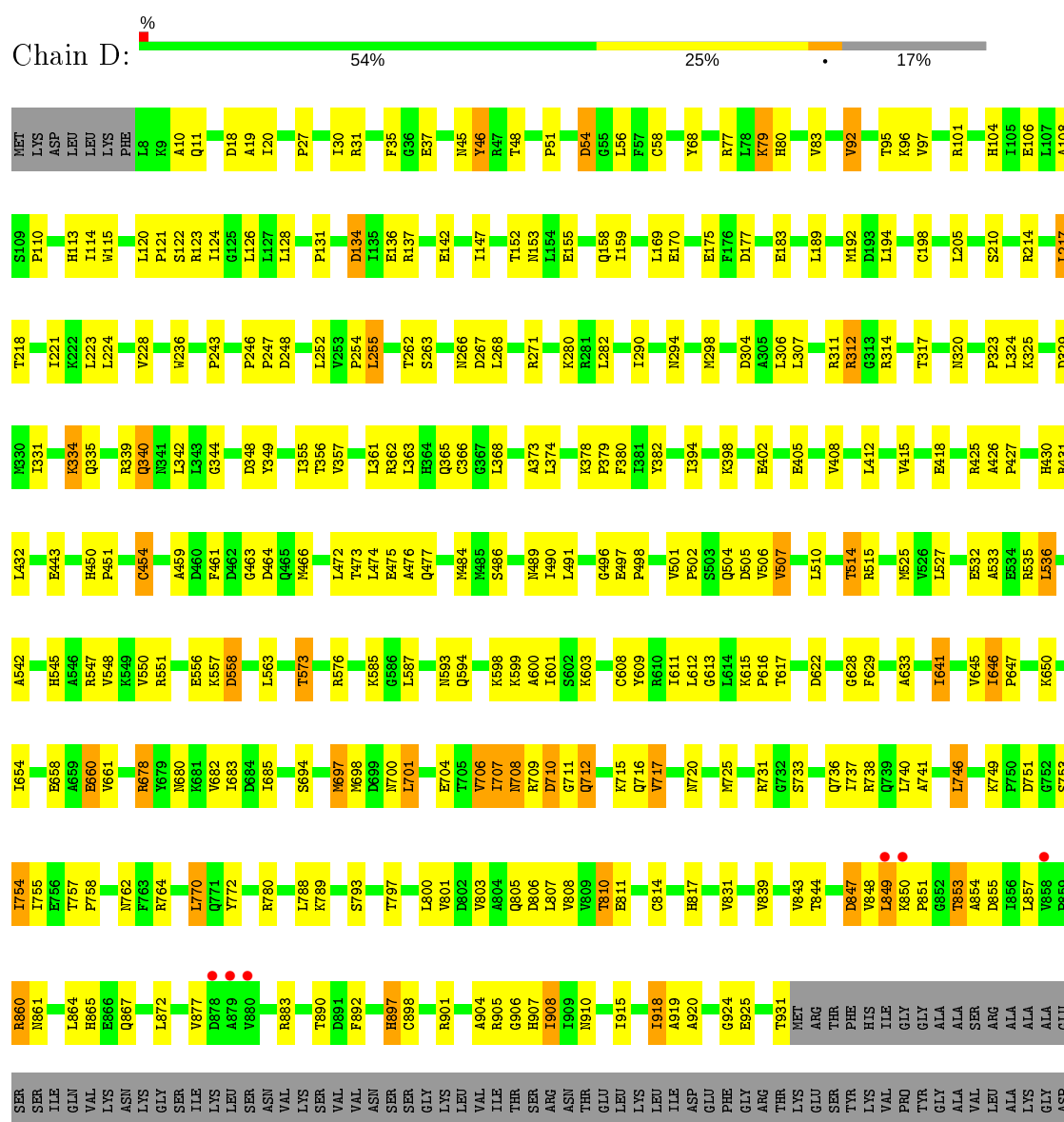


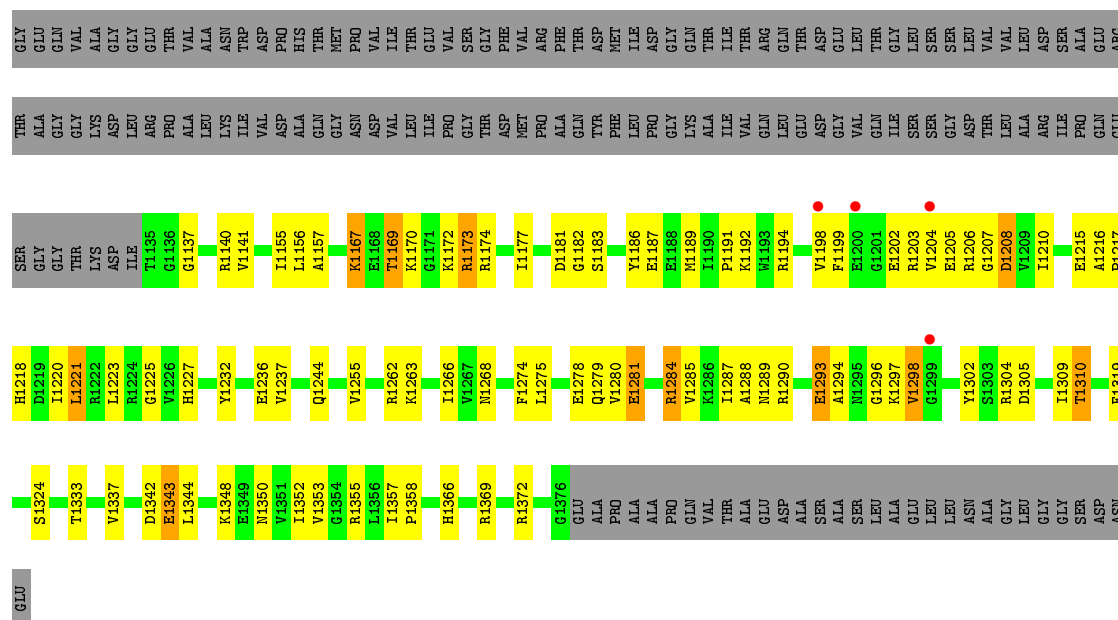
• Molecule 2: DNA-directed RNA polymerase subunit beta



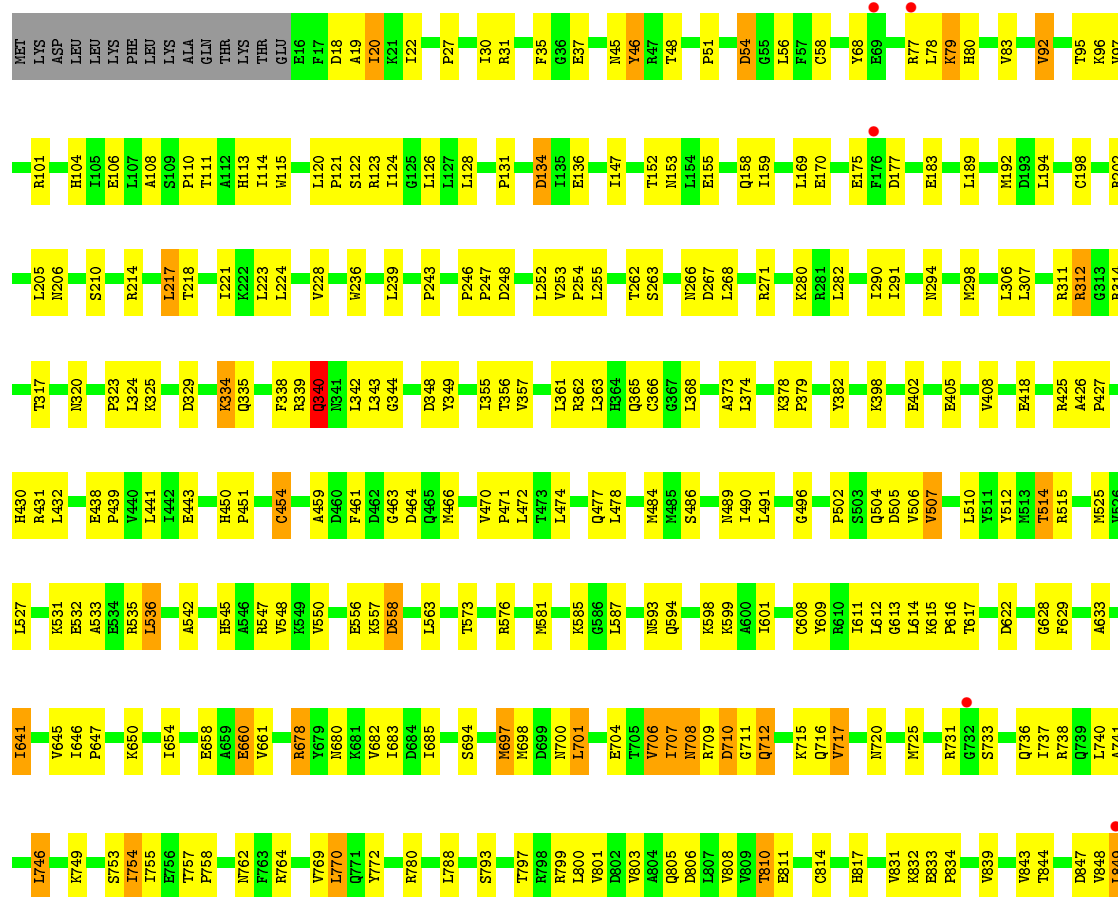


- Molecule 3: DNA-directed RNA polymerase subunit beta'

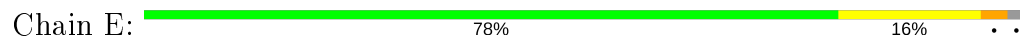




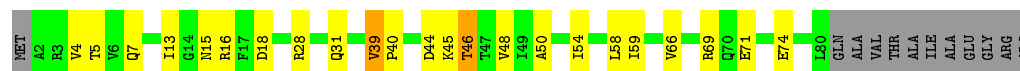
• Molecule 3: DNA-directed RNA polymerase subunit beta'



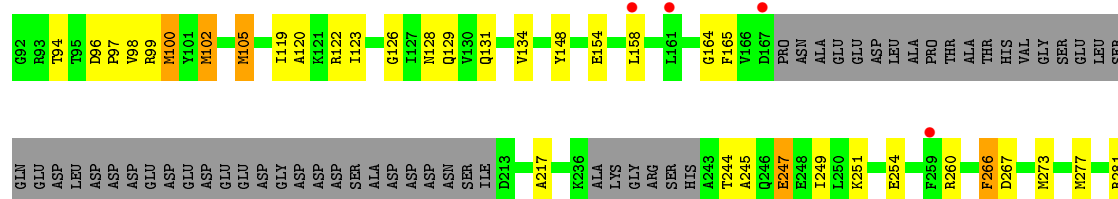
- Molecule 4: DNA-directed RNA polymerase subunit omega

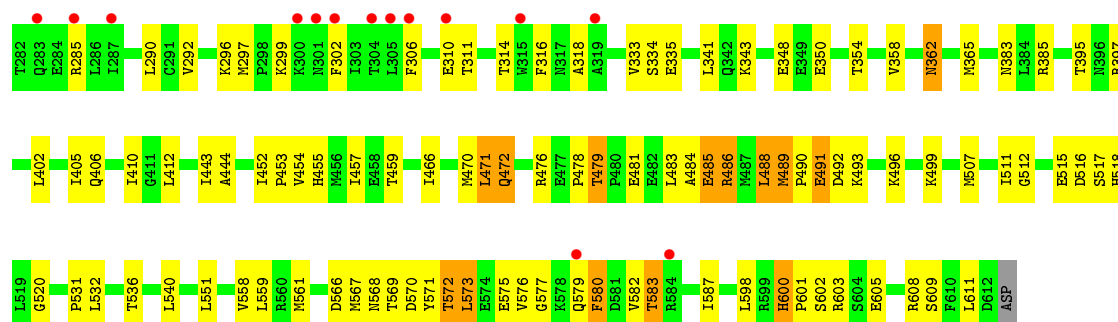


- Molecule 4: DNA-directed RNA polymerase subunit omega

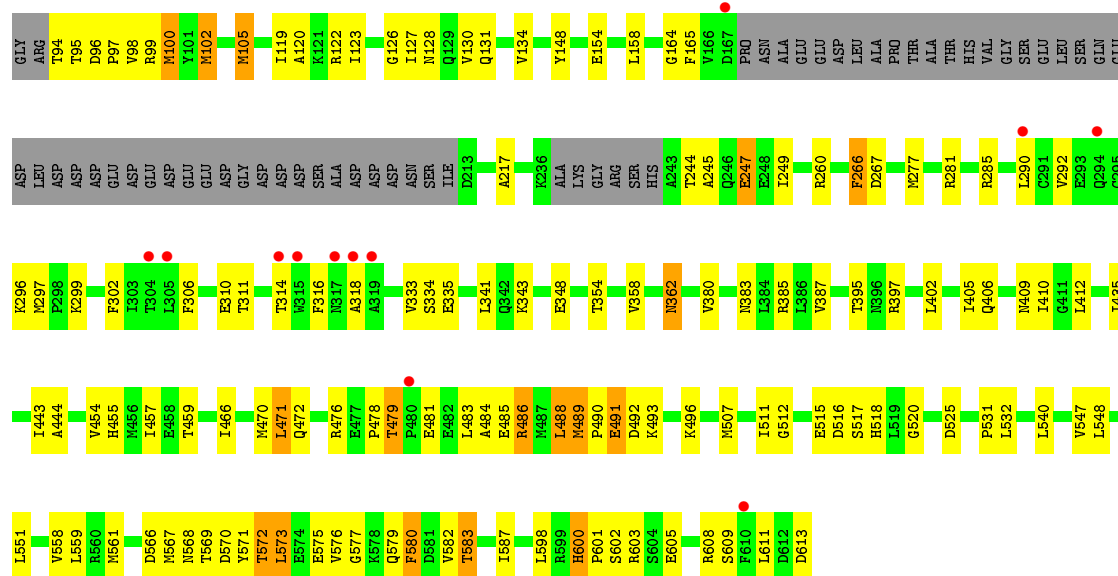


- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.39Å 206.77Å 310.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.36 – 4.01 40.36 – 4.01	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.36-4.01) 96.0 (40.36-4.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.270 0.235 , 0.271	Depositor DCC
R_{free} test set	4849 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	195.8	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55746	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 42T

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	0.26	0/1751	0.51	0/2373
1	B	0.28	0/1707	0.52	0/2314
1	G	0.26	0/1771	0.52	0/2401
1	H	0.27	0/1686	0.51	0/2285
2	C	0.28	0/10739	0.50	0/14489
2	I	0.27	0/10735	0.49	0/14484
3	D	0.27	0/9246	0.49	0/12478
3	J	0.27	0/9785	0.49	0/13206
4	E	0.27	0/693	0.51	0/935
4	K	0.28	0/629	0.52	0/847
5	F	0.29	0/3873	0.48	0/5206
5	L	0.29	0/3872	0.48	0/5205
All	All	0.28	0/56487	0.49	0/76223

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1161	LEU	Peptide
2	C	648	ASP	Peptide
3	D	1169	THR	Peptide
3	D	1296	GLY	Peptide
2	I	1161	LEU	Peptide
2	I	648	ASP	Peptide
3	J	1169	THR	Peptide
3	J	1296	GLY	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	1730	0	1756	48	0
1	B	1687	0	1700	60	0
1	G	1750	0	1764	56	0
1	H	1667	0	1689	61	0
2	C	10570	0	10582	265	0
2	I	10566	0	10576	248	0
3	D	9107	0	9308	260	0
3	J	9638	0	9853	271	0
4	E	691	0	695	12	0
4	K	627	0	634	13	0
5	F	3822	0	3885	86	0
5	L	3821	0	3884	87	0
6	C	32	0	14	0	0
6	J	32	0	14	0	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	55746	0	56354	1330	0

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

All (1330) 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	1.45	0.96
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.95
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.57	0.87
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.57	0.86
1:G:45:ARG:NH1	1:H:34:GLY:O	2.10	0.85
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.56	0.85
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.58	0.84
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.59	0.83
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.59	0.82
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.63	0.80
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.61	0.80
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.64	0.78
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.49	0.78
2:C:115:LYS:HE3	2:C:116:ASP:H	1.49	0.78
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.67	0.77
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.50	0.76
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.69	0.75
3:D:418:GLU:HG3	4:E:45:LYS:H	1.52	0.75
2:I:115:LYS:HE3	2:I:116:ASP:H	1.49	0.74
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.69	0.74
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.53	0.73
2:I:452:ARG:NH1	2:I:584:TYR:O	2.21	0.72
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.52	0.72
2:C:452:ARG:NH1	2:C:584:TYR:O	2.22	0.72
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.69	0.72
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.56	0.71
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.24	0.71
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.56	0.71
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.73	0.71
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.72	0.70
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.73	0.70
5:F:292:VAL:HG21	5:F:299:LYS:HG2	1.73	0.70
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.73	0.70
5:L:292:VAL:HG21	5:L:299:LYS:HG2	1.74	0.70
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.74	0.70
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.71	0.70
1:G:226:GLU:HG2	1:H:10:LYS:HE3	1.74	0.70
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.74	0.70
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.70
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.74	0.70
5:L:97:PRO:HA	5:L:100:MET:HG3	1.73	0.69
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.74	0.69
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.73	0.69
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.74	0.69
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.26	0.69
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.73	0.69
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.68
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.76	0.68
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.76	0.68
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.76	0.67
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.75	0.67
2:C:444:ASP:O	2:C:450:ASN:ND2	2.27	0.67
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.76	0.67
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.26	0.67
5:F:602:SER:H	5:F:605:GLU:HG3	1.60	0.67
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.76	0.67
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.77	0.67
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.76	0.66
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.77	0.66
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.76	0.66
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.77	0.66
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.78	0.66
3:J:576:ARG:NH1	3:J:593:ASN:O	2.29	0.66
1:A:12:ARG:H	1:A:30:PRO:HD2	1.61	0.66
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.77	0.66
1:G:12:ARG:H	1:G:30:PRO:HD2	1.61	0.66
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.77	0.66
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.76	0.66
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.77	0.66
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.78	0.65
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.77	0.65
3:D:576:ARG:NH1	3:D:593:ASN:O	2.29	0.65
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.65
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.77	0.65
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.62	0.65
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.61	0.65
1:A:166:ARG:O	1:A:168:ILE:N	2.30	0.64
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.77	0.64
5:L:602:SER:H	5:L:605:GLU:HG3	1.62	0.64
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.80	0.64
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.79	0.64
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.80	0.64
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.30	0.64
3:J:1216:ALA:HB1	3:J:1218:HIS:HD2	1.63	0.64
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.80	0.64
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.64
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.80	0.63
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.31	0.63
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.80	0.63
2:I:324:LYS:O	2:I:327:GLN:NE2	2.29	0.63
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.80	0.63
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.64	0.63
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.79	0.63
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.80	0.63
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.81	0.63
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.80	0.63
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.80	0.63
1:H:90:VAL:HG11	1:H:146:VAL:HG11	1.81	0.63
3:D:1297:LYS:HG2	3:J:1302:TYR:O	1.99	0.62
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.64	0.62
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.79	0.62
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.62
2:I:864:LYS:NZ	2:I:876:GLU:O	2.33	0.62
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.80	0.62
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.80	0.62
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.82	0.62
3:D:362:ARG:H	3:D:365:GLN:HE21	1.48	0.62
3:D:325:LYS:HG3	3:D:329:ASP:HB2	1.82	0.61
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.65	0.61
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.83	0.61
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.80	0.61
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.82	0.61
1:H:182:ARG:NH1	3:J:581:MET:SD	2.74	0.61
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.81	0.61
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.65	0.61
2:C:324:LYS:O	2:C:327:GLN:NE2	2.29	0.61
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.82	0.61
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.82	0.61
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.61
3:D:1225:GLY:HA2	3:J:1296:GLY:HA2	1.82	0.61
3:J:362:ARG:H	3:J:365:GLN:HE21	1.48	0.61
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.15	0.61
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.83	0.61
2:C:829:THR:HA	2:C:1059:ARG:HA	1.83	0.61
3:D:77:ARG:HG3	3:D:79:LYS:H	1.65	0.61
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.82	0.61
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.82	0.61
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.67	0.60
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.82	0.60
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.66	0.60
5:L:479:THR:HG23	5:L:481:GLU:H	1.67	0.60
2:C:864:LYS:NZ	2:C:876:GLU:O	2.32	0.60
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.66	0.60
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.60
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.83	0.60
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.83	0.60
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.66	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.67	0.60
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.84	0.60
2:C:250:THR:HA	2:C:268:ARG:HA	1.84	0.60
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.67	0.60
2:C:18:ARG:NH1	2:C:621:SER:O	2.35	0.60
1:G:23:HIS:HB2	1:G:205:MET:O	2.02	0.60
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.66	0.60
3:J:514:THR:HB	3:J:576:ARG:HG2	1.83	0.60
2:C:136:PHE:O	2:C:143:ARG:N	2.31	0.60
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.83	0.59
2:C:598:VAL:HG22	2:C:628:HIS:HE1	1.67	0.59
3:D:1216:ALA:HB1	3:D:1218:HIS:HD2	1.67	0.59
2:I:829:THR:HA	2:I:1059:ARG:HA	1.83	0.59
3:J:77:ARG:HG3	3:J:79:LYS:H	1.67	0.59
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.84	0.59
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.66	0.59
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.83	0.59
3:D:340:GLN:HA	3:D:340:GLN:HE21	1.65	0.59
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.68	0.59
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.66	0.59
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.83	0.59
1:A:45:ARG:NH1	1:B:34:GLY:O	2.31	0.59
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.85	0.59
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.59
2:I:250:THR:HA	2:I:268:ARG:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:561:MET:HA	5:L:567:MET:HE1	1.84	0.59
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.85	0.59
5:F:573:LEU:H	5:F:573:LEU:HD23	1.67	0.59
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.83	0.59
3:D:741:ALA:O	3:D:762:ASN:ND2	2.35	0.59
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.38	0.59
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.85	0.59
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	1.85	0.58
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.68	0.58
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.84	0.58
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.84	0.58
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.85	0.58
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.84	0.58
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.86	0.58
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.58
2:I:18:ARG:NH1	2:I:621:SER:O	2.36	0.58
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.86	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.85	0.58
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.86	0.58
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.84	0.58
1:A:45:ARG:HG2	1:B:38:THR:HB	1.85	0.58
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.69	0.58
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.85	0.58
1:A:23:HIS:HB2	1:A:205:MET:O	2.04	0.58
3:D:1227:HIS:CD2	3:J:1292:LEU:HB3	2.37	0.58
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.85	0.58
3:D:514:THR:HB	3:D:576:ARG:HG2	1.83	0.58
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.86	0.58
1:B:101:THR:H	1:B:116:THR:HG22	1.69	0.58
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.86	0.58
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.85	0.58
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.04	0.58
5:L:573:LEU:H	5:L:573:LEU:HD23	1.69	0.58
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.85	0.57
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.04	0.57
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.86	0.57
2:I:349:GLU:HA	2:I:352:ARG:HG3	1.85	0.57
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.86	0.57
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.68	0.57
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.87	0.57
1:H:101:THR:H	1:H:116:THR:HG22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:GLU:HA	2:C:352:ARG:HG3	1.86	0.57
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.86	0.57
3:D:843:VAL:HG11	3:D:897:HIS:O	2.05	0.57
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.69	0.57
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.85	0.57
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.87	0.57
2:I:560:PRO:O	3:J:780:ARG:NH2	2.37	0.57
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.87	0.57
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.87	0.57
5:F:515:GLU:HG2	5:F:516:ASP:H	1.70	0.57
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.86	0.57
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.87	0.57
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.87	0.57
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.87	0.57
3:J:741:ALA:O	3:J:762:ASN:ND2	2.38	0.57
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.86	0.56
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.70	0.56
5:L:548:LEU:HD23	5:L:551:LEU:HD12	1.87	0.56
2:C:560:PRO:O	3:D:780:ARG:NH2	2.39	0.56
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.88	0.56
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.86	0.56
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.87	0.56
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.87	0.56
5:F:561:MET:HA	5:F:567:MET:HE1	1.87	0.56
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.87	0.56
1:B:86:LYS:HD2	1:B:174:ASP:HB2	1.88	0.56
3:D:361:LEU:HD13	3:D:366:CYS:HA	1.88	0.56
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.87	0.56
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.87	0.56
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.87	0.56
3:D:853:THR:HG22	3:D:854:ALA:H	1.70	0.56
1:B:101:THR:HG22	1:B:116:THR:HB	1.88	0.56
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.86	0.56
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.88	0.56
5:F:466:ILE:HB	5:F:483:LEU:HD23	1.87	0.56
1:H:101:THR:HG22	1:H:116:THR:HB	1.87	0.56
3:J:843:VAL:HG11	3:J:897:HIS:O	2.04	0.56
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.71	0.56
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.71	0.56
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.54	0.56
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.87	0.56
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.88	0.56
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.56
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.88	0.56
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.87	0.56
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.05	0.55
2:C:138:ILE:HD13	2:C:143:ARG:HD3	1.88	0.55
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.70	0.55
1:H:57:THR:HG22	1:H:58:GLU:HG2	1.87	0.55
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.89	0.55
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.70	0.55
3:J:963:VAL:HB	3:J:980:THR:HG23	1.88	0.55
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.88	0.55
1:A:231:PHE:HZ	1:B:221:ALA:HB3	1.71	0.55
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.86	0.55
5:F:98:VAL:HB	5:F:402:LEU:HD11	1.89	0.55
2:I:1072:ASN:ND2	2:I:1111:GLN:OE1	2.39	0.55
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.87	0.55
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.88	0.55
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.87	0.55
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.38	0.55
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.55
2:I:1105:SER:O	3:J:736:GLN:NE2	2.40	0.55
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.71	0.55
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.89	0.55
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.39	0.55
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.55
2:I:1160:ASP:HB2	2:I:1163:THR:OG1	2.06	0.55
3:J:1010:GLN:HG3	3:J:1011:VAL:H	1.71	0.55
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.55
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.88	0.55
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.88	0.55
3:J:978:ARG:HB2	3:J:1199:PHE:CZ	2.42	0.55
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.89	0.55
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.88	0.55
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.88	0.55
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.89	0.55
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.88	0.55
5:F:483:LEU:H	5:F:483:LEU:HD12	1.71	0.55
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.88	0.55
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.87	0.55
5:L:483:LEU:H	5:L:483:LEU:HD12	1.72	0.55
2:C:1105:SER:O	3:D:736:GLN:NE2	2.40	0.54
3:D:682:VAL:O	3:D:685:ILE:HG12	2.06	0.54
2:C:101:ARG:HE	2:C:118:LYS:HE2	1.72	0.54
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.89	0.54
1:H:86:LYS:HD2	1:H:174:ASP:HB2	1.87	0.54
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.41	0.54
2:I:980:VAL:O	2:I:984:VAL:HB	2.08	0.54
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.89	0.54
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.43	0.54
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.73	0.54
2:I:1298:VAL:HG21	3:J:96:LYS:HE3	1.89	0.54
5:L:511:ILE:HG13	5:L:512:GLY:H	1.72	0.54
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.90	0.54
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.90	0.54
2:C:980:VAL:O	2:C:984:VAL:HB	2.08	0.54
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.89	0.54
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.40	0.54
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.42	0.54
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.89	0.54
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.88	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.73	0.54
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.90	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.89	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.90	0.54
2:C:1298:VAL:HG21	3:D:96:LYS:HE3	1.90	0.54
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.88	0.54
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.90	0.54
3:J:682:VAL:O	3:J:685:ILE:HG12	2.07	0.54
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.88	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.71	0.53
2:C:1142:ARG:HD3	2:C:1161:LEU:HD13	1.89	0.53
3:J:853:THR:HG22	3:J:854:ALA:H	1.72	0.53
2:C:808:ASN:H	3:D:633:ALA:HB2	1.73	0.53
2:C:1304:MET:HE2	3:D:472:LEU:HB3	1.90	0.53
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.38	0.53
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.90	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.74	0.53
5:L:515:GLU:HG2	5:L:516:ASP:H	1.72	0.53
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.91	0.53
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.90	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.90	0.53
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.91	0.53
5:F:348:GLU:HG2	5:F:354:THR:HA	1.91	0.53
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.74	0.53
2:I:396:ASP:HA	2:I:418:GLY:O	2.09	0.53
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.90	0.53
2:I:101:ARG:HE	2:I:118:LYS:HE2	1.73	0.53
3:J:527:LEU:HD22	3:J:533:ALA:HA	1.91	0.53
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.91	0.53
1:B:64:VAL:HG12	1:B:65:LEU:H	1.74	0.53
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.90	0.53
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.31	0.53
3:J:683:ILE:HD11	3:J:754:ILE:HG12	1.91	0.53
5:L:348:GLU:HG2	5:L:354:THR:HA	1.91	0.53
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.91	0.53
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.91	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.53
2:C:396:ASP:HA	2:C:418:GLY:O	2.08	0.53
2:C:757:THR:O	2:C:833:ILE:HD12	2.09	0.53
5:F:343:LYS:H	5:F:343:LYS:HD2	1.73	0.53
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.74	0.53
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.90	0.53
1:B:73:GLY:O	1:B:134:THR:N	2.30	0.52
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.30	0.52
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.91	0.52
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.74	0.52
1:H:181:GLU:O	3:J:531:LYS:HB3	2.10	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.11	0.52
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.92	0.52
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.92	0.52
2:C:90:VAL:HG12	2:C:91:THR:H	1.74	0.52
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.91	0.52
2:I:206:ALA:O	2:I:209:ILE:HG22	2.10	0.52
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.75	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.11	0.52
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.91	0.52
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.74	0.52
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.44	0.52
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.92	0.52
3:D:847:ASP:N	3:D:847:ASP:OD1	2.30	0.52
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.92	0.52
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.91	0.52
2:C:206:ALA:O	2:C:209:ILE:HG22	2.10	0.52
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.91	0.52
1:H:59:VAL:O	1:H:171:LEU:N	2.43	0.52
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.90	0.52
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.90	0.52
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	1.92	0.52
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.91	0.52
3:J:979:ASN:N	3:J:979:ASN:OD1	2.43	0.52
5:L:127:ILE:O	5:L:130:VAL:HG22	2.10	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.92	0.52
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.90	0.52
2:C:543:ALA:HB1	2:C:547:VAL:HG21	1.92	0.52
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.74	0.52
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.75	0.52
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.74	0.52
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.92	0.52
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.91	0.51
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.93	0.51
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.93	0.51
2:I:543:ALA:HB1	2:I:547:VAL:HG21	1.92	0.51
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.91	0.51
2:C:974:ARG:HD2	2:C:1014:LEU:HD11	1.92	0.51
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.92	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.44	0.51
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.91	0.51
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.93	0.51
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.92	0.51
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.45	0.51
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.57	0.51
3:J:749:LYS:HG2	3:J:753:SER:O	2.11	0.51
5:L:94:THR:OG1	5:L:95:THR:N	2.42	0.51
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.43	0.51
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.93	0.51
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.92	0.51
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.58	0.51
3:D:683:ILE:HD11	3:D:754:ILE:HG12	1.92	0.51
5:L:343:LYS:H	5:L:343:LYS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.41	0.51
1:A:14:VAL:HG22	1:A:15:ASP:H	1.76	0.51
1:B:8:PHE:HE1	1:B:32:GLU:HG3	1.76	0.51
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.44	0.51
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.74	0.51
2:I:499:SER:O	2:I:503:LYS:HB2	2.11	0.51
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.92	0.51
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.93	0.51
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.93	0.51
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.92	0.51
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.75	0.51
2:I:90:VAL:HG12	2:I:91:THR:H	1.74	0.51
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.44	0.51
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.92	0.51
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.93	0.51
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.25	0.50
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.93	0.50
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.91	0.50
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.50
2:I:782:VAL:HG11	2:I:792:GLY:HA2	1.93	0.50
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.93	0.50
3:D:110:PRO:HG2	3:D:183:GLU:HG2	1.93	0.50
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.11	0.50
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.93	0.50
2:I:446:ASP:N	2:I:446:ASP:OD1	2.44	0.50
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.93	0.50
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.94	0.50
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.11	0.50
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.93	0.50
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.93	0.50
3:J:514:THR:OG1	3:J:594:GLN:O	2.27	0.50
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.93	0.50
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.46	0.50
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.93	0.50
1:G:207:THR:HG22	1:G:208:ASN:H	1.77	0.50
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.93	0.50
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.76	0.50
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.93	0.50
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.94	0.50
3:D:749:LYS:HG2	3:D:753:SER:O	2.12	0.50
3:D:931:THR:OG1	3:D:1244:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:340:GLN:HA	3:J:340:GLN:HE21	1.76	0.50
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.93	0.50
1:A:74:VAL:HG22	1:A:76:GLU:H	1.77	0.50
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.26	0.50
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.93	0.50
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	1.92	0.50
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.93	0.50
3:J:1266:ILE:HA	3:J:1302:TYR:HA	1.94	0.50
1:B:6:THR:O	1:B:6:THR:OG1	2.30	0.50
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.12	0.50
3:D:514:THR:OG1	3:D:594:GLN:O	2.28	0.50
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.94	0.50
5:F:455:HIS:O	5:F:459:THR:OG1	2.28	0.50
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.47	0.50
3:J:950:ILE:HG13	3:J:1020:TRP:HZ3	1.77	0.50
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.94	0.50
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.45	0.49
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.77	0.49
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.92	0.49
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.94	0.49
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.93	0.49
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.92	0.49
2:I:600:THR:HB	2:I:602:GLU:HG2	1.95	0.49
3:J:709:ARG:O	3:J:711:GLY:N	2.42	0.49
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.95	0.49
3:D:356:THR:OG1	3:D:357:VAL:N	2.45	0.49
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.93	0.49
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.77	0.49
5:L:575:GLU:O	5:L:579:GLN:HG2	2.13	0.49
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.93	0.49
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.47	0.49
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.93	0.49
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.47	0.49
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.93	0.49
1:A:207:THR:HG22	1:A:208:ASN:H	1.77	0.49
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.94	0.49
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.93	0.49
3:D:853:THR:HG21	3:J:1375:ALA:CB	2.42	0.49
5:F:126:GLY:O	5:F:129:GLN:HB2	2.12	0.49
5:F:600:HIS:CG	5:F:601:PRO:HD2	2.47	0.49
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.94	0.49
3:J:356:THR:OG1	3:J:357:VAL:N	2.45	0.49
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.94	0.49
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.94	0.49
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.93	0.49
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.94	0.49
3:J:557:LYS:HA	3:J:563:LEU:HA	1.95	0.49
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.94	0.49
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.94	0.49
1:G:14:VAL:HG22	1:G:15:ASP:H	1.78	0.49
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.94	0.49
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.95	0.49
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.12	0.49
3:D:263:SER:HB2	5:F:507:MET:HE2	1.95	0.49
1:G:74:VAL:HG22	1:G:76:GLU:H	1.77	0.49
2:I:150:HIS:CD2	2:I:454:ARG:HE	2.31	0.49
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.27	0.49
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.48	0.49
3:J:45:ASN:HB3	3:J:48:THR:O	2.13	0.49
4:K:58:LEU:HD12	4:K:59:ILE:HG12	1.93	0.49
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.95	0.49
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.94	0.49
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.94	0.49
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.27	0.49
3:J:398:LYS:O	3:J:402:GLU:HB2	2.13	0.49
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.31	0.49
2:C:518:ASN:O	2:C:691:PRO:HD3	2.13	0.49
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.95	0.49
2:I:562:GLU:OE2	2:I:662:SER:OG	2.23	0.49
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.95	0.49
2:I:518:ASN:O	2:I:691:PRO:HD3	2.12	0.48
5:L:531:PRO:HG2	5:L:532:LEU:HD12	1.95	0.48
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.95	0.48
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.95	0.48
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.96	0.48
5:L:600:HIS:CG	5:L:601:PRO:HD2	2.47	0.48
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.13	0.48
5:F:164:GLY:O	5:F:260:ARG:HB2	2.13	0.48
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.95	0.48
3:D:807:LEU:HD23	3:D:915:ILE:HG13	1.95	0.48
5:F:531:PRO:HG2	5:F:532:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1227:HIS:NE2	3:J:1292:LEU:HB3	2.28	0.48
3:J:110:PRO:HG2	3:J:183:GLU:HG2	1.93	0.48
5:L:164:GLY:O	5:L:260:ARG:HB2	2.13	0.48
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.95	0.48
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.47	0.48
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.95	0.48
3:D:557:LYS:HA	3:D:563:LEU:HA	1.96	0.48
2:I:488:MET:O	2:I:490:GLN:N	2.37	0.48
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.95	0.48
2:C:600:THR:HB	2:C:602:GLU:HG2	1.95	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.79	0.48
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.96	0.48
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.31	0.48
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.96	0.48
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.96	0.48
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.94	0.48
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.78	0.48
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.96	0.48
3:J:901:ARG:HA	3:J:908:ILE:HA	1.96	0.48
1:B:134:THR:HG23	1:B:135:ASP:N	2.29	0.48
2:C:170:VAL:HG23	2:C:171:LEU:N	2.29	0.48
3:D:290:ILE:HD12	3:D:290:ILE:H	1.79	0.48
3:D:613:GLY:O	3:D:617:THR:OG1	2.25	0.48
5:F:575:GLU:O	5:F:579:GLN:HG2	2.14	0.48
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.48	0.48
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.96	0.48
2:C:499:SER:O	2:C:503:LYS:HB2	2.13	0.48
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.94	0.48
3:D:398:LYS:O	3:D:402:GLU:HB2	2.14	0.48
1:H:35:PHE:HA	1:H:38:THR:HG22	1.95	0.48
2:I:930:ASP:OD2	2:I:931:VAL:N	2.47	0.48
3:J:113:HIS:HD1	3:J:115:TRP:H	1.62	0.48
2:C:446:ASP:OD1	2:C:446:ASP:N	2.46	0.48
2:C:562:GLU:OE2	2:C:662:SER:OG	2.23	0.48
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.95	0.48
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.95	0.48
3:D:817:HIS:CD2	3:D:860:ARG:HH21	2.32	0.48
4:E:50:ALA:O	4:E:54:ILE:HG12	2.14	0.48
1:G:10:LYS:HE3	1:H:226:GLU:O	2.14	0.48
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:290:ILE:HD12	3:J:290:ILE:H	1.79	0.48
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.96	0.47
4:E:58:LEU:HD12	4:E:59:ILE:HG12	1.96	0.47
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.96	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.96	0.47
2:I:101:ARG:HG3	2:I:118:LYS:HG3	1.96	0.47
2:I:742:TYR:O	2:I:974:ARG:NH2	2.46	0.47
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.79	0.47
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.33	0.47
1:H:73:GLY:O	1:H:134:THR:N	2.31	0.47
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.96	0.47
2:I:616:ILE:HG13	2:I:652:TYR:HB2	1.96	0.47
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.96	0.47
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.48	0.47
2:C:148:GLN:NE2	2:C:535:PRO:O	2.34	0.47
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.96	0.47
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.96	0.47
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.15	0.47
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.97	0.47
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.95	0.47
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.49	0.47
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.96	0.47
1:B:82:LEU:O	1:B:86:LYS:HG3	2.14	0.47
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.44	0.47
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.96	0.47
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.30	0.47
1:G:113:ALA:HB2	1:G:126:PRO:HB3	1.95	0.47
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.96	0.47
3:J:1173:ARG:HB2	3:J:1192:LYS:HB3	1.97	0.47
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.95	0.47
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.96	0.47
1:H:82:LEU:O	1:H:86:LYS:HG3	2.14	0.47
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.97	0.47
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.96	0.47
2:I:739:ASP:N	2:I:739:ASP:OD1	2.46	0.47
3:J:152:THR:OG1	3:J:153:ASN:N	2.47	0.47
1:B:35:PHE:HA	1:B:38:THR:HG22	1.95	0.47
3:D:314:ARG:NH2	3:D:323:PRO:HG3	2.30	0.47
3:D:806:ASP:O	3:D:808:VAL:HG23	2.15	0.47
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.54	0.47
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:793:SER:O	3:D:797:THR:HG23	2.14	0.47
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.47
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.80	0.47
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	1.97	0.47
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.54	0.47
2:I:170:VAL:HG23	2:I:171:LEU:N	2.30	0.47
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.97	0.47
3:D:700:ASN:O	3:D:704:GLU:HB2	2.15	0.47
5:F:281:ARG:O	5:F:285:ARG:HG3	2.14	0.47
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.44	0.47
5:L:316:PHE:HZ	5:L:334:SER:HA	1.79	0.47
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.96	0.47
2:C:488:MET:O	2:C:490:GLN:N	2.37	0.47
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.96	0.47
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.12	0.47
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.95	0.47
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.14	0.47
3:J:340:GLN:HA	3:J:340:GLN:NE2	2.30	0.47
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.95	0.47
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.96	0.47
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.15	0.47
1:H:134:THR:HG23	1:H:135:ASP:N	2.29	0.47
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.97	0.47
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.50	0.47
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.97	0.47
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.96	0.47
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.33	0.47
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.97	0.47
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.15	0.46
2:C:101:ARG:HG3	2:C:118:LYS:HG3	1.97	0.46
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.44	0.46
3:D:45:ASN:HB3	3:D:48:THR:O	2.15	0.46
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.95	0.46
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.12	0.46
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.46
3:D:1173:ARG:HB2	3:D:1192:LYS:HB3	1.97	0.46
3:D:152:THR:OG1	3:D:153:ASN:N	2.46	0.46
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.96	0.46
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.75	0.46
2:I:148:GLN:NE2	2:I:535:PRO:O	2.35	0.46
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.50	0.46
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.98	0.46
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.98	0.46
2:C:1329:GLU:O	2:C:1332:SER:OG	2.28	0.46
2:C:886:LYS:H	2:C:917:SER:HB3	1.80	0.46
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.30	0.46
2:I:23:ASP:N	2:I:23:ASP:OD1	2.47	0.46
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.67	0.46
3:J:700:ASN:O	3:J:704:GLU:HB2	2.15	0.46
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.97	0.46
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.98	0.46
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.44	0.46
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.46
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.97	0.46
3:D:901:ARG:HA	3:D:908:ILE:HA	1.96	0.46
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.78	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.80	0.46
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.31	0.46
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.62	0.46
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.98	0.46
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.98	0.46
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.97	0.46
1:A:172:LEU:H	1:A:172:LEU:HD12	1.81	0.46
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.98	0.46
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.97	0.46
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.55	0.46
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.78	0.46
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.98	0.46
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.38	0.46
2:C:930:ASP:OD2	2:C:931:VAL:N	2.48	0.46
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.51	0.46
3:D:113:HIS:HD1	3:D:115:TRP:H	1.63	0.46
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.77	0.46
2:I:745:GLU:HG2	2:I:1021:LEU:HD11	1.98	0.46
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.48	0.46
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.80	0.46
2:I:1242:LYS:O	2:I:1244:HIS:ND1	2.46	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.46
5:L:567:MET:HE3	5:L:571:TYR:HE2	1.79	0.46
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.98	0.46
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.15	0.46
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.98	0.46
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.98	0.46
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.97	0.46
5:F:485:GLU:H	5:F:485:GLU:HG3	1.49	0.46
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.98	0.46
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.46
3:J:263:SER:HB2	5:L:507:MET:HE2	1.97	0.46
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.80	0.46
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.98	0.46
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.31	0.46
3:D:298:MET:SD	5:F:402:LEU:HB3	2.56	0.46
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.97	0.46
3:J:425:ARG:NH1	3:J:464:ASP:HB3	2.31	0.46
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.96	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.16	0.46
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.49	0.46
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.51	0.46
3:D:210:SER:O	3:D:214:ARG:HG2	2.16	0.46
3:D:425:ARG:NH1	3:D:464:ASP:HB3	2.31	0.46
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.96	0.46
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.97	0.46
3:D:789:LYS:HE3	3:D:931:THR:C	2.36	0.46
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.97	0.46
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.29	0.46
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.49	0.46
3:D:755:ILE:HG22	3:D:757:THR:H	1.81	0.46
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.98	0.46
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.98	0.46
2:I:3:TYR:HE1	2:I:11:ILE:HD11	1.81	0.46
3:J:755:ILE:HG22	3:J:757:THR:H	1.81	0.46
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.31	0.45
2:C:1326:LEU:HD21	3:D:339:ARG:HH12	1.80	0.45
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.80	0.45
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.80	0.45
2:I:557:ARG:HG2	2:I:587:LEU:HB3	1.98	0.45
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.98	0.45
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.97	0.45
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.80	0.45
2:C:23:ASP:N	2:C:23:ASP:OD1	2.46	0.45
3:D:515:ARG:NH2	3:D:717:VAL:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:810:THR:HG23	3:D:811:GLU:H	1.81	0.45
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.97	0.45
1:G:172:LEU:HD12	1:G:172:LEU:H	1.81	0.45
1:G:22:THR:HB	1:G:206:GLU:OE2	2.16	0.45
2:I:174:ALA:HB2	2:I:432:LEU:HD13	1.98	0.45
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.56	0.45
5:F:96:ASP:HA	5:F:97:PRO:HD2	1.84	0.45
1:G:91:ARG:HD3	1:G:210:THR:O	2.16	0.45
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.98	0.45
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.98	0.45
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	1.98	0.45
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.51	0.45
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.49	0.45
3:J:298:MET:SD	5:L:402:LEU:HB3	2.56	0.45
3:J:694:SER:OG	3:J:738:ARG:NE	2.48	0.45
5:L:314:THR:O	5:L:318:ALA:HB3	2.17	0.45
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.98	0.45
2:C:3:TYR:HE1	2:C:11:ILE:HD11	1.81	0.45
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.52	0.45
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.98	0.45
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.80	0.45
2:C:557:ARG:HG2	2:C:587:LEU:HB3	1.98	0.45
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.45
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.99	0.45
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.97	0.45
2:C:1304:MET:CE	3:D:472:LEU:HB3	2.47	0.45
5:F:567:MET:HE3	5:F:571:TYR:HE2	1.81	0.45
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.98	0.45
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.45	0.45
2:I:886:LYS:H	2:I:917:SER:HB3	1.81	0.45
3:J:210:SER:O	3:J:214:ARG:HG2	2.17	0.45
3:J:806:ASP:O	3:J:808:VAL:HG23	2.17	0.45
1:A:22:THR:HB	1:A:206:GLU:OE2	2.16	0.45
1:B:74:VAL:HG11	1:B:81:ILE:HD11	1.98	0.45
2:C:1242:LYS:O	2:C:1244:HIS:ND1	2.45	0.45
1:G:222:THR:O	1:G:226:GLU:HB2	2.17	0.45
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.50	0.45
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.98	0.45
2:I:1326:LEU:HD21	3:J:339:ARG:HH12	1.81	0.45
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.98	0.45
5:L:96:ASP:HA	5:L:97:PRO:HD2	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.65	0.45
2:I:119:GLU:HB2	2:I:489:PRO:HD2	1.98	0.45
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.98	0.45
3:J:1348:LYS:O	3:J:1352:ILE:HG12	2.17	0.45
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.50	0.45
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.98	0.45
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.45
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.99	0.45
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.82	0.45
3:D:694:SER:OG	3:D:738:ARG:NE	2.49	0.45
2:I:1329:GLU:O	2:I:1332:SER:OG	2.27	0.45
2:I:349:GLU:O	2:I:353:VAL:HG23	2.17	0.45
2:I:959:ASP:O	2:I:963:GLU:HG2	2.17	0.45
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.98	0.45
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.97	0.45
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.97	0.45
3:D:645:VAL:HB	3:D:701:LEU:HD23	1.99	0.45
5:F:601:PRO:HB3	5:F:608:ARG:HH22	1.82	0.45
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.99	0.45
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.31	0.45
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.81	0.45
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.52	0.45
2:I:596:ASP:OD2	2:I:598:VAL:HG23	2.16	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.45
3:J:314:ARG:NH2	3:J:323:PRO:HG3	2.31	0.45
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.99	0.45
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.50	0.45
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.52	0.45
3:J:654:ILE:O	3:J:658:GLU:HB2	2.17	0.45
5:L:548:LEU:HD21	5:L:559:LEU:HB3	1.97	0.45
1:B:8:PHE:HD1	1:B:9:LEU:H	1.66	0.44
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.98	0.44
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.99	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.44
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.54	0.44
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.88	0.44
1:G:214:GLU:HA	1:G:217:ILE:HG22	1.99	0.44
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.31	0.44
3:J:425:ARG:HH12	3:J:464:ASP:HB3	1.82	0.44
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.32	0.44
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HD3	1:A:210:THR:O	2.16	0.44
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.50	0.44
3:D:147:ILE:O	3:D:177:ASP:HB3	2.17	0.44
3:D:475:GLU:OE1	4:E:28:ARG:NH1	2.48	0.44
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.99	0.44
3:D:654:ILE:O	3:D:658:GLU:HB2	2.17	0.44
3:J:147:ILE:O	3:J:177:ASP:HB3	2.17	0.44
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.98	0.44
5:L:126:GLY:O	5:L:130:VAL:HG13	2.17	0.44
1:A:222:THR:O	1:A:226:GLU:HB2	2.17	0.44
1:A:64:VAL:HG11	1:A:78:ILE:HG13	2.00	0.44
2:C:349:GLU:O	2:C:353:VAL:HG23	2.17	0.44
2:C:898:GLU:N	2:C:898:GLU:OE1	2.47	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.17	0.44
3:D:114:ILE:HD11	3:D:311:ARG:HB2	2.00	0.44
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.83	0.44
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.64	0.44
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.99	0.44
2:I:582:ASN:HB3	2:I:586:PHE:H	1.81	0.44
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.98	0.44
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.64	0.44
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.99	0.44
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.48	0.44
3:J:793:SER:O	3:J:797:THR:HG23	2.17	0.44
1:A:78:ILE:HA	1:A:81:ILE:HD12	2.00	0.44
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.17	0.44
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.53	0.44
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.98	0.44
3:D:425:ARG:HH12	3:D:464:ASP:HB3	1.83	0.44
5:F:517:SER:O	5:F:518:HIS:HD2	2.00	0.44
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.44
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.52	0.44
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.44
2:C:1313:HIS:ND1	4:E:31:GLN:OE1	2.51	0.44
2:C:582:ASN:HB3	2:C:586:PHE:H	1.81	0.44
3:D:54:ASP:N	3:D:54:ASP:OD1	2.50	0.44
5:F:471:LEU:HD23	5:F:476:ARG:O	2.17	0.44
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.82	0.44
3:J:515:ARG:NH2	3:J:717:VAL:O	2.51	0.44
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.00	0.44
3:J:950:ILE:HG13	3:J:1020:TRP:CZ3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.99	0.44
5:F:245:ALA:O	5:F:249:ILE:HG13	2.18	0.44
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.99	0.44
2:I:316:GLU:CD	2:I:316:GLU:H	2.21	0.44
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.51	0.44
3:J:426:ALA:HB3	3:J:427:PRO:HD3	2.00	0.44
3:J:797:THR:O	3:J:801:VAL:HG22	2.17	0.44
5:L:471:LEU:HD23	5:L:476:ARG:O	2.18	0.44
5:L:551:LEU:HD11	5:L:598:LEU:HD11	1.98	0.44
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.98	0.44
1:H:51:MET:HA	1:H:52:PRO:HD3	1.83	0.44
2:I:1061:GLN:NE2	2:I:1240:ASP:OD2	2.51	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.30	0.44
5:L:470:MET:O	5:L:478:PRO:HD3	2.18	0.44
1:A:228:LEU:HD13	1:A:228:LEU:HA	1.80	0.44
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.99	0.44
2:C:245:ARG:HG2	2:C:337:PHE:CZ	2.53	0.44
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.49	0.44
4:E:15:ASN:HB3	4:E:18:ASP:HB2	2.00	0.44
5:F:314:THR:O	5:F:318:ALA:HB3	2.18	0.44
1:G:78:ILE:HA	1:G:81:ILE:HD12	1.99	0.44
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.99	0.44
2:I:699:LEU:HA	2:I:699:LEU:HD22	1.81	0.44
1:B:80:GLU:HG3	3:D:551:ARG:NH2	2.33	0.43
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.51	0.43
2:C:959:ASP:O	2:C:963:GLU:HG2	2.18	0.43
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.99	0.43
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.43
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.18	0.43
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.18	0.43
3:J:658:GLU:O	3:J:661:VAL:HG22	2.18	0.43
3:J:905:ARG:NH1	3:J:910:ASN:HD21	2.15	0.43
5:L:245:ALA:O	5:L:249:ILE:HG13	2.18	0.43
5:L:517:SER:O	5:L:518:HIS:HD2	2.00	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.01	0.43
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.15	0.43
2:C:898:GLU:HB3	5:F:540:LEU:HD22	2.00	0.43
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.58	0.43
2:I:462:ASN:O	2:I:465:ARG:HB3	2.18	0.43
2:I:578:TYR:HE1	2:I:658:GLN:HB2	1.83	0.43
3:J:1170:LYS:C	3:J:1172:LYS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.54	0.43
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.79	0.43
2:I:95:PRO:HA	2:I:126:GLU:HG2	2.00	0.43
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.53	0.43
3:J:349:TYR:CE1	3:J:472:LEU:HD11	2.53	0.43
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.01	0.43
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.00	0.43
1:A:118:ASP:H	1:A:121:VAL:HB	1.83	0.43
2:C:1109:ILE:HA	2:C:1109:ILE:HD12	1.76	0.43
2:C:174:ALA:HB2	2:C:432:LEU:HD13	1.99	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.43
3:D:598:LYS:O	3:D:601:ILE:HG22	2.18	0.43
1:G:46:ILE:HD12	1:H:35:PHE:CZ	2.54	0.43
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.83	0.43
2:I:618:GLN:HG3	3:J:770:LEU:HD21	2.01	0.43
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.98	0.43
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	2.01	0.43
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.53	0.43
3:J:491:LEU:HD22	3:J:496:GLY:O	2.18	0.43
3:J:708:ASN:HB3	3:J:712:GLN:O	2.19	0.43
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.00	0.43
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	2.00	0.43
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.54	0.43
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.52	0.43
3:D:797:THR:O	3:D:801:VAL:HG22	2.18	0.43
1:G:118:ASP:H	1:G:121:VAL:HB	1.83	0.43
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	2.01	0.43
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.18	0.43
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.83	0.43
3:J:56:LEU:HD12	3:J:56:LEU:H	1.83	0.43
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.83	0.43
5:L:484:ALA:C	5:L:491:GLU:HB2	2.38	0.43
1:B:178:SER:HA	1:B:179:PRO:HD3	1.87	0.43
1:A:66:HIS:HB3	2:C:874:GLY:HA2	1.99	0.43
5:F:281:ARG:HG2	5:F:285:ARG:HD2	2.01	0.43
1:H:41:ASN:O	1:H:45:ARG:HG3	2.18	0.43
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.53	0.43
2:I:548:ARG:HB3	2:I:569:ILE:O	2.19	0.43
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.32	0.43
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:601:PRO:HB3	5:L:608:ARG:HH22	1.84	0.43
1:B:41:ASN:O	1:B:45:ARG:HG3	2.19	0.43
2:C:964:LEU:HD11	2:C:1022:LYS:HD2	2.01	0.43
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.19	0.43
3:D:405:GLU:O	3:D:408:VAL:HG22	2.18	0.43
3:D:491:LEU:HD22	3:D:496:GLY:O	2.19	0.43
3:D:770:LEU:H	3:D:770:LEU:HD22	1.84	0.43
1:G:10:LYS:HE2	1:H:229:GLU:HB3	2.01	0.43
2:I:1007:LYS:O	2:I:1011:LEU:HG	2.18	0.43
2:I:964:LEU:HD11	2:I:1022:LYS:HD2	2.01	0.43
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.53	0.43
5:L:281:ARG:HG2	5:L:285:ARG:HD2	2.00	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.87	0.43
5:L:569:THR:OG1	5:L:570:ASP:N	2.52	0.43
5:L:98:VAL:O	5:L:102:MET:HB2	2.19	0.43
1:A:208:ASN:N	1:A:208:ASN:OD1	2.48	0.43
1:A:49:SER:OG	1:A:50:SER:N	2.51	0.43
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	2.01	0.43
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.18	0.43
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.79	0.43
2:C:462:ASN:O	2:C:465:ARG:HB3	2.19	0.43
2:C:557:ARG:HH21	2:C:607:SER:C	2.22	0.43
3:D:349:TYR:CE1	3:D:472:LEU:HD11	2.54	0.43
3:D:51:PRO:HB2	3:D:58:CYS:HA	2.01	0.43
3:D:678:ARG:O	3:D:682:VAL:HG23	2.19	0.43
5:F:120:ALA:HA	5:F:123:ILE:HD12	2.01	0.43
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.99	0.43
5:L:455:HIS:O	5:L:459:THR:OG1	2.29	0.43
1:B:18:GLN:HA	1:B:24:ALA:HA	2.01	0.43
1:B:51:MET:HA	1:B:52:PRO:HD3	1.83	0.43
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.54	0.43
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.54	0.43
2:C:548:ARG:HB3	2:C:569:ILE:O	2.18	0.43
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.43
3:D:1170:LYS:C	3:D:1172:LYS:H	2.22	0.43
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.83	0.43
3:D:658:GLU:O	3:D:661:VAL:HG22	2.19	0.43
3:D:801:VAL:O	3:D:805:GLN:HB2	2.19	0.43
5:F:484:ALA:C	5:F:491:GLU:HB2	2.38	0.43
1:H:102:LEU:HD12	1:H:142:MET:HG2	2.00	0.43
2:I:486:THR:HG23	2:I:487:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HG23	2:I:775:GLU:O	2.19	0.43
2:I:767:GLN:HG2	2:I:786:GLY:HA2	2.01	0.43
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.88	0.43
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.01	0.43
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.18	0.43
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.99	0.43
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.19	0.43
1:G:9:LEU:H	1:G:9:LEU:HD23	1.84	0.43
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.32	0.43
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	2.01	0.43
3:J:54:ASP:N	3:J:54:ASP:OD1	2.50	0.43
2:C:578:TYR:HE1	2:C:658:GLN:HB2	1.84	0.42
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.54	0.42
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.19	0.42
1:H:51:MET:HB3	1:H:178:SER:HA	2.01	0.42
1:H:67:GLU:O	1:H:78:ILE:HB	2.19	0.42
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.18	0.42
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.53	0.42
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.78	0.42
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.49	0.42
5:L:547:VAL:CG1	5:L:598:LEU:HD22	2.49	0.42
1:B:112:ALA:HB2	1:B:128:HIS:HB3	2.01	0.42
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	2.01	0.42
2:C:829:THR:HG23	2:C:1059:ARG:HA	2.00	0.42
2:C:95:PRO:HA	2:C:126:GLU:HG2	2.01	0.42
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.54	0.42
2:C:696:ASP:O	2:C:697:LYS:HB3	2.18	0.42
3:D:708:ASN:HB3	3:D:712:GLN:O	2.19	0.42
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.49	0.42
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.49	0.42
1:H:19:VAL:HB	1:H:23:HIS:HD2	1.84	0.42
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.82	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.49	0.42
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.53	0.42
2:I:660:VAL:HG13	2:I:661:VAL:HG13	2.00	0.42
2:I:720:ARG:HH21	2:I:736:VAL:HG11	1.85	0.42
2:I:705:GLU:HB2	2:I:794:LEU:HB3	2.00	0.42
3:J:108:ALA:HB2	3:J:280:LYS:HG2	2.01	0.42
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.77	0.42
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.84	0.42
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:ILE:H	2:C:117:ILE:HG12	1.49	0.42
3:D:267:ASP:OD1	3:D:271:ARG:NH2	2.53	0.42
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.54	0.42
1:G:49:SER:OG	1:G:50:SER:N	2.52	0.42
5:L:120:ALA:HA	5:L:123:ILE:HD12	2.01	0.42
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.90	0.42
1:A:12:ARG:H	1:A:30:PRO:CD	2.30	0.42
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.19	0.42
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.01	0.42
2:I:169:LYS:O	2:I:170:VAL:HG22	2.19	0.42
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.53	0.42
2:I:696:ASP:O	2:I:697:LYS:HB3	2.19	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.54	0.42
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.52	0.42
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.36	0.42
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.16	0.42
1:B:102:LEU:HD12	1:B:142:MET:HG2	2.00	0.42
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	2.00	0.42
2:C:316:GLU:CD	2:C:316:GLU:H	2.22	0.42
2:C:60:GLN:H	2:C:60:GLN:HG2	1.73	0.42
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.65	0.42
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	2.01	0.42
3:D:340:GLN:HA	3:D:340:GLN:NE2	2.33	0.42
1:B:80:GLU:HG3	3:D:551:ARG:HH21	1.84	0.42
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.17	0.42
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.85	0.42
5:F:569:THR:OG1	5:F:570:ASP:N	2.52	0.42
2:I:804:PHE:HB3	2:I:1100:PRO:HG3	2.01	0.42
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.53	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.89	0.42
1:B:34:GLY:HA3	2:C:1083:GLU:OE1	2.19	0.42
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	2.00	0.42
2:C:169:LYS:HG2	2:C:169:LYS:O	2.19	0.42
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.01	0.42
3:D:56:LEU:H	3:D:56:LEU:HD12	1.84	0.42
3:D:661:VAL:HG12	3:D:685:ILE:HD11	2.01	0.42
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.89	0.42
2:I:860:ALA:O	2:I:863:SER:OG	2.35	0.42
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	2.02	0.42
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:488:LEU:H	5:L:488:LEU:HD12	1.85	0.42
1:A:214:GLU:HA	1:A:217:ILE:HG22	2.00	0.42
1:A:19:VAL:HG12	1:A:24:ALA:HA	2.02	0.42
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.52	0.42
2:C:618:GLN:HG3	3:D:770:LEU:HD21	2.01	0.42
5:F:244:THR:O	5:F:247:GLU:HG2	2.20	0.42
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.69	0.42
5:L:244:THR:O	5:L:247:GLU:HG2	2.19	0.42
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.01	0.42
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.69	0.42
2:C:724:VAL:HG23	2:C:775:GLU:O	2.19	0.42
2:C:720:ARG:HH21	2:C:736:VAL:HG11	1.84	0.42
1:A:65:LEU:HB3	2:C:874:GLY:HA3	2.02	0.42
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.02	0.42
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.69	0.42
2:I:730:SER:O	2:I:753:LEU:HB2	2.20	0.42
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.79	0.42
3:J:51:PRO:HB2	3:J:58:CYS:HA	2.02	0.42
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.58	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
2:C:520:PRO:HB3	2:C:714:VAL:HG21	2.01	0.42
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.54	0.42
5:F:611:LEU:HA	5:F:611:LEU:HD23	1.88	0.42
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.02	0.42
2:I:1271:GLY:HA2	3:J:344:GLY:HA2	2.02	0.42
2:I:494:ASN:HB3	2:I:497:PRO:HD2	2.01	0.42
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.02	0.42
5:L:572:THR:O	5:L:576:VAL:HG23	2.20	0.42
1:B:80:GLU:O	1:B:83:LEU:HB2	2.20	0.42
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.54	0.42
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.35	0.42
5:F:481:GLU:O	5:F:484:ALA:HB3	2.20	0.42
5:F:551:LEU:HD11	5:F:598:LEU:HD11	2.01	0.42
2:I:1124:ILE:HB	2:I:1180:MET:HB2	2.01	0.42
2:I:169:LYS:O	2:I:169:LYS:HG2	2.20	0.42
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.42
2:I:736:VAL:HG23	2:I:748:ILE:HA	2.02	0.42
3:J:746:LEU:HD23	3:J:758:PRO:HG3	2.02	0.42
5:L:105:MET:HE3	5:L:105:MET:HB2	1.80	0.42
2:C:13:LYS:HZ3	2:C:1151:LEU:HB2	1.85	0.41
2:C:169:LYS:O	2:C:170:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.02	0.41
3:D:461:PHE:HA	3:D:461:PHE:HD2	1.78	0.41
3:D:525:MET:O	3:D:548:VAL:HG13	2.20	0.41
3:D:800:LEU:HB3	3:D:920:ALA:HB1	2.01	0.41
1:G:47:LEU:O	1:G:180:VAL:HG21	2.20	0.41
2:I:24:VAL:HG21	2:I:704:MET:SD	2.60	0.41
2:I:660:VAL:HG11	3:J:769:VAL:HG13	2.02	0.41
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.85	0.41
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.20	0.41
3:J:218:THR:HA	3:J:221:ILE:HG22	2.02	0.41
3:J:461:PHE:HA	3:J:461:PHE:HD2	1.79	0.41
3:J:614:LEU:HD23	4:K:7:GLN:HB2	2.02	0.41
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.02	0.41
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.57	0.41
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	2.02	0.41
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.35	0.41
5:F:98:VAL:O	5:F:102:MET:HB2	2.19	0.41
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.20	0.41
2:I:84:GLU:HG3	2:I:1035:LYS:NZ	2.35	0.41
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.02	0.41
3:J:998:PRO:HG2	3:J:1020:TRP:CE2	2.55	0.41
3:J:111:THR:O	3:J:239:LEU:N	2.49	0.41
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.88	0.41
3:J:525:MET:O	3:J:548:VAL:HG13	2.20	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.20	0.41
2:C:13:LYS:NZ	2:C:1151:LEU:HB2	2.35	0.41
2:C:176:ILE:HB	2:C:184:LEU:HB3	2.01	0.41
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.51	0.41
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.02	0.41
1:G:64:VAL:HG11	1:G:78:ILE:HG13	2.01	0.41
1:H:62:ASP:OD1	1:H:62:ASP:N	2.53	0.41
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.35	0.41
2:I:557:ARG:HH21	2:I:607:SER:C	2.23	0.41
2:I:91:THR:HG21	2:I:503:LYS:CE	2.50	0.41
3:J:405:GLU:O	3:J:408:VAL:HG22	2.19	0.41
5:L:311:THR:HG21	5:L:348:GLU:OE2	2.20	0.41
1:B:67:GLU:O	1:B:78:ILE:HB	2.21	0.41
2:C:297:VAL:HG12	2:C:315:MET:O	2.21	0.41
2:C:486:THR:HG23	2:C:487:LEU:H	1.84	0.41
2:C:736:VAL:HG23	2:C:748:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.56	0.41
3:D:45:ASN:O	3:D:46:TYR:HD2	2.03	0.41
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.86	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.20	0.41
3:D:905:ARG:HH21	3:D:907:HIS:HB3	1.85	0.41
1:G:178:SER:HA	1:G:179:PRO:HD3	1.94	0.41
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.41
2:I:538:LEU:H	2:I:538:LEU:HG	1.49	0.41
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.21	0.41
3:J:801:VAL:O	3:J:805:GLN:HB2	2.20	0.41
2:C:130:MET:HB2	2:C:136:PHE:CZ	2.55	0.41
5:F:134:VAL:HG22	5:F:273:MET:HE3	2.03	0.41
1:G:85:LEU:HA	1:G:85:LEU:HD23	1.87	0.41
2:I:358:ASP:OD1	2:I:360:LEU:HB3	2.20	0.41
2:I:387:ASN:HA	2:I:391:SER:HB2	2.02	0.41
3:J:77:ARG:HG3	3:J:79:LYS:HB3	2.02	0.41
1:B:95:LYS:HB2	1:B:120:ASP:OD2	2.21	0.41
2:C:60:GLN:HB3	2:C:67:GLU:HG3	2.03	0.41
3:D:901:ARG:HD2	3:D:906:GLY:O	2.20	0.41
1:G:12:ARG:H	1:G:30:PRO:CD	2.30	0.41
3:J:267:ASP:OD1	3:J:271:ARG:NH2	2.53	0.41
3:J:334:LYS:HA	3:J:334:LYS:HD2	1.57	0.41
3:J:661:VAL:HG12	3:J:685:ILE:HD11	2.01	0.41
3:J:770:LEU:HD22	3:J:770:LEU:H	1.86	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.41
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.54	0.41
1:B:102:LEU:HB2	1:B:142:MET:H	1.85	0.41
1:B:18:GLN:NE2	1:B:20:SER:O	2.53	0.41
2:C:387:ASN:HA	2:C:391:SER:HB2	2.02	0.41
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.54	0.41
3:D:1141:VAL:HG13	3:D:1237:VAL:HG23	2.03	0.41
5:F:251:LYS:HA	5:F:254:GLU:HG2	2.03	0.41
5:F:470:MET:O	5:F:478:PRO:HD3	2.20	0.41
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.03	0.41
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.19	0.41
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.03	0.41
2:C:1124:ILE:HB	2:C:1180:MET:HB2	2.01	0.41
2:C:379:GLU:CD	2:C:379:GLU:H	2.24	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.01	0.41
2:C:739:ASP:OD1	2:C:739:ASP:N	2.45	0.41
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1271:GLY:HA2	3:D:344:GLY:HA2	2.03	0.41
3:D:473:THR:HG23	3:D:476:ALA:H	1.86	0.41
2:I:1223:ARG:HD2	3:J:512:TYR:HE1	1.86	0.41
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.56	0.41
2:I:292:ILE:HB	2:I:322:LEU:HD11	2.02	0.41
2:I:379:GLU:H	2:I:379:GLU:CD	2.23	0.41
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.20	0.41
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.56	0.41
3:J:478:LEU:HD23	3:J:478:LEU:HA	1.89	0.41
5:L:481:GLU:O	5:L:484:ALA:HB3	2.21	0.41
5:L:489:MET:HG2	5:L:489:MET:H	1.53	0.41
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.41
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.91	0.41
2:C:528:ARG:NH2	2:C:576:SER:O	2.53	0.41
2:C:577:VAL:HG23	2:C:661:VAL:O	2.21	0.41
2:C:730:SER:O	2:C:753:LEU:HB2	2.20	0.41
3:D:746:LEU:HD23	3:D:758:PRO:HG3	2.02	0.41
3:D:77:ARG:HG3	3:D:79:LYS:HB3	2.03	0.41
3:D:918:ILE:HG13	3:D:919:ALA:N	2.35	0.41
5:F:350:GLU:HG3	5:F:350:GLU:H	1.69	0.41
1:G:90:VAL:HG23	1:G:123:ILE:HD13	2.03	0.41
1:G:167:PRO:HB2	1:G:170:ARG:HG3	2.03	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.21	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.41
3:J:678:ARG:O	3:J:682:VAL:HG23	2.20	0.41
3:J:972:LYS:HA	3:J:972:LYS:NZ	2.36	0.41
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.21	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.90	0.41
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.76	0.41
5:F:489:MET:HB2	5:F:490:PRO:HD2	2.02	0.41
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.03	0.41
1:H:124:VAL:HG11	1:H:209:GLY:HA3	2.02	0.41
3:J:613:GLY:O	3:J:617:THR:OG1	2.25	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.56	0.41
3:J:905:ARG:HH21	3:J:907:HIS:HB3	1.86	0.41
2:C:138:ILE:HG22	2:C:139:ASN:N	2.36	0.41
2:C:153:PRO:HB2	2:C:401:GLY:HA2	2.03	0.41
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.02	0.41
3:D:1309:ILE:HG13	3:D:1310:THR:H	1.86	0.41
3:D:218:THR:HA	3:D:221:ILE:HG22	2.02	0.41
3:D:254:PRO:O	3:D:255:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.86	0.41
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.03	0.41
3:D:749:LYS:HE2	3:D:751:ASP:HB3	2.03	0.41
4:E:31:GLN:HB2	4:E:31:GLN:HE21	1.64	0.41
5:F:488:LEU:H	5:F:488:LEU:HD12	1.85	0.41
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.56	0.41
1:H:147:GLN:HG3	1:H:148:ARG:N	2.36	0.41
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.02	0.41
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	2.02	0.41
3:J:68:TYR:HA	3:J:92:VAL:HG23	2.02	0.41
3:J:918:ILE:HG13	3:J:919:ALA:N	2.36	0.41
5:L:354:THR:O	5:L:358:VAL:HG23	2.21	0.41
1:B:147:GLN:HG3	1:B:148:ARG:N	2.36	0.40
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.21	0.40
2:C:356:THR:HG21	2:C:362:ALA:HA	2.02	0.40
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	2.02	0.40
2:C:758:ARG:HD3	2:C:835:GLU:HB2	2.03	0.40
3:D:137:ARG:HG2	3:D:142:GLU:HB2	2.03	0.40
3:D:224:LEU:O	3:D:228:VAL:HG23	2.20	0.40
1:B:196:THR:HG23	3:D:443:GLU:HG3	2.03	0.40
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.56	0.40
5:F:452:ILE:HA	5:F:453:PRO:HD3	1.98	0.40
5:F:572:THR:O	5:F:576:VAL:HG23	2.21	0.40
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.54	0.40
1:H:18:GLN:NE2	1:H:20:SER:O	2.54	0.40
1:H:95:LYS:HB2	1:H:120:ASP:OD2	2.21	0.40
2:I:130:MET:HB2	2:I:136:PHE:CZ	2.56	0.40
2:I:898:GLU:OE1	2:I:898:GLU:N	2.47	0.40
3:J:1168:GLU:HB3	3:J:1169:THR:H	1.80	0.40
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.86	0.40
1:A:9:LEU:HD23	1:A:9:LEU:H	1.86	0.40
2:C:120:GLN:O	2:C:120:GLN:HG3	2.20	0.40
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.91	0.40
2:C:658:GLN:O	2:C:661:VAL:HG22	2.21	0.40
2:C:985:GLU:HG2	2:C:988:LYS:HD2	2.04	0.40
3:D:1262:ARG:O	3:D:1280:VAL:HG23	2.22	0.40
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	2.03	0.40
3:D:600:ALA:O	3:D:603:LYS:HG2	2.20	0.40
5:F:354:THR:O	5:F:358:VAL:HG23	2.20	0.40
1:H:102:LEU:HB2	1:H:142:MET:H	1.85	0.40
1:H:16:ILE:HG13	1:H:26:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.53	0.40
2:I:339:ASN:O	2:I:344:GLY:HA2	2.21	0.40
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.01	0.40
3:J:224:LEU:O	3:J:228:VAL:HG23	2.21	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.86	0.40
3:J:77:ARG:HD2	3:J:78:LEU:H	1.86	0.40
1:A:219:ARG:O	1:A:222:THR:HB	2.21	0.40
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.51	0.40
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.75	0.40
2:C:967:LEU:HG	2:C:1021:LEU:HD13	2.03	0.40
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	2.04	0.40
2:C:198:ILE:O	2:C:201:ARG:HB2	2.21	0.40
2:C:206:ALA:HB3	2:C:350:THR:HG21	2.04	0.40
2:C:816:ILE:HG22	2:C:818:VAL:HG23	2.03	0.40
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.40
3:D:198:CYS:HA	3:D:221:ILE:HD13	2.03	0.40
3:D:27:PRO:HD3	3:D:236:TRP:CD1	2.56	0.40
3:D:451:PRO:O	3:D:454:CYS:HB2	2.21	0.40
1:G:137:ASN:N	1:G:137:ASN:OD1	2.54	0.40
1:G:19:VAL:HG12	1:G:24:ALA:HA	2.02	0.40
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.22	0.40
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	2.02	0.40
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.21	0.40
3:J:19:ALA:O	3:J:20:ILE:HG13	2.21	0.40
3:J:198:CYS:HA	3:J:221:ILE:HD13	2.03	0.40
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.88	0.40
3:J:451:PRO:O	3:J:454:CYS:HB2	2.21	0.40
3:J:45:ASN:O	3:J:46:TYR:HD2	2.04	0.40
3:J:470:VAL:HA	3:J:471:PRO:HD3	1.87	0.40
2:C:4:SER:OG	2:C:5:TYR:N	2.53	0.40
2:C:91:THR:HG21	2:C:503:LYS:CE	2.52	0.40
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.86	0.40
3:D:108:ALA:HB2	3:D:280:LYS:HG2	2.04	0.40
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.40
3:D:646:ILE:H	3:D:646:ILE:HG12	1.63	0.40
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.03	0.40
1:G:61:ILE:HG22	1:G:62:ASP:H	1.86	0.40
2:I:1017:GLN:O	2:I:1021:LEU:HG	2.21	0.40
2:I:229:ILE:HB	2:I:240:GLU:HB2	2.04	0.40
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.40
2:I:4:SER:OG	2:I:5:TYR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.21	0.40
3:J:510:LEU:HD22	3:J:601:ILE:HD11	2.03	0.40
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.57	0.40
5:L:489:MET:HB2	5:L:490:PRO:HD2	2.02	0.40
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.90	0.40
3:D:19:ALA:CB	3:D:1343:GLU:HA	2.52	0.40
3:D:114:ILE:HD12	3:D:304:ASP:HB3	2.03	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.04	0.40
3:D:425:ARG:HG2	3:D:426:ALA:H	1.86	0.40
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.88	0.40
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.03	0.40
2:I:103:VAL:HB	2:I:113:THR:HG21	2.02	0.40
2:I:27:LEU:O	2:I:528:ARG:NH1	2.44	0.40
2:I:582:ASN:HB3	2:I:586:PHE:N	2.37	0.40
3:J:598:LYS:O	3:J:601:ILE:HG22	2.21	0.40
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.36	0.40
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.04	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	222/239 (93%)	191 (86%)	28 (13%)	3 (1%)	11	46
1	B	216/239 (90%)	189 (88%)	27 (12%)	0	100	100
1	G	226/239 (95%)	193 (85%)	30 (13%)	3 (1%)	12	48
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100	100
2	C	1338/1342 (100%)	1224 (92%)	109 (8%)	5 (0%)	34	71
2	I	1338/1342 (100%)	1220 (91%)	113 (8%)	5 (0%)	34	71
3	D	1162/1407 (83%)	1066 (92%)	93 (8%)	3 (0%)	41	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1230/1407 (87%)	1131 (92%)	96 (8%)	3 (0%)	47	79
4	E	87/91 (96%)	83 (95%)	4 (5%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	464/522 (89%)	418 (90%)	46 (10%)	0	100	100
5	L	463/522 (89%)	420 (91%)	43 (9%)	0	100	100
All	All	7036/7680 (92%)	6399 (91%)	615 (9%)	22 (0%)	41	75

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1159	VAL
2	C	170	VAL
2	I	170	VAL
2	I	1159	VAL
2	C	238	GLN
2	I	238	GLN
3	J	340	GLN
2	C	697	LYS
3	D	710	ASP
2	I	697	LYS
3	J	710	ASP
1	A	167	PRO
1	G	62	ASP
1	G	167	PRO
1	A	14	VAL
1	A	62	ASP
3	D	10	ALA
1	G	14	VAL
3	D	831	VAL
3	J	831	VAL
2	C	1186	VAL
2	I	1186	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	191/206 (93%)	181 (95%)	10 (5%)	23	51
1	B	184/206 (89%)	170 (92%)	14 (8%)	13	40
1	G	191/206 (93%)	181 (95%)	10 (5%)	23	51
1	H	183/206 (89%)	172 (94%)	11 (6%)	19	47
2	C	1155/1157 (100%)	1058 (92%)	97 (8%)	11	37
2	I	1154/1157 (100%)	1054 (91%)	100 (9%)	10	35
3	D	975/1168 (84%)	880 (90%)	95 (10%)	8	30
3	J	1036/1168 (89%)	934 (90%)	102 (10%)	8	29
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	30
4	K	67/75 (89%)	64 (96%)	3 (4%)	27	55
5	F	417/462 (90%)	381 (91%)	36 (9%)	10	37
5	L	418/462 (90%)	382 (91%)	36 (9%)	10	37
All	All	6043/6548 (92%)	5522 (91%)	521 (9%)	10	37

All (521) 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	61	ILE
1	A	77	ASP
1	A	145	LYS
1	A	165	GLU
1	A	215	GLU
1	A	219	ARG
1	B	6	THR
1	B	8	PHE
1	B	50	SER
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	79	LEU
1	B	80	GLU
1	B	97	GLU
1	B	105	SER

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Mol	Chain	Res	Type
1	B	133	LEU
1	B	134	THR
1	B	160	HIS
1	B	183	ILE
2	C	4	SER
2	C	11	ILE
2	C	39	ILE
2	C	91	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	120	GLN
2	C	121	GLU
2	C	124	MET
2	C	131	THR
2	C	132	ASP
2	C	160	ASP
2	C	197	ARG
2	C	238	GLN
2	C	285	ILE
2	C	306	THR
2	C	316	GLU
2	C	320	ASP
2	C	369	MET
2	C	377	THR
2	C	419	ILE
2	C	423	ASP
2	C	446	ASP
2	C	471	VAL
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	496	LYS
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	554	HIS
2	C	563	THR
2	C	604	HIS

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Mol	Chain	Res	Type
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	637	ARG
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	693	LEU
2	C	697	LYS
2	C	699	LEU
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	779	ARG
2	C	788	SER
2	C	814	ASP
2	C	815	SER
2	C	817	LEU
2	C	859	GLU
2	C	868	SER
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	913	VAL
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	992	LEU
2	C	1006	GLU
2	C	1014	LEU
2	C	1082	ILE
2	C	1108	ASN
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN

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Mol	Chain	Res	Type
2	C	1146	GLN
2	C	1156	ARG
2	C	1159	VAL
2	C	1160	ASP
2	C	1163	THR
2	C	1198	LEU
2	C	1233	LEU
2	C	1238	LEU
2	C	1240	ASP
2	C	1246	ARG
2	C	1248	THR
2	C	1264	GLN
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1331	ARG
2	C	1342	GLU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	92	VAL
3	D	95	THR
3	D	134	ASP
3	D	159	ILE
3	D	169	LEU
3	D	170	GLU
3	D	175	GLU
3	D	217	LEU
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	312	ARG
3	D	324	LEU
3	D	334	LYS
3	D	335	GLN
3	D	340	GLN
3	D	363	LEU
3	D	374	LEU
3	D	431	ARG

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Mol	Chain	Res	Type
3	D	454	CYS
3	D	486	SER
3	D	490	ILE
3	D	507	VAL
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	558	ASP
3	D	573	THR
3	D	622	ASP
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	678	ARG
3	D	680	ASN
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	706	VAL
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	772	TYR
3	D	788	LEU
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	855	ASP
3	D	857	LEU
3	D	860	ARG

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Mol	Chain	Res	Type
3	D	897	HIS
3	D	898	CYS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1167	LYS
3	D	1173	ARG
3	D	1177	ILE
3	D	1186	TYR
3	D	1189	MET
3	D	1208	ASP
3	D	1221	LEU
3	D	1255	VAL
3	D	1268	ASN
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1305	ASP
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
3	D	1344	LEU
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	28	ARG
4	E	31	GLN
4	E	39	VAL
4	E	46	THR
5	F	94	THR
5	F	100	MET
5	F	102	MET
5	F	105	MET
5	F	154	GLU
5	F	247	GLU
5	F	266	PHE

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Mol	Chain	Res	Type
5	F	267	ASP
5	F	297	MET
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	362	ASN
5	F	395	THR
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	492	ASP
5	F	558	VAL
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	582	VAL
5	F	583	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	609	SER
1	G	9	LEU
1	G	13	LEU
1	G	35	PHE
1	G	54	CYS
1	G	61	ILE
1	G	77	ASP
1	G	145	LYS
1	G	165	GLU
1	G	215	GLU
1	G	219	ARG
1	H	50	SER
1	H	60	GLU
1	H	65	LEU

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Mol	Chain	Res	Type
1	H	75	GLN
1	H	79	LEU
1	H	80	GLU
1	H	97	GLU
1	H	105	SER
1	H	133	LEU
1	H	134	THR
1	H	183	ILE
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	91	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	121	GLU
2	I	124	MET
2	I	131	THR
2	I	132	ASP
2	I	160	ASP
2	I	197	ARG
2	I	238	GLN
2	I	285	ILE
2	I	306	THR
2	I	316	GLU
2	I	320	ASP
2	I	369	MET
2	I	377	THR
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	446	ASP
2	I	471	VAL
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	496	LYS
2	I	538	LEU
2	I	539	THR

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Mol	Chain	Res	Type
2	I	540	ARG
2	I	542	ARG
2	I	554	HIS
2	I	563	THR
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	637	ARG
2	I	639	LYS
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	693	LEU
2	I	697	LYS
2	I	699	LEU
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	778	GLU
2	I	779	ARG
2	I	788	SER
2	I	814	ASP
2	I	815	SER
2	I	817	LEU
2	I	857	VAL
2	I	859	GLU
2	I	868	SER
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	913	VAL
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU

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Mol	Chain	Res	Type
2	I	1014	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1156	ARG
2	I	1159	VAL
2	I	1160	ASP
2	I	1163	THR
2	I	1198	LEU
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1246	ARG
2	I	1248	THR
2	I	1264	GLN
2	I	1310	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1331	ARG
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	134	ASP
3	J	159	ILE
3	J	169	LEU
3	J	170	GLU
3	J	175	GLU
3	J	217	LEU
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	312	ARG
3	J	324	LEU

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Mol	Chain	Res	Type
3	J	334	LYS
3	J	335	GLN
3	J	340	GLN
3	J	363	LEU
3	J	374	LEU
3	J	431	ARG
3	J	454	CYS
3	J	486	SER
3	J	490	ILE
3	J	507	VAL
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	558	ASP
3	J	573	THR
3	J	622	ASP
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	680	ASN
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	764	ARG
3	J	770	LEU
3	J	772	TYR
3	J	788	LEU
3	J	810	THR
3	J	844	THR
3	J	847	ASP

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Mol	Chain	Res	Type
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	897	HIS
3	J	898	CYS
3	J	908	ILE
3	J	918	ILE
3	J	960	LEU
3	J	963	VAL
3	J	972	LYS
3	J	979	ASN
3	J	987	GLU
3	J	988	PHE
3	J	997	VAL
3	J	1011	VAL
3	J	1017	VAL
3	J	1155	ILE
3	J	1167	LYS
3	J	1173	ARG
3	J	1177	ILE
3	J	1186	TYR
3	J	1189	MET
3	J	1208	ASP
3	J	1221	LEU
3	J	1255	VAL
3	J	1268	ASN
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1305	ASP
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
3	J	1344	LEU

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Mol	Chain	Res	Type
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
5	L	100	MET
5	L	102	MET
5	L	105	MET
5	L	154	GLU
5	L	247	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	362	ASN
5	L	395	THR
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	492	ASP
5	L	558	VAL
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	583	THR
5	L	587	ILE
5	L	600	HIS
5	L	603	ARG
5	L	609	SER
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	B	18	GLN
1	B	75	GLN
1	B	132	HIS
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	620	ASN
2	C	628	HIS
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1288	GLN
2	C	1314	GLN
3	D	200	GLN
3	D	340	GLN
3	D	365	GLN
3	D	435	GLN
3	D	450	HIS
3	D	477	GLN
3	D	702	GLN
3	D	792	ASN
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
3	D	1244	GLN
5	F	131	GLN
5	F	246	GLN
5	F	345	GLN
5	F	362	ASN
5	F	406	GLN
5	F	446	GLN
5	F	518	HIS
1	G	23	HIS
1	H	18	GLN
1	H	75	GLN
1	H	132	HIS
2	I	69	GLN
2	I	139	ASN
2	I	494	ASN
2	I	620	ASN

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Mol	Chain	Res	Type
2	I	628	HIS
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	200	GLN
3	J	340	GLN
3	J	365	GLN
3	J	435	GLN
3	J	450	HIS
3	J	477	GLN
3	J	702	GLN
3	J	792	ASN
3	J	910	ASN
3	J	929	GLN
3	J	1218	HIS
3	J	1244	GLN
5	L	131	GLN
5	L	246	GLN
5	L	345	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	518	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	42T	J	1501	-	34,34,34	1.94	5 (14%)	47,48,48	2.21	9 (19%)
6	42T	C	1401	-	34,34,34	1.92	5 (14%)	47,48,48	2.24	9 (19%)

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	42T	J	1501	-	-	0/23/24/24	0/3/3/3
6	42T	C	1401	-	-	0/23/24/24	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	42T	C13-N14	-6.51	1.28	1.41
6	J	1501	42T	C13-N14	-6.49	1.28	1.41
6	J	1501	42T	C08-N07	6.27	1.38	1.28
6	C	1401	42T	C08-N07	6.25	1.38	1.28
6	J	1501	42T	C15-N17	3.41	1.44	1.37
6	J	1501	42T	O20-N19	-3.30	1.31	1.40
6	C	1401	42T	O20-N19	-3.29	1.31	1.40
6	C	1401	42T	C15-N17	3.20	1.44	1.37
6	C	1401	42T	C08-N19	-2.19	1.30	1.35
6	J	1501	42T	C08-N19	-2.15	1.30	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	42T	C09-C08-N19	-7.22	102.86	114.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1501	42T	C09-C08-N19	-7.04	103.14	114.63
6	C	1401	42T	C18-C19-CL1	5.75	125.85	119.27
6	J	1501	42T	C18-C19-CL1	5.53	125.61	119.27
6	J	1501	42T	C04-N07-C08	5.40	132.15	120.41
6	C	1401	42T	C04-N07-C08	5.24	131.80	120.41
6	C	1401	42T	O16-C15-N17	-4.82	115.46	123.62
6	J	1501	42T	O16-C15-N17	-4.65	115.76	123.62
6	J	1501	42T	C18-N17-C15	-4.25	115.54	121.82
6	C	1401	42T	C18-N17-C15	-4.24	115.55	121.82
6	C	1401	42T	C19-C18-N17	4.22	126.19	121.14
6	J	1501	42T	C19-C18-N17	4.20	126.16	121.14
6	J	1501	42T	C21-C19-CL1	-3.57	111.24	118.41
6	J	1501	42T	N17-C15-N14	3.45	118.51	112.49
6	C	1401	42T	C21-C19-CL1	-3.43	111.52	118.41
6	C	1401	42T	N17-C15-N14	3.36	118.35	112.49
6	C	1401	42T	C02-C03-C04	2.75	123.43	119.74
6	J	1501	42T	C02-C03-C04	2.67	123.33	119.74

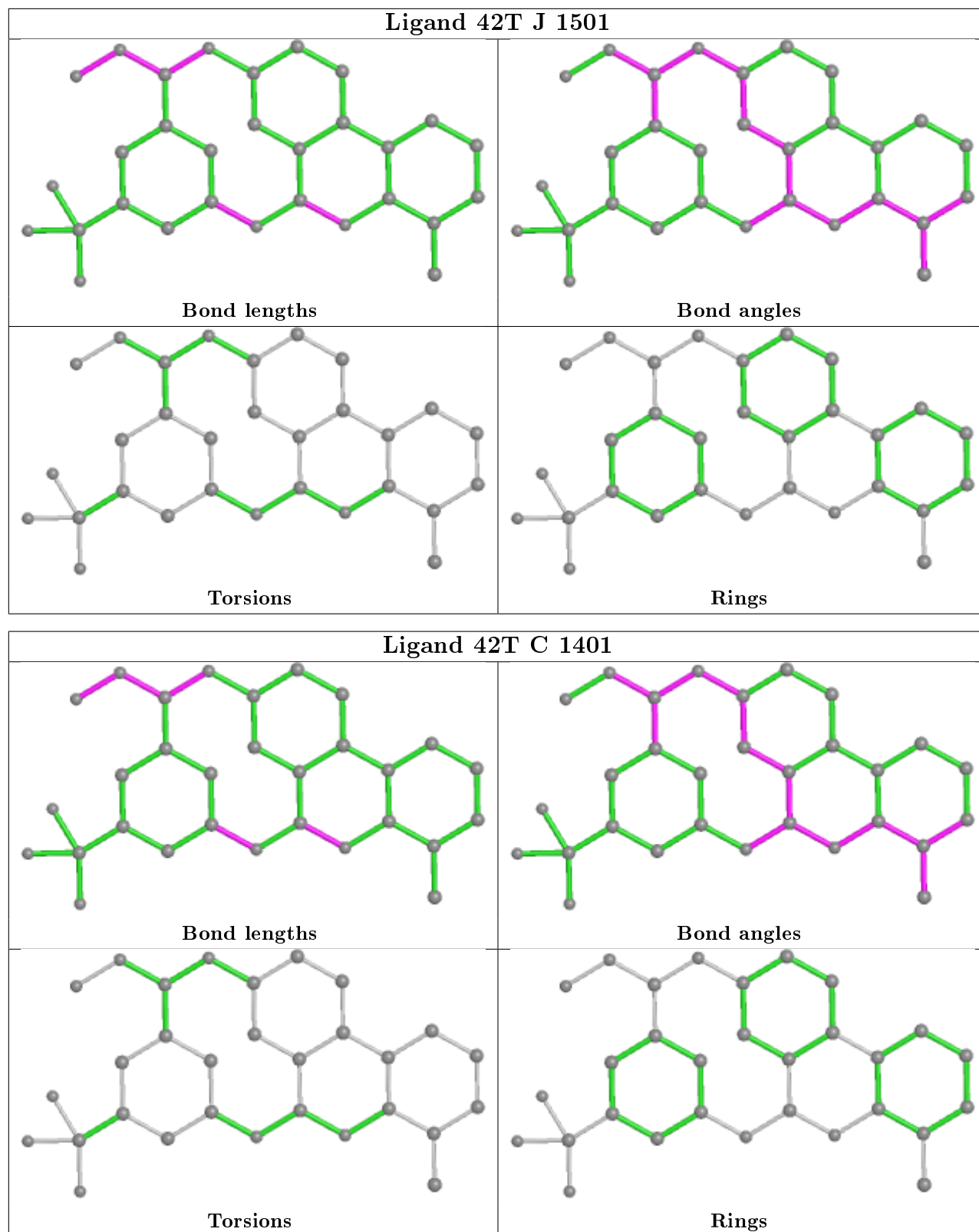
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/239 (93%)	-0.20	0 100 100	53, 89, 135, 163	0
1	B	220/239 (92%)	0.06	10 (4%) 33 27	59, 126, 160, 181	0
1	G	228/239 (95%)	-0.02	7 (3%) 49 38	78, 121, 145, 188	0
1	H	217/239 (90%)	-0.01	3 (1%) 75 65	79, 127, 150, 167	0
2	C	1340/1342 (99%)	-0.23	16 (1%) 79 70	22, 78, 132, 165	0
2	I	1340/1342 (99%)	-0.17	28 (2%) 63 54	41, 98, 145, 179	0
3	D	1166/1407 (82%)	-0.22	10 (0%) 84 77	23, 77, 140, 177	0
3	J	1236/1407 (87%)	-0.12	20 (1%) 72 62	31, 96, 144, 169	0
4	E	89/91 (97%)	-0.40	0 100 100	36, 80, 122, 124	0
4	K	79/91 (86%)	-0.34	0 100 100	58, 94, 137, 160	0
5	F	470/522 (90%)	-0.21	18 (3%) 40 32	43, 116, 156, 171	0
5	L	469/522 (89%)	-0.21	12 (2%) 56 46	49, 115, 154, 180	0
All	All	7078/7680 (92%)	-0.17	124 (1%) 68 59	22, 96, 147, 188	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	8.0
1	B	69	SER	6.3
2	C	1000	LEU	5.7
3	J	1294	ALA	5.6
3	D	878	ASP	5.5
1	B	66	HIS	5.4
3	J	1295	ASN	5.2
1	B	68	TYR	5.1
1	B	159	ILE	5.0
2	I	982	GLY	4.9
3	J	1188	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	158	ARG	4.8
2	C	1001	GLY	4.8
5	F	167	ASP	4.6
5	L	167	ASP	4.4
2	I	999	GLU	4.4
5	F	301	ASN	4.2
3	D	1198	VAL	4.1
5	L	305	LEU	4.1
3	D	879	ALA	4.0
1	B	146	VAL	3.9
2	I	1002	LEU	3.7
5	L	318	ALA	3.7
1	G	89	ALA	3.6
5	L	290	LEU	3.6
1	B	78	ILE	3.5
3	J	975	ILE	3.5
3	J	998	PRO	3.5
3	J	732	GLY	3.5
1	B	160	HIS	3.4
2	C	251	ALA	3.4
2	I	979	LEU	3.4
2	C	282	VAL	3.3
2	C	266	GLY	3.3
2	I	1003	THR	3.2
2	C	540	ARG	3.0
1	G	184	ALA	3.0
1	G	90	VAL	3.0
3	D	1204	VAL	3.0
3	J	1186	TYR	3.0
5	F	306	PHE	3.0
2	I	987	GLU	2.9
2	I	1001	GLY	2.9
1	H	67	GLU	2.9
5	L	315	TRP	2.9
3	J	69	GLU	2.9
2	I	975	ILE	2.8
5	L	480	PRO	2.8
5	L	304	THR	2.8
2	I	996	ARG	2.7
5	L	317	ASN	2.7
2	I	981	ALA	2.7
3	J	974	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
5	L	319	ALA	2.7
5	F	285	ARG	2.6
5	L	314	THR	2.6
2	C	999	GLU	2.6
5	F	579	GLN	2.6
2	I	169	LYS	2.6
3	J	1161	GLY	2.6
1	H	172	LEU	2.6
5	F	584	ARG	2.6
3	J	1198	VAL	2.6
5	F	319	ALA	2.6
5	F	283	GLN	2.6
5	F	300	LYS	2.5
2	C	982	GLY	2.5
2	I	978	VAL	2.5
5	L	610	PHE	2.5
1	G	194	GLN	2.5
2	C	252	SER	2.4
5	F	305	LEU	2.4
5	L	294	GLN	2.4
2	I	980	VAL	2.4
5	F	315	TRP	2.4
3	J	930	LEU	2.4
5	F	259	PHE	2.4
2	I	720	ARG	2.4
2	I	983	GLY	2.4
5	F	304	THR	2.3
2	C	265	LYS	2.3
1	G	211	ILE	2.3
3	J	1187	GLU	2.3
1	B	157	THR	2.3
2	I	21	VAL	2.2
2	I	882	ILE	2.2
2	I	1010	GLN	2.2
3	J	1010	GLN	2.2
3	D	849	LEU	2.2
2	C	319	LEU	2.2
2	I	264	GLU	2.2
2	I	974	ARG	2.2
1	G	209	GLY	2.2
3	J	849	LEU	2.2
5	F	310	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	231	GLU	2.2
2	I	782	VAL	2.2
2	I	1165	SER	2.2
2	C	165	HIS	2.1
3	J	77	ARG	2.1
3	J	856	ILE	2.1
2	C	585	GLY	2.1
5	F	287	ILE	2.1
3	D	1200	GLU	2.1
3	D	850	LYS	2.1
5	F	161	LEU	2.1
3	D	880	VAL	2.1
3	D	1299	GLY	2.1
3	J	999	TYR	2.1
5	F	158	LEU	2.1
1	H	210	THR	2.1
2	C	998	LEU	2.1
2	C	893	THR	2.1
3	J	176	PHE	2.1
2	C	333	ILE	2.0
2	I	247	ARG	2.0
2	I	740	GLU	2.0
2	I	266	GLY	2.0
5	F	302	PHE	2.0
2	I	977	ALA	2.0
2	I	243	PRO	2.0
3	J	957	SER	2.0
1	G	148	ARG	2.0
3	D	858	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

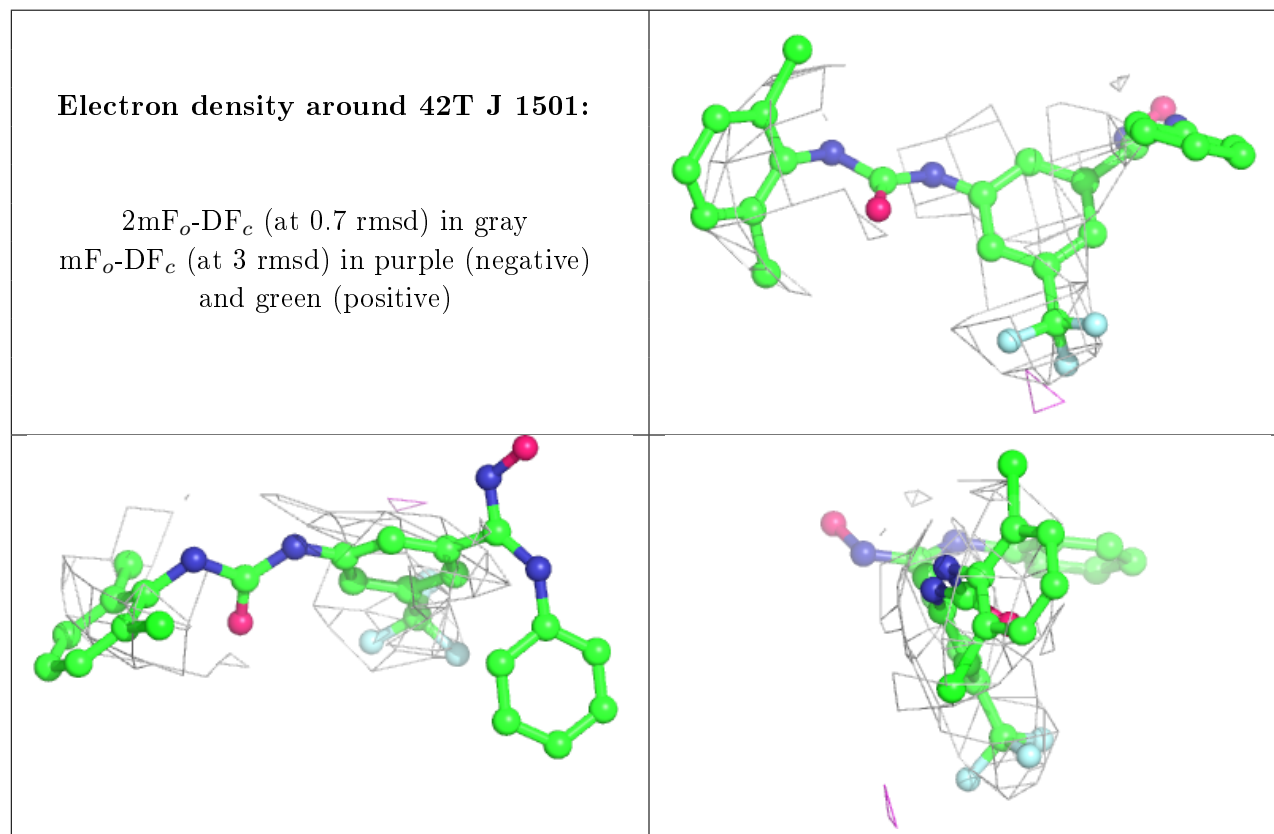
There are no carbohydrates in this entry.

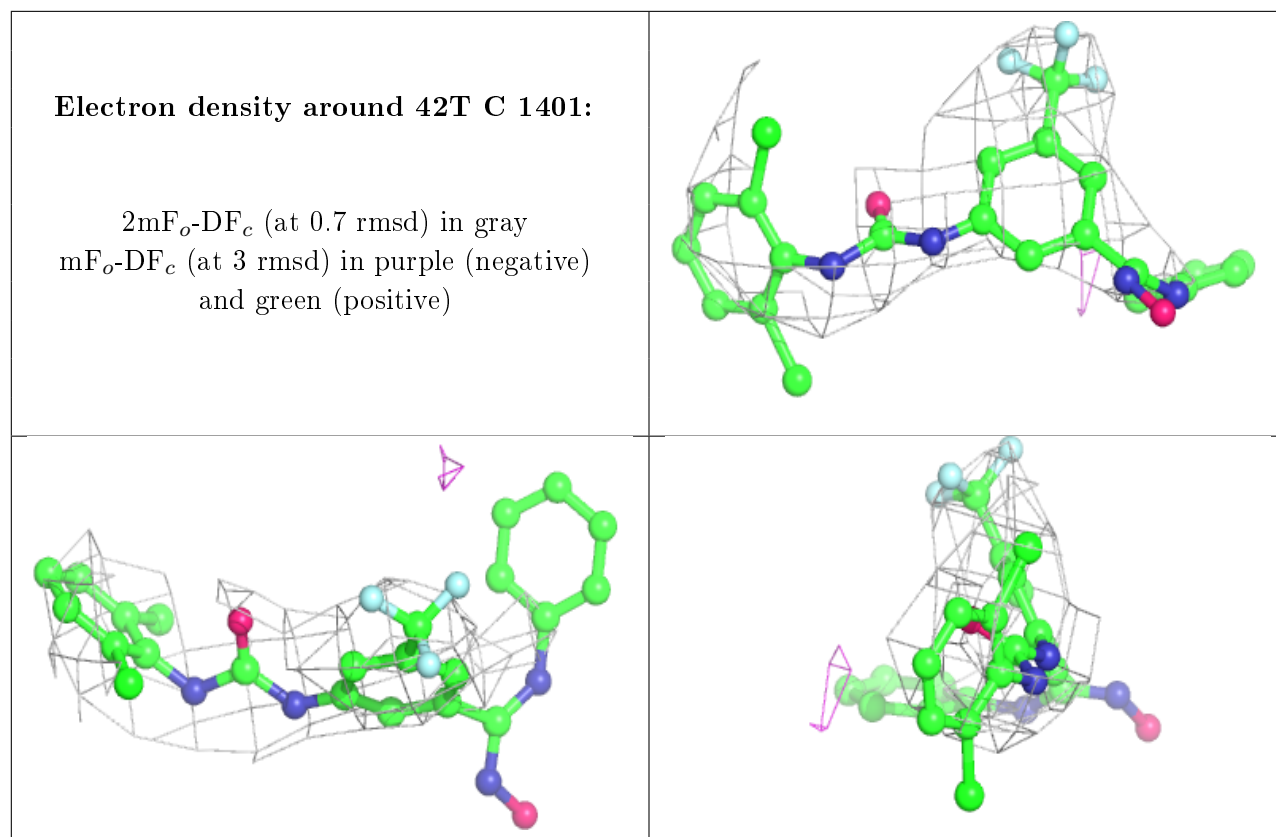
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ZN	D	1502	1/1	0.83	0.17	227,227,227,227	0
8	ZN	J	1503	1/1	0.83	0.20	422,422,422,422	0
8	ZN	D	1503	1/1	0.84	0.39	331,331,331,331	0
6	42T	J	1501	32/32	0.85	0.38	59,111,153,156	0
6	42T	C	1401	32/32	0.90	0.41	56,88,113,134	0
7	MG	J	1502	1/1	0.90	0.55	68,68,68,68	0
8	ZN	J	1504	1/1	0.95	0.35	333,333,333,333	0
7	MG	D	1501	1/1	0.97	0.51	74,74,74,74	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.