Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:28 PM GMT

PDB ID	:	4LK1
Title	:	Crystal Structure Analysis of the E.coli holoenzyme
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2013-07-05
Resolution	:	3.84 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

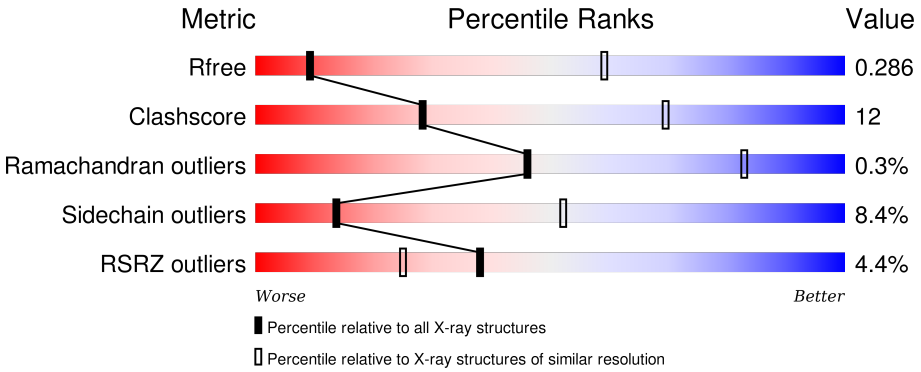
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.84 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}	91344	1334 (4.18-3.50)
Clashscore	102246	1036 (4.16-3.52)
Ramachandran outliers	100387	1415 (4.18-3.50)
Sidechain outliers	100360	1410 (4.18-3.50)
RSRZ outliers	91569	1342 (4.18-3.50)

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. 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 <=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	64% 28% • 6%
1	B	239	6% 59% 30% • 8%
1	G	239	3% 64% 28% • 5%
1	H	239	9% 57% 31% • 9%
2	C	1342	2% 68% 29% •

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Mol	Chain	Length	Quality of chain
2	I	1342	4% 69% 29%
3	D	1407	2% 55% 25% 17%
3	J	1407	7% 62% 29% 5%
4	E	91	68% 26%
4	K	91	% 62% 23% 13%
5	F	613	6% 61% 25% 12%
5	L	613	5% 61% 25% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ZN	D	1503	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 57170 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 C9QXI7
A	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
A	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
A	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
A	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
B	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
B	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
B	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
B	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
B	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
G	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
G	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
G	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
G	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
G	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
H	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
H	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
H	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
H	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
H	239	GLN	-	EXPRESSION TAG	UNP C9QXI7

- 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	1334	Total	C	N	O	S	0	0	0
			10369	6513	1850	1957	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

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

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

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

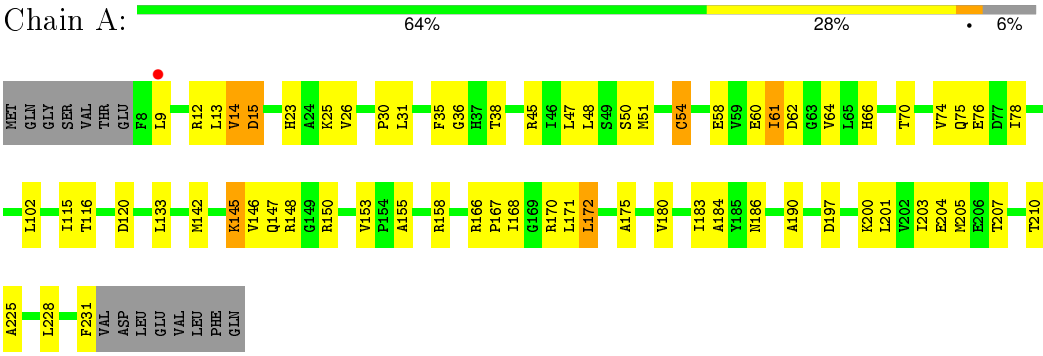
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	2	Total Zn 2 2	0	0
7	D	2	Total Zn 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

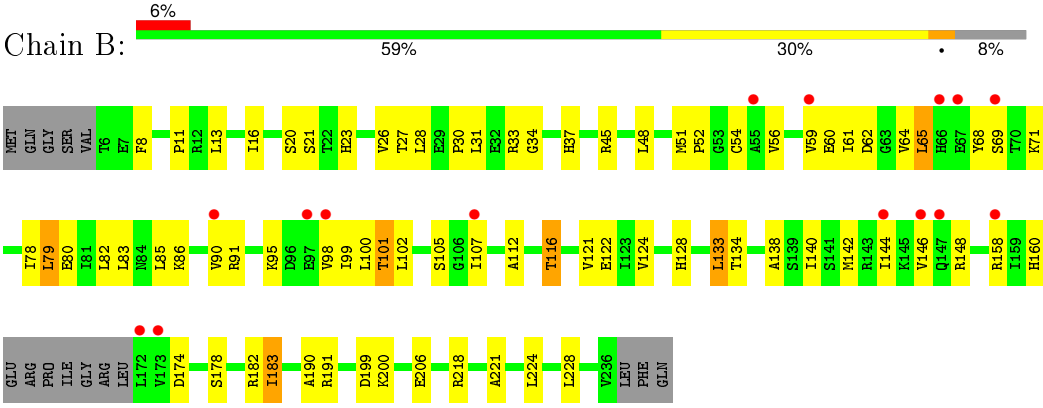
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



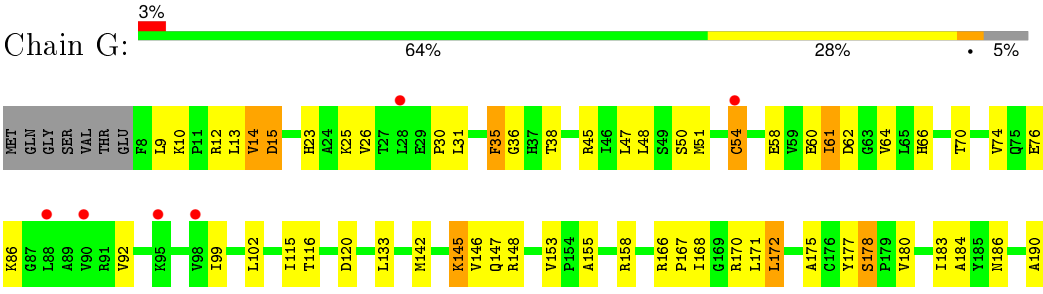
- Molecule 1: DNA-directed RNA polymerase subunit alpha

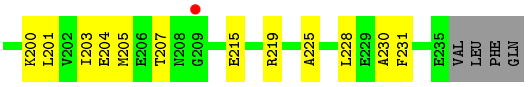
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

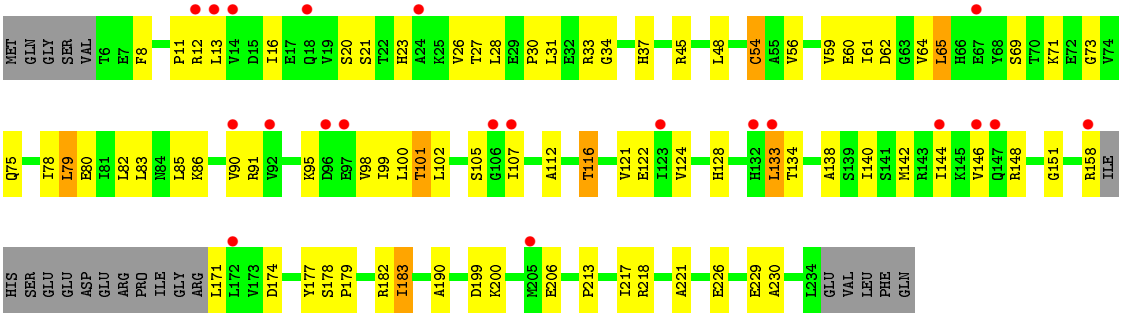
Chain G:





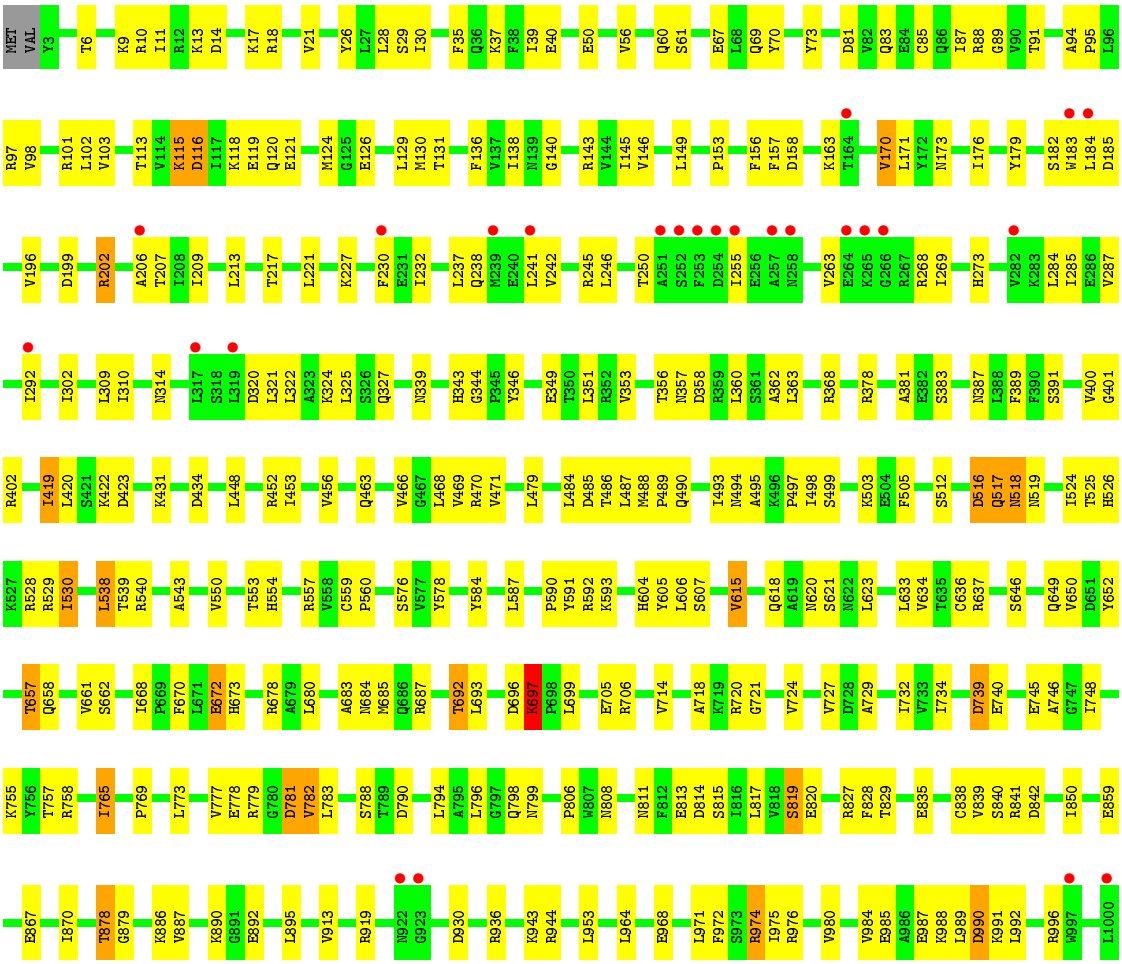
- Molecule 1: DNA-directed RNA polymerase subunit alpha

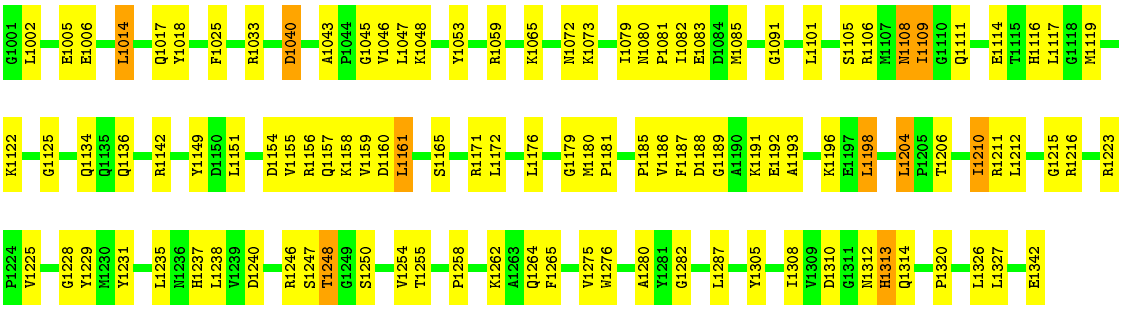
Chain H:

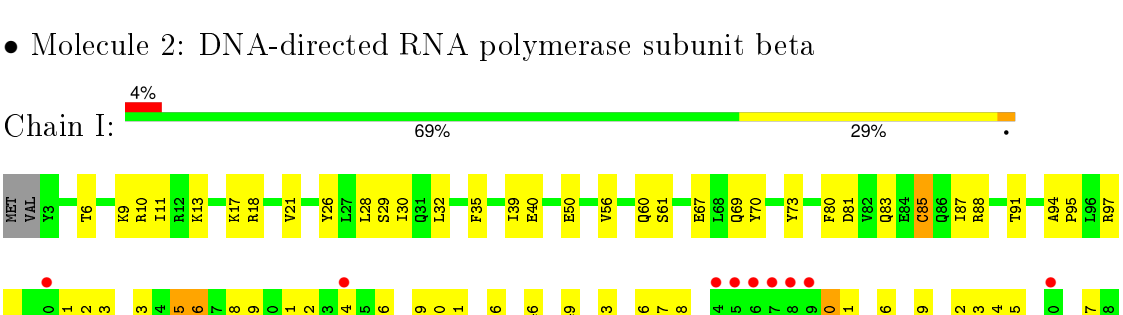


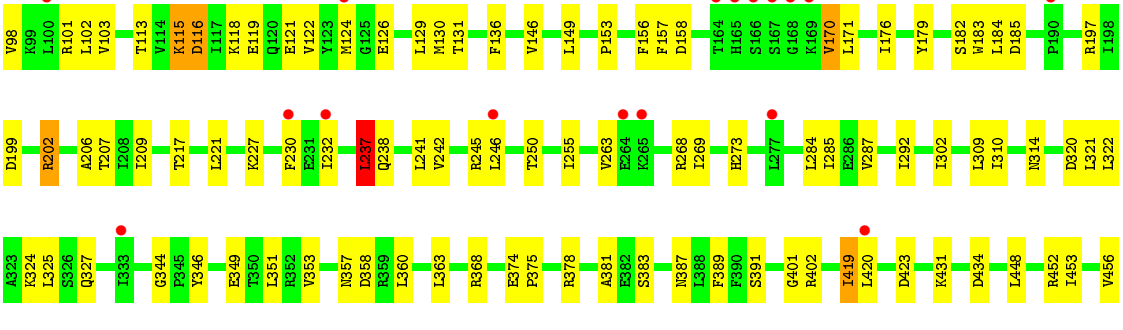
- Molecule 2: DNA-directed RNA polymerase subunit beta

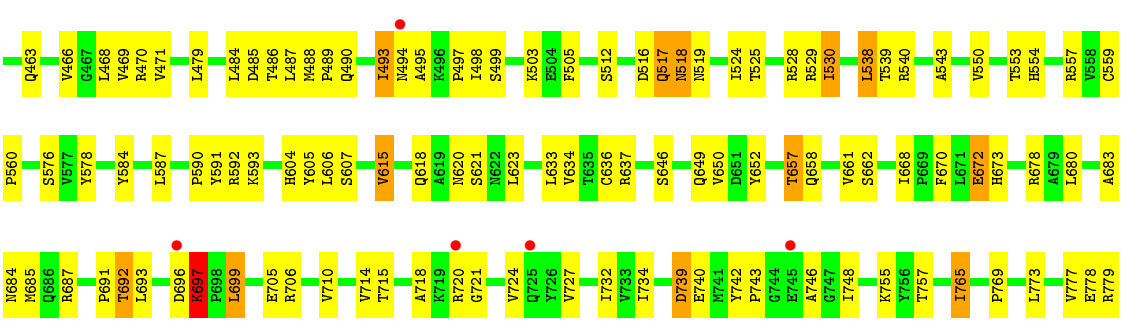
Chain C:

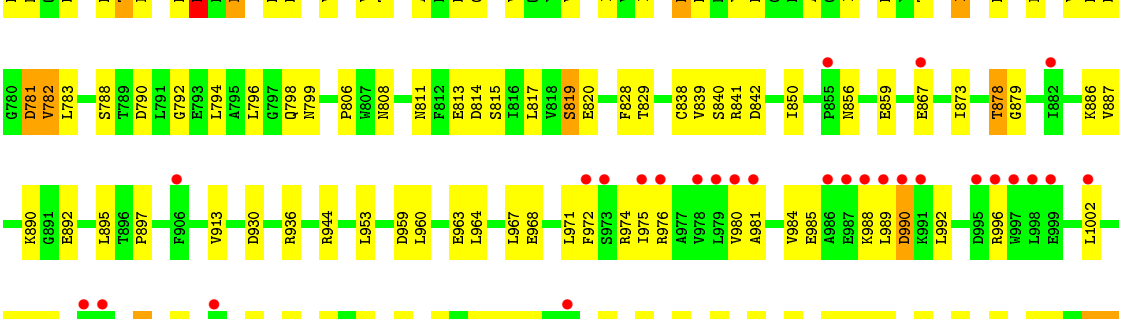


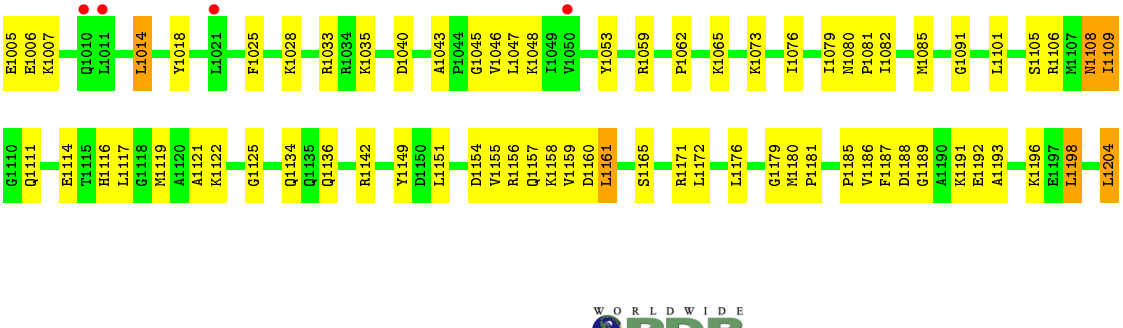






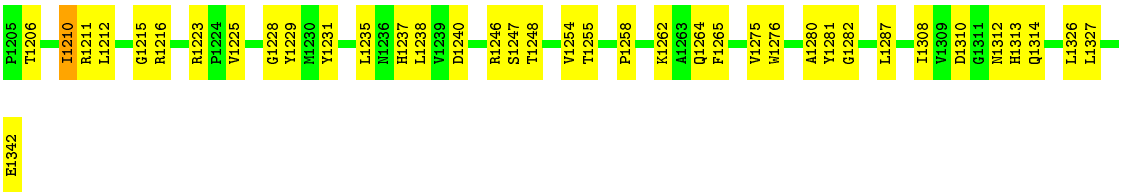






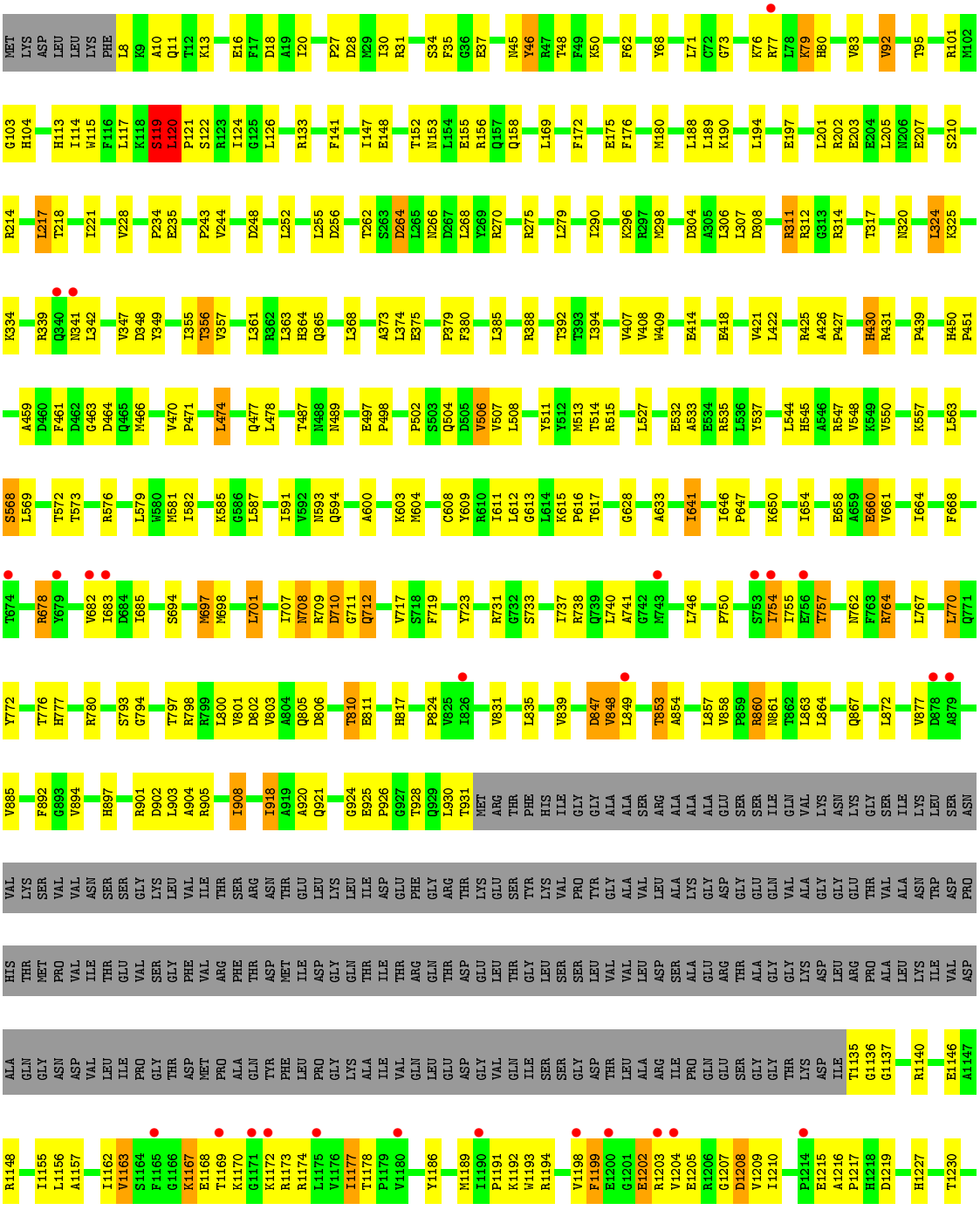
• Molecule 2: DNA-directed RNA polymerase subunit beta

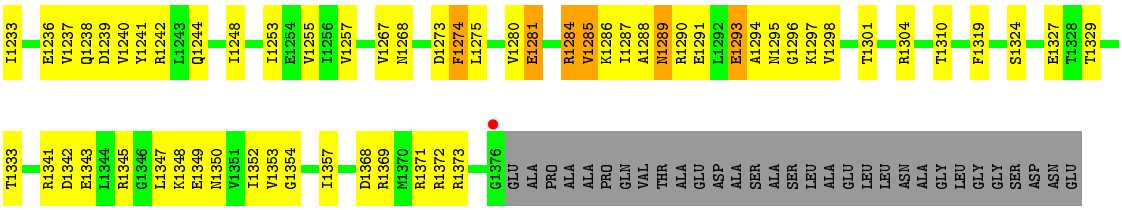
Chain I: 4% 69% 29%



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

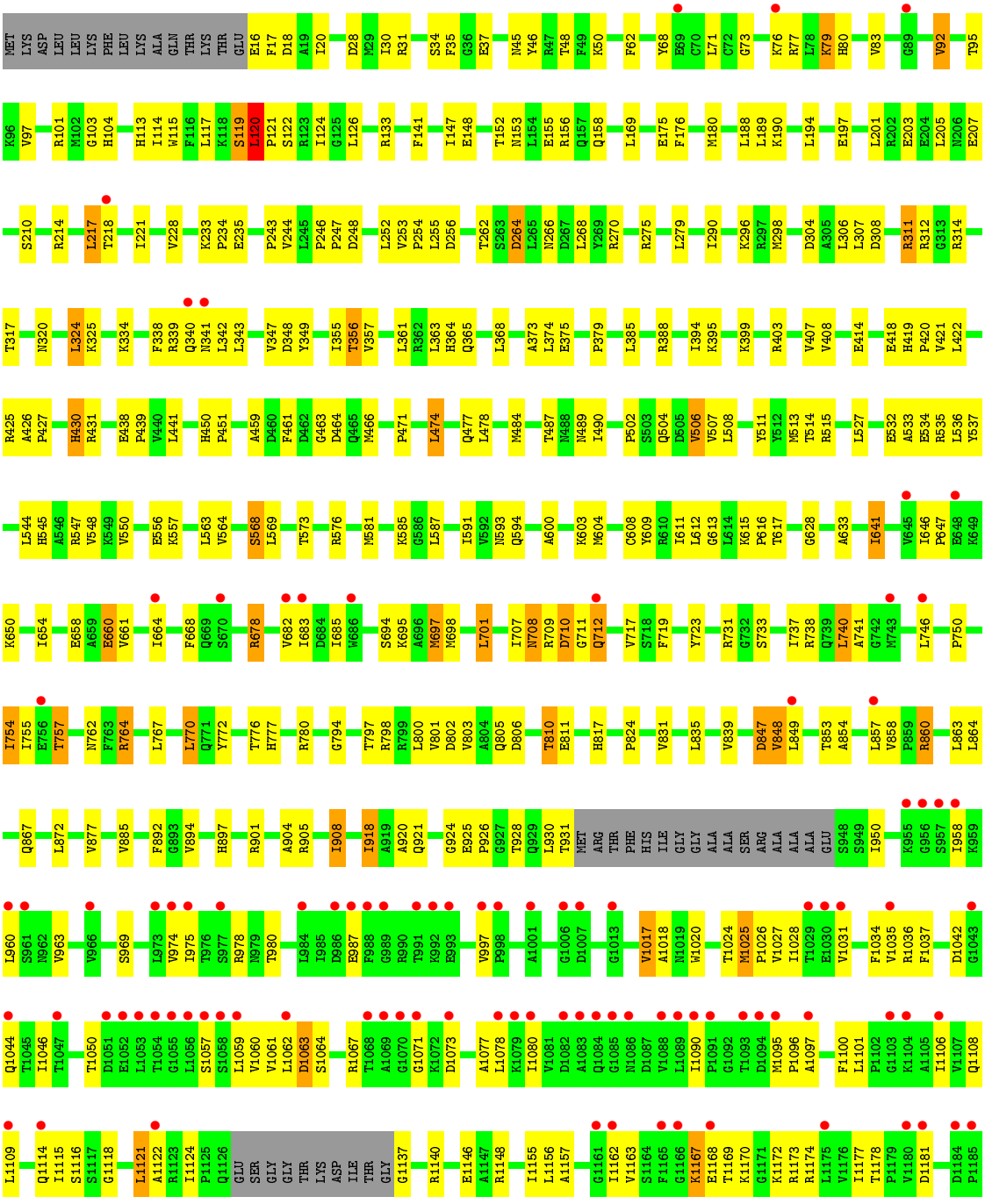
Chain D:

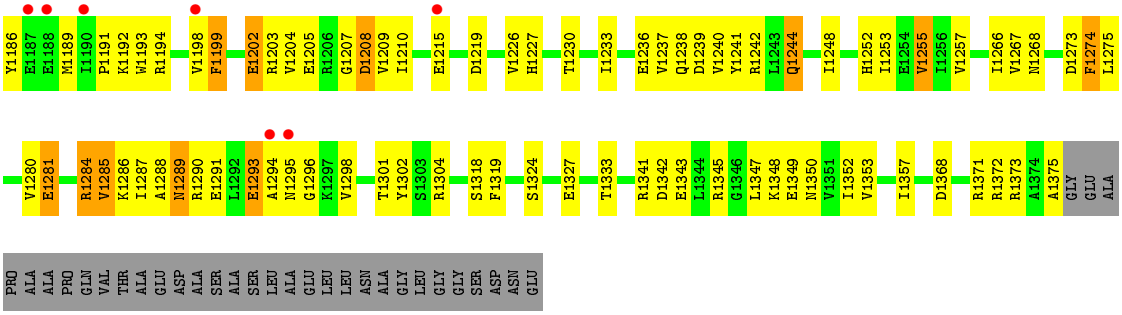




• Molecule 3: DNA-directed RNA polymerase subunit beta'

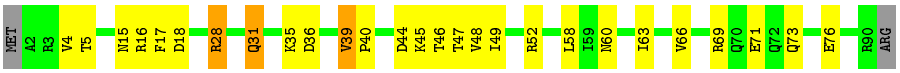
Chain J:





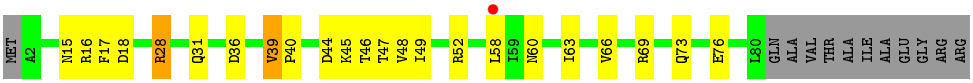
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



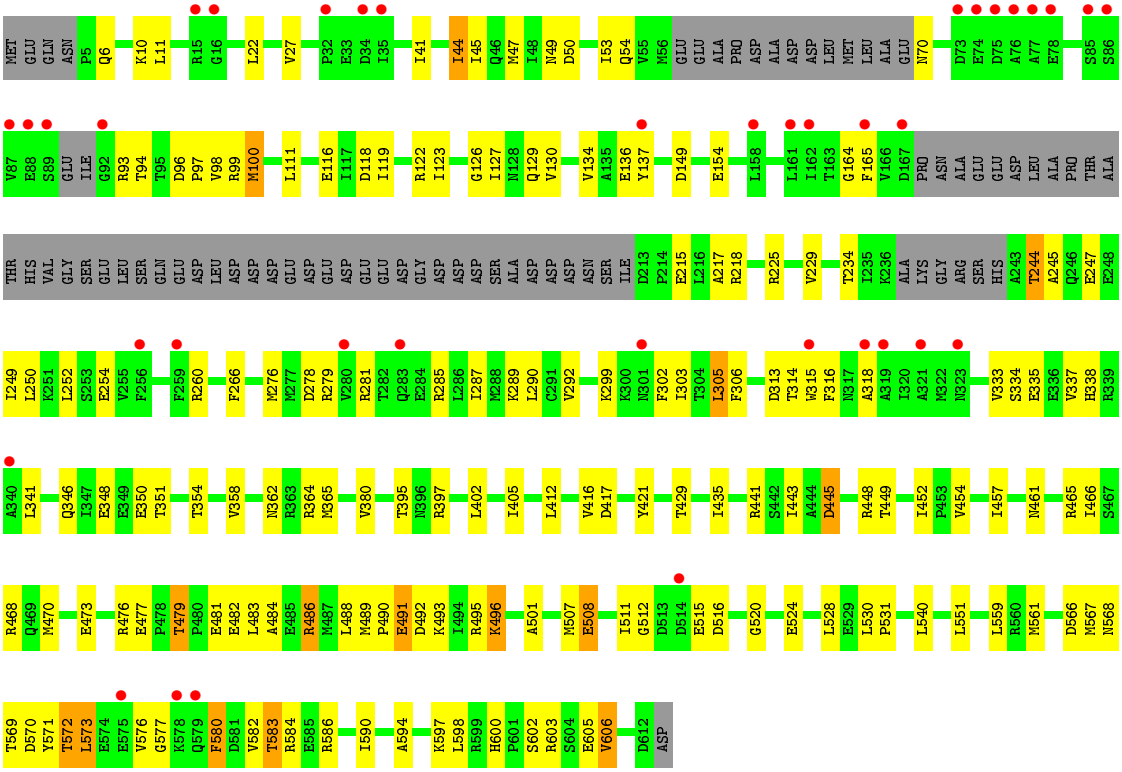
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



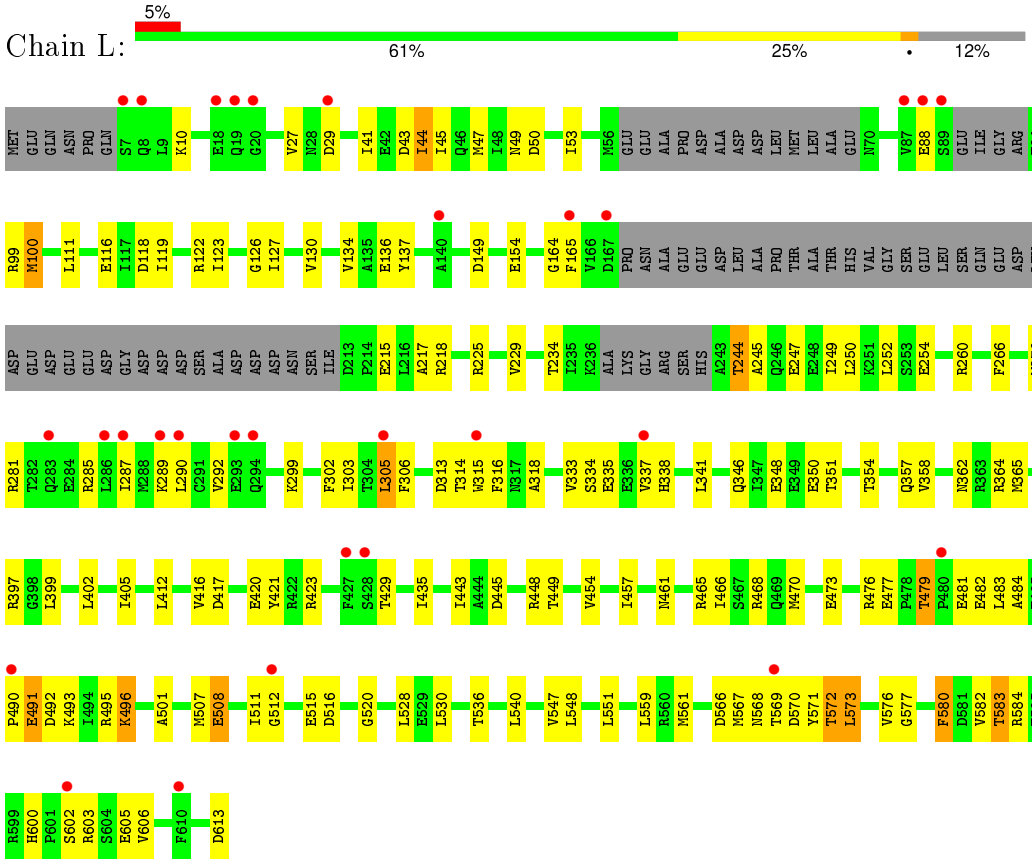
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.68Å 206.39Å 308.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.78 – 3.84 44.78 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.78-3.84) 98.3 (44.78-3.84)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.224 , 0.272 0.247 , 0.286	Depositor DCC
R_{free} test set	5631 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	142.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 112457 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	57170	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.25	0/1751	0.51	0/2373
1	B	0.26	0/1707	0.49	0/2314
1	G	0.25	0/1771	0.53	0/2401
1	H	0.26	0/1686	0.49	0/2285
2	C	0.26	0/10739	0.48	1/14489 (0.0%)
2	I	0.26	0/10735	0.48	2/14484 (0.0%)
3	D	0.26	0/9246	0.48	1/12478 (0.0%)
3	J	0.26	0/10525	0.48	1/14212 (0.0%)
4	E	0.24	0/693	0.48	0/935
4	K	0.24	0/629	0.48	0/847
5	F	0.29	0/4254	0.51	2/5731 (0.0%)
5	L	0.29	0/4246	0.49	1/5720 (0.0%)
All	All	0.27	0/57982	0.49	8/78269 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	4
3	J	0	2
5	F	0	2
5	L	0	1
All	All	0	10

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	11	LEU	N-CA-C	-9.14	86.33	111.00
2	I	237	LEU	N-CA-C	5.38	125.53	111.00
3	D	120	LEU	N-CA-C	5.26	125.21	111.00
3	J	120	LEU	N-CA-C	5.25	125.18	111.00
2	C	516	ASP	CB-CG-OD2	5.23	123.01	118.30
2	I	516	ASP	CB-CG-OD2	5.21	122.99	118.30
5	F	149	ASP	CB-CG-OD2	5.21	122.99	118.30
5	L	149	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1161	LEU	Peptide
3	D	119	SER	Mainchain,Peptide
3	D	120	LEU	Peptide
3	D	1296	GLY	Peptide
5	F	10	LYS	Peptide
5	F	6	GLN	Peptide
3	J	120	LEU	Peptide
3	J	1296	GLY	Peptide
5	L	10	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	48	0
1	B	1687	0	1700	53	0
1	G	1750	0	1764	54	0
1	H	1667	0	1689	53	0
2	C	10570	0	10582	254	0
2	I	10566	0	10576	243	0
3	D	9107	0	9308	249	0
3	J	10369	0	10589	284	0
4	E	691	0	695	17	0
4	K	627	0	634	13	0
5	F	4204	0	4106	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	4196	0	4103	97	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	57170	0	57502	1328	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 (1328) 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:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.96
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.47	0.92
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.84
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.42	0.84
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.43	0.84
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.27	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.62	0.82
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.26	0.82
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.62	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.62	0.81
3:J:418:GLU:HG3	4:K:45:LYS:H	1.45	0.81
3:D:418:GLU:HG3	4:E:45:LYS:H	1.46	0.81
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.64	0.80
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.46	0.79
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.48	0.79
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.78
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.67	0.77
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.66	0.77
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.77
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.48	0.77
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.64	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.66	0.76
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.67	0.76
1:A:231:PHE:HZ	1:B:221:ALA:HB3	1.51	0.76
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.67	0.75
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.68	0.75
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.69	0.75
5:F:561:MET:HA	5:F:567:MET:HE1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.69	0.74
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.68	0.74
5:F:470:MET:HA	5:F:473:GLU:HB3	1.68	0.74
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.70	0.74
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.69	0.74
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.68	0.73
5:L:470:MET:HA	5:L:473:GLU:HB3	1.69	0.73
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.69	0.73
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.69	0.73
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.22	0.73
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.73
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.71	0.73
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.70	0.72
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.71	0.72
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.70	0.72
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.71	0.72
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.71	0.72
1:H:59:VAL:O	1:H:171:LEU:N	2.23	0.72
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.71
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.72	0.71
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.71
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.72	0.71
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.73	0.71
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.70	0.71
5:L:561:MET:HA	5:L:567:MET:HE1	1.71	0.71
1:H:101:THR:HG22	1:H:116:THR:HB	1.73	0.70
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.73	0.70
2:C:452:ARG:NH1	2:C:584:TYR:O	2.25	0.70
1:B:101:THR:HG22	1:B:116:THR:HB	1.73	0.70
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.73	0.70
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.71	0.70
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.73	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.26	0.69
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.74	0.69
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.73	0.69
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.74	0.68
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.58	0.68
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.59	0.68
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.73	0.68
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.75	0.68
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.59	0.68
2:I:829:THR:HA	2:I:1059:ARG:HA	1.76	0.68
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.75	0.68
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.76	0.67
2:I:528:ARG:NH2	2:I:576:SER:O	2.26	0.67
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.75	0.67
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.76	0.67
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.75	0.67
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.27	0.67
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.76	0.67
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.77	0.67
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.59	0.67
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.27	0.66
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.61	0.66
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.61	0.66
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.77	0.66
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.66
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.28	0.66
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.78	0.66
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.78	0.66
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.76	0.66
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.29	0.66
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.77	0.66
2:C:136:PHE:O	2:C:143:ARG:N	2.24	0.66
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.78	0.66
2:I:18:ARG:NH1	2:I:621:SER:O	2.29	0.65
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.77	0.65
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.77	0.65
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.77	0.65
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.78	0.65
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.76	0.65
2:C:829:THR:HA	2:C:1059:ARG:HA	1.77	0.65
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.78	0.65
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.77	0.65
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.78	0.65
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.78	0.65
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.79	0.65
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.79	0.65
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.65
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.79	0.65
1:A:166:ARG:O	1:A:168:ILE:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.60	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:C:18:ARG:NH1	2:C:621:SER:O	2.30	0.65
3:J:478:LEU:HG	4:K:47:THR:HG23	1.79	0.65
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.79	0.65
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.62	0.65
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.77	0.64
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.78	0.64
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.33	0.64
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.78	0.64
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.64
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.78	0.64
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.79	0.64
3:D:478:LEU:HG	4:E:47:THR:HG23	1.79	0.64
1:G:230:ALA:HA	1:H:12:ARG:HG2	1.78	0.64
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.80	0.64
3:D:755:ILE:HG22	3:D:757:THR:H	1.62	0.64
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.78	0.64
3:J:755:ILE:HG22	3:J:757:THR:H	1.62	0.63
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.61	0.63
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.63	0.63
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.79	0.63
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.32	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.63
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.63
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.31	0.63
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.81	0.63
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.63	0.62
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.81	0.62
2:C:339:ASN:HB3	2:C:343:HIS:H	1.64	0.62
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.81	0.62
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.64	0.62
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.81	0.62
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.32	0.62
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.81	0.62
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.32	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.80	0.62
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.82	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
2:I:518:ASN:N	2:I:518:ASN:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:30:ILE:HD12	2:I:30:ILE:H	1.65	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.63	0.61
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.82	0.61
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.61
2:C:518:ASN:OD1	2:C:518:ASN:N	2.33	0.61
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.82	0.61
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.83	0.61
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.83	0.61
1:H:182:ARG:NH1	3:J:581:MET:SD	2.74	0.61
2:I:560:PRO:O	3:J:780:ARG:NH2	2.34	0.61
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.83	0.61
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.83	0.60
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.81	0.60
3:D:847:ASP:N	3:D:847:ASP:OD1	2.34	0.60
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.82	0.60
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.83	0.60
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.33	0.60
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.81	0.60
3:J:148:GLU:H	3:J:156:ARG:HG3	1.65	0.60
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.84	0.60
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.83	0.60
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.60
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.83	0.60
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.84	0.60
2:I:494:ASN:OD1	2:I:495:ALA:N	2.33	0.60
2:C:494:ASN:OD1	2:C:495:ALA:N	2.32	0.60
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.34	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.84	0.60
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.83	0.59
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.84	0.59
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.84	0.59
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.84	0.59
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.84	0.59
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.84	0.59
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.84	0.59
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.84	0.59
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.85	0.59
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.84	0.59
3:D:148:GLU:H	3:D:156:ARG:HG3	1.67	0.59
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.84	0.59
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.84	0.59
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.85	0.59
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.33	0.59
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.68	0.59
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.85	0.59
2:C:560:PRO:O	3:D:780:ARG:NH2	2.35	0.58
3:D:356:THR:OG1	3:D:357:VAL:N	2.36	0.58
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.58
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.35	0.58
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.36	0.58
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.35	0.58
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.84	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.58
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.36	0.58
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.85	0.58
3:J:356:THR:OG1	3:J:357:VAL:N	2.36	0.58
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.37	0.58
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.84	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.84	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.68	0.58
3:J:741:ALA:O	3:J:762:ASN:ND2	2.37	0.58
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.85	0.58
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.86	0.58
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.85	0.58
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.85	0.58
3:J:847:ASP:N	3:J:847:ASP:OD1	2.34	0.58
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.85	0.57
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.86	0.57
3:D:741:ALA:O	3:D:762:ASN:ND2	2.37	0.57
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.57
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.85	0.57
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.86	0.57
5:F:276:MET:SD	5:F:279:ARG:NH1	2.77	0.57
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.37	0.57
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.85	0.57
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.86	0.57
3:J:77:ARG:HE	5:L:569:THR:HA	1.69	0.57
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.85	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.57
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.87	0.57
2:C:30:ILE:H	2:C:30:ILE:HD12	1.69	0.57
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.57
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.69	0.57
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.37	0.57
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.87	0.57
5:L:482:GLU:O	5:L:486:ARG:NH2	2.38	0.57
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.87	0.57
2:I:40:GLU:O	2:I:73:TYR:OH	2.22	0.57
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.57
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.85	0.57
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.87	0.57
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.87	0.57
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.87	0.57
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.70	0.57
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.86	0.57
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.87	0.56
2:C:40:GLU:O	2:C:73:TYR:OH	2.22	0.56
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.87	0.56
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.86	0.56
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.70	0.56
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.70	0.56
3:J:613:GLY:O	3:J:617:THR:OG1	2.23	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.86	0.56
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.68	0.56
3:J:152:THR:OG1	3:J:153:ASN:N	2.37	0.56
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.86	0.56
5:L:276:MET:SD	5:L:279:ARG:NH1	2.77	0.56
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.86	0.56
3:D:794:GLY:O	3:D:797:THR:OG1	2.21	0.56
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.24	0.56
5:F:482:GLU:O	5:F:486:ARG:NH2	2.38	0.56
1:A:14:VAL:HG22	1:A:15:ASP:H	1.71	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.70	0.56
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.87	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.38	0.56
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.38	0.56
1:B:64:VAL:HG12	1:B:65:LEU:H	1.71	0.56
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.88	0.56
1:A:23:HIS:HB2	1:A:205:MET:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.70	0.56
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.88	0.56
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.86	0.56
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.88	0.56
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.88	0.56
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.70	0.56
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.23	0.56
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.88	0.56
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.88	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
3:J:682:VAL:O	3:J:685:ILE:HG12	2.05	0.55
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.36	0.55
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.88	0.55
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.88	0.55
2:C:227:LYS:O	2:C:245:ARG:NH2	2.39	0.55
2:C:207:THR:HG21	2:C:351:LEU:HG	1.88	0.55
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.89	0.55
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.88	0.55
3:J:794:GLY:O	3:J:797:THR:OG1	2.21	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.34	0.55
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.88	0.55
1:G:14:VAL:HG22	1:G:15:ASP:H	1.72	0.55
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.89	0.55
1:B:16:ILE:HG13	1:B:26:VAL:HG22	1.88	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.55
3:J:120:LEU:HD12	5:L:43:ASP:HB3	1.88	0.55
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.88	0.55
3:D:613:GLY:O	3:D:617:THR:OG1	2.24	0.55
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.89	0.55
2:I:227:LYS:O	2:I:245:ARG:NH2	2.40	0.55
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.37	0.54
2:I:207:THR:HG21	2:I:351:LEU:HG	1.88	0.54
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.90	0.54
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.89	0.54
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.41	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.05	0.54
5:L:602:SER:H	5:L:605:GLU:HG3	1.72	0.54
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.90	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.72	0.54
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:515:GLU:HG2	5:L:516:ASP:H	1.71	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.08	0.54
3:J:425:ARG:HG2	3:J:426:ALA:H	1.72	0.54
2:I:488:MET:O	2:I:490:GLN:N	2.35	0.54
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.89	0.54
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.41	0.54
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.90	0.54
3:D:770:LEU:H	3:D:770:LEU:HD22	1.72	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.71	0.54
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.90	0.54
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.54
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.89	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.21	0.54
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.89	0.54
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.42	0.54
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.88	0.54
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.88	0.54
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.89	0.54
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.89	0.54
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.90	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.54
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.90	0.54
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.89	0.54
3:D:210:SER:O	3:D:214:ARG:HG2	2.08	0.54
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.90	0.54
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.90	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.90	0.54
5:F:573:LEU:H	5:F:573:LEU:HD23	1.72	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.90	0.54
3:D:425:ARG:HG2	3:D:426:ALA:H	1.73	0.54
3:J:34:SER:OG	3:J:104:HIS:ND1	2.28	0.54
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.90	0.54
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.90	0.54
3:J:770:LEU:HD22	3:J:770:LEU:H	1.73	0.53
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.90	0.53
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.53
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.90	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.73	0.53
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.44	0.53
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.73	0.53
5:F:602:SER:H	5:F:605:GLU:HG3	1.72	0.53
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.91	0.53
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.73	0.53
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.90	0.53
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.90	0.53
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.73	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.91	0.53
5:L:49:ASN:HA	5:L:53:ILE:HA	1.90	0.53
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.90	0.53
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.44	0.53
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.53
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.91	0.53
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.41	0.53
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.89	0.53
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.53
1:A:74:VAL:HG22	1:A:76:GLU:H	1.73	0.53
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.41	0.53
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.90	0.53
3:D:34:SER:OG	3:D:104:HIS:ND1	2.29	0.53
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.89	0.53
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.89	0.53
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.53
1:B:11:PRO:HB3	1:B:30:PRO:O	2.08	0.53
5:L:511:ILE:HG13	5:L:512:GLY:H	1.74	0.53
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.53
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.91	0.53
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.90	0.53
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.91	0.53
2:C:324:LYS:O	2:C:327:GLN:NE2	2.42	0.53
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.09	0.52
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.42	0.52
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.08	0.52
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.10	0.52
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.90	0.52
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.90	0.52
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.90	0.52
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.91	0.52
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.09	0.52
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.90	0.52
1:A:172:LEU:H	1:A:172:LEU:HD12	1.74	0.52
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.52
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.92	0.52
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.91	0.52
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.52
1:A:61:ILE:HG22	1:A:62:ASP:H	1.74	0.52
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.21	0.52
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.52
2:I:324:LYS:O	2:I:327:GLN:NE2	2.43	0.52
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.27	0.52
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.39	0.52
1:G:74:VAL:HG22	1:G:76:GLU:H	1.74	0.52
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.91	0.52
3:J:119:SER:O	3:J:121:PRO:HD2	2.10	0.52
3:D:77:ARG:HE	5:F:569:THR:HA	1.74	0.52
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.90	0.52
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.90	0.52
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.44	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.52
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.91	0.52
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.36	0.52
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.90	0.52
1:G:61:ILE:HG22	1:G:62:ASP:H	1.74	0.52
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.92	0.52
5:F:126:GLY:O	5:F:129:GLN:HB2	2.10	0.52
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.52
5:L:547:VAL:HG12	5:L:598:LEU:HD22	1.92	0.52
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.73	0.52
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.92	0.52
5:F:49:ASN:HA	5:F:53:ILE:HA	1.91	0.52
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.42	0.52
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.92	0.52
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.92	0.52
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.92	0.52
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.91	0.52
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.43	0.52
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.92	0.52
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.92	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.45	0.51
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.91	0.51
5:L:483:LEU:H	5:L:483:LEU:HD12	1.74	0.51
2:I:103:VAL:HB	2:I:113:THR:HG21	1.91	0.51
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.74	0.51
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.76	0.51
3:D:73:GLY:O	3:D:76:LYS:NZ	2.33	0.51
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.92	0.51
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.92	0.51
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.92	0.51
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.91	0.51
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.75	0.51
2:C:349:GLU:O	2:C:353:VAL:HG23	2.10	0.51
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.46	0.51
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.92	0.51
2:C:103:VAL:HB	2:C:113:THR:HG21	1.91	0.51
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.92	0.51
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.93	0.51
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.43	0.51
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.75	0.51
1:H:11:PRO:HB3	1:H:30:PRO:O	2.10	0.51
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.76	0.51
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.93	0.51
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.93	0.51
1:G:172:LEU:HD12	1:G:172:LEU:H	1.76	0.51
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.93	0.51
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.51
3:J:568:SER:OG	3:J:569:LEU:N	2.43	0.51
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.27	0.51
5:L:448:ARG:NH1	5:L:501:ALA:O	2.35	0.51
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.92	0.51
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.51
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.93	0.51
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.26	0.51
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.92	0.51
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.92	0.51
5:F:316:PHE:HZ	5:F:334:SER:HA	1.76	0.51
5:L:126:GLY:O	5:L:130:VAL:HG13	2.11	0.51
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.46	0.51
3:D:1268:ASN:HD22	3:J:1268:ASN:HD22	1.59	0.51
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.92	0.51
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.46	0.51
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.92	0.51
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.51
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.44	0.51
5:F:483:LEU:H	5:F:483:LEU:HD12	1.75	0.51
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.93	0.50
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.92	0.50
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.93	0.50
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.44	0.50
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.94	0.50
1:A:91:ARG:HD3	1:A:210:THR:O	2.12	0.50
5:F:164:GLY:O	5:F:260:ARG:HB2	2.10	0.50
3:J:73:GLY:O	3:J:76:LYS:NZ	2.34	0.50
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.45	0.50
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.92	0.50
3:D:568:SER:OG	3:D:569:LEU:N	2.44	0.50
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.50
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.76	0.50
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.93	0.50
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.45	0.50
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.93	0.50
2:C:867:GLU:OE1	2:C:943:LYS:NZ	2.42	0.50
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.46	0.50
5:L:316:PHE:HZ	5:L:334:SER:HA	1.76	0.50
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.26	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.10	0.50
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.94	0.50
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.94	0.50
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.27	0.50
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.93	0.50
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.94	0.50
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.93	0.50
5:L:573:LEU:HD23	5:L:573:LEU:H	1.76	0.50
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.94	0.50
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.93	0.50
5:F:461:ASN:O	5:F:465:ARG:HG2	2.11	0.50
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.50
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.94	0.50
2:C:250:THR:HA	2:C:268:ARG:HA	1.93	0.50
2:C:842:ASP:N	2:C:1045:GLY:O	2.45	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:461:ASN:O	5:L:465:ARG:HG2	2.12	0.49
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.93	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.47	0.49
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.94	0.49
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.94	0.49
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.93	0.49
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.93	0.49
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.95	0.49
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.94	0.49
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.95	0.49
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.94	0.49
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.95	0.49
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.94	0.49
2:I:739:ASP:N	2:I:739:ASP:OD1	2.38	0.49
5:F:281:ARG:O	5:F:285:ARG:HG3	2.13	0.49
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.93	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.49
2:I:402:ARG:NH2	2:I:419:ILE:O	2.46	0.49
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.49
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.94	0.49
2:I:842:ASP:N	2:I:1045:GLY:O	2.45	0.49
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.94	0.49
2:I:897:PRO:HG3	3:J:77:ARG:HH22	1.77	0.49
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.94	0.49
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.95	0.49
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.49
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.95	0.49
1:G:231:PHE:HB3	1:H:218:ARG:NH1	2.27	0.49
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.95	0.49
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.95	0.49
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.77	0.49
3:J:122:SER:O	3:J:126:LEU:HG	2.13	0.49
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.95	0.49
2:I:250:THR:HA	2:I:268:ARG:HA	1.94	0.49
1:A:13:LEU:H	1:A:13:LEU:HD23	1.78	0.49
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.95	0.49
3:D:266:ASN:O	3:D:270:ARG:HB2	2.13	0.49
5:F:244:THR:O	5:F:247:GLU:HG2	2.13	0.49
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.93	0.49
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.95	0.49
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.94	0.49
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.61	0.49
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.95	0.48
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.94	0.48
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.78	0.48
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.95	0.48
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.78	0.48
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.46	0.48
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.94	0.48
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.78	0.48
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.94	0.48
3:D:392:THR:HG21	5:F:606:VAL:HA	1.95	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.48
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.94	0.48
2:C:255:ILE:HB	2:C:263:VAL:HB	1.96	0.48
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.95	0.48
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.48	0.48
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.39	0.48
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.96	0.48
5:F:583:THR:HG22	5:F:584:ARG:H	1.79	0.48
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.78	0.48
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.94	0.48
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.94	0.48
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.96	0.48
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.95	0.48
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.33	0.48
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.93	0.48
3:J:266:ASN:O	3:J:270:ARG:HB2	2.13	0.48
3:D:1268:ASN:HD22	3:J:1268:ASN:ND2	2.11	0.48
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.78	0.48
2:C:778:GLU:O	2:C:781:ASP:HB2	2.14	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.46	0.48
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.95	0.48
3:J:341:ASN:HB2	3:J:1352:ILE:HD13	1.95	0.48
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.96	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.95	0.48
1:G:13:LEU:H	1:G:13:LEU:HD23	1.78	0.48
3:D:77:ARG:HG3	3:D:79:LYS:H	1.78	0.48
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.48
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.48	0.48
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.94	0.48
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.95	0.48
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.94	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.35	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.48
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.49	0.48
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.47	0.48
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.53	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.48
3:J:77:ARG:HG3	3:J:79:LYS:H	1.78	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.14	0.48
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.77	0.48
2:I:878:THR:OG1	2:I:879:GLY:N	2.46	0.48
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.95	0.48
5:L:244:THR:O	5:L:247:GLU:HG2	2.13	0.48
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.48	0.48
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.96	0.48
2:I:778:GLU:O	2:I:781:ASP:HB2	2.14	0.48
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.96	0.48
3:J:708:ASN:HB3	3:J:712:GLN:O	2.14	0.48
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.14	0.48
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.95	0.48
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.29	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.47
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.47
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.96	0.47
3:D:115:TRP:O	3:D:119:SER:HB2	2.14	0.47
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.54	0.47
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.96	0.47
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.29	0.47
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.96	0.47
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.95	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.62	0.47
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.95	0.47
2:I:115:LYS:HE3	2:I:116:ASP:H	1.79	0.47
3:J:733:SER:O	3:J:737:ILE:HG12	2.15	0.47
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.97	0.47
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.62	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.95	0.47
5:L:137:TYR:HE1	5:L:351:THR:HB	1.80	0.47
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.70	0.47
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.29	0.47
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.49	0.47
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.96	0.47
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.47
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.95	0.47
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.96	0.47
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.96	0.47
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.96	0.47
5:F:137:TYR:HE1	5:F:351:THR:HB	1.80	0.47
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.49	0.47
3:J:395:LYS:HE2	5:L:536:THR:HG21	1.96	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.97	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.13	0.47
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.97	0.47
2:I:517:GLN:O	2:I:517:GLN:HG2	2.15	0.47
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.74	0.47
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.97	0.47
2:C:115:LYS:HE3	2:C:116:ASP:H	1.78	0.47
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.96	0.47
5:L:127:ILE:O	5:L:130:VAL:HG22	2.14	0.47
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.96	0.47
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.30	0.47
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.47	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.95	0.47
2:I:448:LEU:HB2	2:I:553:THR:HB	1.96	0.47
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.97	0.47
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.97	0.47
3:J:709:ARG:C	3:J:711:GLY:H	2.18	0.47
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.97	0.47
3:D:708:ASN:HB3	3:D:712:GLN:O	2.14	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.97	0.47
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.97	0.47
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.95	0.47
2:C:232:ILE:HG12	2:C:237:LEU:HD13	1.96	0.47
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.97	0.47
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.47	0.47
2:I:170:VAL:HG23	2:I:171:LEU:H	1.80	0.47
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.97	0.47
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.50	0.47
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.96	0.47
5:L:225:ARG:O	5:L:229:VAL:HG13	2.15	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.96	0.47
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.80	0.47
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.47
5:F:225:ARG:O	5:F:229:VAL:HG13	2.15	0.47
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.97	0.47
5:L:583:THR:HG22	5:L:584:ARG:H	1.79	0.47
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.96	0.47
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.46
1:G:228:LEU:HA	1:G:228:LEU:HD13	1.79	0.46
2:I:170:VAL:HG23	2:I:171:LEU:N	2.30	0.46
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.30	0.46
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.97	0.46
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.46
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.97	0.46
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.81	0.46
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.80	0.46
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.97	0.46
3:D:133:ARG:NH2	5:F:93:ARG:O	2.47	0.46
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.96	0.46
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.95	0.46
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.55	0.46
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.50	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.97	0.46
3:J:79:LYS:HB2	5:L:569:THR:N	2.31	0.46
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.98	0.46
3:D:708:ASN:N	3:D:708:ASN:OD1	2.48	0.46
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.95	0.46
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.97	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.96	0.46
2:C:170:VAL:HG23	2:C:171:LEU:N	2.31	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.28	0.46
5:L:380:VAL:HG22	5:L:416:VAL:HG21	1.98	0.46
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.55	0.46
3:J:385:LEU:HD11	3:J:408:VAL:HG12	1.98	0.46
2:I:255:ILE:HB	2:I:263:VAL:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.97	0.46
3:D:709:ARG:C	3:D:711:GLY:H	2.18	0.46
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.31	0.46
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.50	0.46
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.98	0.46
3:D:1170:LYS:C	3:D:1172:LYS:H	2.18	0.46
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.81	0.46
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.97	0.46
2:C:448:LEU:HB2	2:C:553:THR:HB	1.96	0.46
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.96	0.46
2:I:721:GLY:N	2:I:740:GLU:OE1	2.45	0.46
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.97	0.46
2:I:657:THR:HG1	2:I:1187:PHE:HB2	1.80	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.97	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.96	0.46
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.72	0.46
1:G:51:MET:HB3	1:G:51:MET:HE3	1.84	0.46
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.98	0.46
1:G:12:ARG:H	1:G:30:PRO:HD2	1.81	0.46
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.64	0.46
2:I:387:ASN:HA	2:I:391:SER:HB2	1.97	0.46
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.97	0.46
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.98	0.46
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.16	0.46
2:C:517:GLN:HG2	2:C:517:GLN:O	2.15	0.46
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.78	0.46
3:J:963:VAL:HB	3:J:980:THR:HG23	1.98	0.45
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.81	0.45
3:D:385:LEU:HD11	3:D:408:VAL:HG12	1.98	0.45
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.97	0.45
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.32	0.45
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.51	0.45
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.97	0.45
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.97	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.81	0.45
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.97	0.45
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.82	0.45
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.45
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.98	0.45
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.81	0.45
1:B:51:MET:HA	1:B:52:PRO:HD3	1.85	0.45
3:D:1349:GLU:N	3:D:1349:GLU:OE2	2.33	0.45
3:J:264:ASP:OD2	3:J:264:ASP:N	2.50	0.45
2:C:721:GLY:N	2:C:740:GLU:OE1	2.45	0.45
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.16	0.45
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.31	0.45
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.51	0.45
2:I:206:ALA:O	2:I:209:ILE:HG22	2.16	0.45
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.97	0.45
5:F:507:MET:HG2	5:F:520:GLY:HA3	1.98	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.83	0.45
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.48	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.45
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.16	0.45
2:C:820:GLU:N	2:C:1080:ASN:O	2.50	0.45
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.98	0.45
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.81	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.97	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.31	0.45
2:C:113:THR:OG1	2:C:116:ASP:OD2	2.24	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.45
2:I:820:GLU:N	2:I:1080:ASN:O	2.49	0.45
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.99	0.45
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.98	0.45
2:C:680:LEU:O	2:C:684:ASN:HB2	2.17	0.45
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.99	0.45
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.99	0.45
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.99	0.45
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.99	0.45
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.98	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.80	0.45
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.45
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.59	0.45
5:F:44:ILE:HA	5:F:47:MET:HB2	1.98	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.45
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.81	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.31	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.51	0.45
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.82	0.45
2:I:217:THR:HG23	2:I:351:LEU:HD13	1.97	0.45
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.51	0.45
2:C:658:GLN:O	2:C:661:VAL:HG22	2.17	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.99	0.45
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.99	0.45
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.99	0.45
3:J:701:LEU:HD13	3:J:723:TYR:HB2	1.99	0.45
1:G:47:LEU:HD13	1:G:183:ILE:HG12	1.99	0.45
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.99	0.45
3:D:264:ASP:N	3:D:264:ASP:OD2	2.50	0.45
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.45
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.98	0.45
3:J:654:ILE:O	3:J:658:GLU:HB2	2.17	0.45
5:L:249:ILE:O	5:L:252:LEU:HB3	2.16	0.45
3:D:50:LYS:HB3	3:D:71:LEU:HD21	1.98	0.45
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.52	0.45
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.85	0.45
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.99	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.32	0.45
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.19	0.45
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.20	0.45
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.32	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.99	0.45
3:J:901:ARG:HA	3:J:908:ILE:HA	1.99	0.45
3:J:708:ASN:N	3:J:708:ASN:OD1	2.48	0.45
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.99	0.45
2:I:680:LEU:O	2:I:684:ASN:HB2	2.17	0.45
3:J:1061:VAL:HG21	3:J:1101:LEU:HB2	1.99	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
5:L:572:THR:O	5:L:576:VAL:HG23	2.17	0.44
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.99	0.44
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.98	0.44
2:I:113:THR:OG1	2:I:116:ASP:OD2	2.23	0.44
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.99	0.44
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.52	0.44
3:J:62:PHE:O	3:J:101:ARG:HD2	2.17	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.17	0.44
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.98	0.44
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.77	0.44
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.31	0.44
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.99	0.44
1:B:79:LEU:HD23	1:B:79:LEU:H	1.82	0.44
1:H:91:ARG:HG2	1:H:122:GLU:O	2.17	0.44
3:J:800:LEU:O	3:J:803:VAL:HG12	2.17	0.44
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.82	0.44
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.82	0.44
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.76	0.44
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.99	0.44
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.53	0.44
2:I:98:VAL:HG21	2:I:124:MET:HE3	2.00	0.44
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.91	0.44
5:F:346:GLN:O	5:F:350:GLU:HG3	2.17	0.44
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.99	0.44
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.48	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
1:G:197:ASP:OD1	1:G:197:ASP:N	2.51	0.44
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.99	0.44
3:D:800:LEU:O	3:D:803:VAL:HG12	2.17	0.44
3:J:709:ARG:O	3:J:711:GLY:N	2.50	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.99	0.44
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.53	0.44
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.82	0.44
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.99	0.44
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.80	0.44
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.82	0.44
1:A:197:ASP:N	1:A:197:ASP:OD1	2.51	0.44
3:D:661:VAL:HG12	3:D:685:ILE:HD11	2.00	0.44
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.99	0.44
3:D:872:LEU:O	3:D:877:VAL:HG12	2.18	0.44
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.82	0.44
2:I:1247:SER:HB3	3:J:375:GLU:O	2.17	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.17	0.44
2:C:466:VAL:O	2:C:469:VAL:HG22	2.18	0.44
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.00	0.44
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.52	0.44
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.44
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.00	0.44
5:L:314:THR:O	5:L:318:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.99	0.44
5:L:547:VAL:CG1	5:L:598:LEU:HD22	2.47	0.44
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.44
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.44
3:D:62:PHE:O	3:D:101:ARG:HD2	2.18	0.44
5:L:346:GLN:O	5:L:350:GLU:HG3	2.18	0.44
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.44
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.00	0.44
2:C:840:SER:O	2:C:1047:LEU:N	2.51	0.44
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.99	0.44
2:C:976:ARG:NH2	2:C:990:ASP:OD2	2.51	0.44
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.33	0.44
3:D:860:ARG:HB3	3:D:861:ASN:H	1.57	0.44
1:B:91:ARG:HG2	1:B:122:GLU:O	2.18	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.99	0.44
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.83	0.44
5:L:97:PRO:HA	5:L:100:MET:HG3	2.00	0.44
3:D:694:SER:OG	3:D:738:ARG:NE	2.42	0.44
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.82	0.44
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.83	0.44
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.98	0.44
1:G:25:LYS:HG2	1:G:204:GLU:HG3	2.00	0.44
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.50	0.44
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.00	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.44
5:L:44:ILE:HA	5:L:47:MET:HB2	2.00	0.44
5:F:249:ILE:O	5:F:252:LEU:HB3	2.17	0.44
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.99	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.99	0.44
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.18	0.44
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.44
1:A:12:ARG:H	1:A:30:PRO:HD2	1.82	0.44
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.00	0.44
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.98	0.44
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.65	0.43
5:F:572:THR:O	5:F:576:VAL:HG23	2.18	0.43
2:C:453:ILE:HD11	2:C:530:ILE:HD12	2.00	0.43
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.83	0.43
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.99	0.43
2:C:383:SER:O	2:C:387:ASN:HB2	2.18	0.43
2:I:658:GLN:O	2:I:661:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:325:LYS:HD3	5:L:508:GLU:HG2	2.00	0.43
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.00	0.43
5:F:136:GLU:OE1	5:F:364:ARG:NH2	2.51	0.43
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.83	0.43
3:D:527:LEU:HD22	3:D:533:ALA:HA	2.00	0.43
2:C:1151:LEU:HA	2:C:1151:LEU:HD23	1.81	0.43
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.82	0.43
3:D:298:MET:SD	5:F:402:LEU:HB3	2.58	0.43
3:D:470:VAL:HA	3:D:471:PRO:HD3	1.79	0.43
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.00	0.43
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.43
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.52	0.43
1:B:98:VAL:HG22	1:B:99:ILE:H	1.84	0.43
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.53	0.43
2:I:466:VAL:O	2:I:469:VAL:HG22	2.18	0.43
3:D:45:ASN:HB3	3:D:48:THR:O	2.18	0.43
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.18	0.43
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.58	0.43
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.16	0.43
3:J:314:ARG:HG2	3:J:314:ARG:HH11	1.83	0.43
1:H:101:THR:HA	1:H:142:MET:O	2.18	0.43
3:D:654:ILE:O	3:D:658:GLU:HB2	2.17	0.43
5:F:493:LYS:HA	5:F:496:LYS:HE2	2.00	0.43
3:J:557:LYS:HA	3:J:563:LEU:HA	2.00	0.43
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.78	0.43
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.00	0.43
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.99	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.16	0.43
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.85	0.43
1:H:98:VAL:HG22	1:H:99:ILE:H	1.84	0.43
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.83	0.43
5:F:119:ILE:O	5:F:123:ILE:HG13	2.18	0.43
2:C:170:VAL:HG23	2:C:171:LEU:H	1.81	0.43
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.54	0.43
3:D:557:LYS:HA	3:D:563:LEU:HA	2.01	0.43
5:L:354:THR:O	5:L:358:VAL:HG23	2.18	0.43
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.53	0.43
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.43
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.00	0.43
5:F:590:ILE:O	5:F:594:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.83	0.43
1:A:231:PHE:HB3	1:B:218:ARG:HH11	1.82	0.43
2:I:840:SER:O	2:I:1047:LEU:N	2.51	0.43
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.00	0.43
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.52	0.43
3:J:527:LEU:HD22	3:J:533:ALA:HA	2.00	0.43
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.01	0.43
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.34	0.43
2:C:98:VAL:HG21	2:C:124:MET:HE3	2.01	0.43
1:A:224:LEU:HD22	1:B:228:LEU:HD11	2.00	0.43
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.43
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.54	0.43
1:H:20:SER:OG	1:H:21:SER:N	2.51	0.43
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.43
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.59	0.43
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.53	0.43
1:H:79:LEU:HD23	1:H:79:LEU:H	1.83	0.43
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.43
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.34	0.43
2:I:453:ILE:HD11	2:I:530:ILE:HD12	2.01	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.83	0.43
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.52	0.43
3:D:203:GLU:O	3:D:207:GLU:HG2	2.18	0.43
2:C:1247:SER:HB3	3:D:375:GLU:O	2.18	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
3:D:701:LEU:HD13	3:D:723:TYR:HB2	2.00	0.43
5:F:314:THR:O	5:F:318:ALA:HB3	2.19	0.43
3:J:661:VAL:HG12	3:J:685:ILE:HD11	2.00	0.43
1:B:101:THR:HA	1:B:142:MET:O	2.19	0.43
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.85	0.43
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.01	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.43
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.48	0.43
1:A:47:LEU:HD13	1:A:183:ILE:HG12	1.99	0.43
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.01	0.43
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.00	0.43
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.65	0.43
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.19	0.43
3:J:872:LEU:O	3:J:877:VAL:HG12	2.18	0.43
3:D:709:ARG:O	3:D:711:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:348:GLU:HG2	5:L:354:THR:HA	2.01	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.43
3:D:314:ARG:HH11	3:D:314:ARG:HG2	1.84	0.43
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.84	0.43
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.54	0.43
3:D:901:ARG:HA	3:D:908:ILE:HA	1.99	0.43
2:I:383:SER:O	2:I:387:ASN:HB2	2.18	0.43
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.43
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.86	0.43
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.01	0.43
1:B:28:LEU:HG	1:B:31:LEU:HD21	2.01	0.43
3:D:537:TYR:CE1	3:D:544:LEU:HB2	2.54	0.43
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.18	0.42
3:J:317:THR:HB	3:J:324:LEU:HB3	2.00	0.42
3:D:317:THR:HB	3:D:324:LEU:HB3	2.00	0.42
3:J:298:MET:SD	5:L:402:LEU:HB3	2.58	0.42
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.19	0.42
1:B:78:ILE:O	1:B:82:LEU:HG	2.19	0.42
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.01	0.42
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.42
1:H:28:LEU:HG	1:H:31:LEU:HD21	2.01	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.01	0.42
1:B:34:GLY:HA3	2:C:1083:GLU:OE1	2.18	0.42
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.84	0.42
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.42	0.42
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.54	0.42
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.54	0.42
3:J:1237:VAL:HG13	3:J:1253:ILE:HD13	2.00	0.42
2:C:964:LEU:HD22	2:C:1025:PHE:CG	2.54	0.42
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.84	0.42
3:D:347:VAL:HG12	3:D:348:ASP:O	2.19	0.42
1:G:115:ILE:HG22	1:G:116:THR:H	1.84	0.42
1:A:115:ILE:HG22	1:A:116:THR:H	1.84	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
1:G:219:ARG:HE	1:G:219:ARG:HB2	1.56	0.42
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.42
1:G:145:LYS:HB3	1:G:145:LYS:HE3	1.84	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.20	0.42
2:C:692:THR:OG1	2:C:827:ARG:O	2.32	0.42
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:537:TYR:CE1	3:J:544:LEU:HB2	2.54	0.42
5:L:580:PHE:C	5:L:582:VAL:H	2.22	0.42
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.59	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.86	0.42
1:A:51:MET:HE3	1:A:51:MET:HB3	1.88	0.42
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.51	0.42
1:B:86:LYS:HD3	1:B:174:ASP:HB2	2.02	0.42
3:J:1162:ILE:HA	3:J:1203:ARG:HA	2.01	0.42
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.54	0.42
5:F:130:VAL:HB	5:F:365:MET:HG3	2.00	0.42
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.01	0.42
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.49	0.42
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.42
1:H:101:THR:H	1:H:116:THR:HG22	1.84	0.42
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.54	0.42
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.02	0.42
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.99	0.42
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.19	0.42
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.02	0.42
5:F:97:PRO:HA	5:F:100:MET:HG3	2.01	0.42
1:A:25:LYS:HG2	1:A:204:GLU:HG3	2.01	0.42
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.01	0.42
3:J:1090:ILE:HG13	3:J:1097:ALA:HB2	2.01	0.42
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.01	0.42
1:H:91:ARG:HG2	1:H:91:ARG:H	1.76	0.42
2:C:758:ARG:HD3	2:C:835:GLU:HB2	2.01	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.01	0.42
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.01	0.42
1:G:10:LYS:HE2	1:H:229:GLU:HB3	2.00	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.01	0.42
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.00	0.42
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.00	0.42
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.53	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.42
2:C:69:GLN:HB3	2:C:69:GLN:HE21	1.67	0.42
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.02	0.42
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.69	0.42
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.83	0.42
1:B:90:VAL:HG11	1:B:146:VAL:HG11	2.01	0.42
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.54	0.42
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	2.01	0.42
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.55	0.42
1:A:54:CYS:HA	1:A:148:ARG:HG3	2.02	0.42
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.35	0.42
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.34	0.42
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.66	0.42
3:J:694:SER:OG	3:J:738:ARG:NE	2.42	0.42
2:I:710:VAL:HA	2:I:715:THR:HG21	2.01	0.42
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.34	0.42
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.89	0.42
3:J:334:LYS:HA	3:J:334:LYS:HD2	1.50	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.35	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.50	0.42
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.96	0.42
1:G:61:ILE:HG23	1:G:142:MET:HB3	2.01	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.87	0.42
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.91	0.42
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.84	0.42
5:F:454:VAL:HA	5:F:457:ILE:HD12	2.02	0.42
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.52	0.42
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.49	0.42
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.53	0.42
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.02	0.42
3:D:668:PHE:HB2	3:D:678:ARG:HG3	2.02	0.42
3:D:1293:GLU:HA	3:J:1226:VAL:H	1.85	0.42
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.42
1:A:61:ILE:HG23	1:A:142:MET:HB3	2.01	0.42
5:L:119:ILE:O	5:L:123:ILE:HG13	2.19	0.42
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.48	0.42
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.84	0.42
2:C:56:VAL:HG11	2:C:468:LEU:HB3	2.01	0.42
2:I:980:VAL:HG13	2:I:984:VAL:HB	2.02	0.42
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.55	0.42
1:G:86:LYS:HE3	1:G:86:LYS:HB2	1.86	0.42
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.02	0.41
5:L:569:THR:OG1	5:L:570:ASP:N	2.53	0.41
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.02	0.41
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.41
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.55	0.41
2:C:153:PRO:O	2:C:401:GLY:HA2	2.20	0.41
1:H:178:SER:HA	1:H:179:PRO:HD3	1.94	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.91	0.41
3:J:347:VAL:HG12	3:J:348:ASP:O	2.20	0.41
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.77	0.41
2:I:518:ASN:O	2:I:691:PRO:HD3	2.20	0.41
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.49	0.41
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.20	0.41
3:D:355:ILE:HD13	3:D:466:MET:HG3	2.02	0.41
1:G:54:CYS:HA	1:G:148:ARG:HG3	2.01	0.41
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.41
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.53	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.88	0.41
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.85	0.41
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.88	0.41
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.50	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.20	0.41
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.69	0.41
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.86	0.41
1:H:86:LYS:HD3	1:H:174:ASP:HB2	2.02	0.41
3:J:124:ILE:HG13	3:J:124:ILE:H	1.63	0.41
5:L:362:ASN:HB2	5:L:365:MET:HE2	2.02	0.41
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.86	0.41
3:J:1156:LEU:HD23	3:J:1219:ASP:HB3	2.02	0.41
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.60	0.41
1:H:151:GLY:O	1:H:177:TYR:HD2	2.04	0.41
2:I:360:LEU:HB2	2:I:378:ARG:HH21	1.84	0.41
5:L:357:GLN:H	5:L:357:GLN:HG3	1.62	0.41
1:H:158:ARG:HD2	1:H:158:ARG:HA	1.91	0.41
1:B:101:THR:H	1:B:116:THR:HG22	1.85	0.41
2:I:550:VAL:HG11	3:J:776:THR:HG22	2.02	0.41
1:B:91:ARG:H	1:B:91:ARG:HG2	1.76	0.41
3:D:190:LYS:HE2	3:D:190:LYS:HB2	1.87	0.41
1:A:54:CYS:O	1:A:146:VAL:HG13	2.20	0.41
3:D:1285:VAL:O	3:D:1289:ASN:HB3	2.20	0.41
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.35	0.41
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.49	0.41
3:D:810:THR:HG23	3:D:811:GLU:H	1.85	0.41
1:B:182:ARG:NH1	3:D:581:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HA	1:B:158:ARG:HD2	1.90	0.41
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.70	0.41
3:D:361:LEU:HD22	3:D:365:GLN:HG3	2.01	0.41
3:D:806:ASP:OD2	3:D:1347:LEU:N	2.48	0.41
5:L:561:MET:HG3	5:L:571:TYR:HD2	1.84	0.41
3:J:79:LYS:HG3	3:J:80:HIS:N	2.35	0.41
1:B:68:TYR:O	1:B:69:SER:OG	2.34	0.41
3:J:1236:GLU:O	3:J:1240:VAL:HG23	2.20	0.41
3:D:27:PRO:O	3:D:31:ARG:HG3	2.21	0.41
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.55	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.21	0.41
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	2.02	0.41
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.02	0.41
5:L:580:PHE:HA	5:L:580:PHE:HD1	1.70	0.41
5:L:582:VAL:HG22	5:L:586:ARG:HG2	2.02	0.41
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.01	0.41
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.41
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.54	0.41
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.55	0.41
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.45	0.41
2:I:499:SER:O	2:I:503:LYS:HB2	2.20	0.41
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.80	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.02	0.41
2:I:699:LEU:HA	2:I:699:LEU:HD22	1.95	0.41
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.90	0.41
3:J:668:PHE:HB2	3:J:678:ARG:HG3	2.02	0.41
3:D:793:SER:O	3:D:797:THR:HG23	2.20	0.41
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.02	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.92	0.41
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.56	0.41
3:J:556:GLU:O	3:J:564:VAL:N	2.33	0.41
2:I:122:VAL:HG21	2:I:493:ILE:HG23	2.03	0.41
1:G:177:TYR:O	1:G:178:SER:HB2	2.20	0.41
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.88	0.41
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.76	0.41
2:C:550:VAL:HG11	3:D:776:THR:HG22	2.03	0.41
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.21	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.91	0.41
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.02	0.41
1:B:34:GLY:N	1:B:199:ASP:OD2	2.53	0.41
1:G:10:LYS:HE3	1:H:226:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:GLN:O	2:C:87:ILE:HG13	2.21	0.41
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.46	0.41
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.01	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.91	0.41
5:F:490:PRO:HG2	5:F:493:LYS:HE3	2.03	0.41
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.03	0.41
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.56	0.41
3:D:461:PHE:HA	3:D:461:PHE:HD2	1.77	0.41
1:B:51:MET:HB3	1:B:178:SER:HA	2.01	0.41
3:D:746:LEU:HD22	3:D:754:ILE:HD11	2.02	0.41
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.02	0.41
1:G:92:VAL:HA	1:G:120:ASP:O	2.21	0.41
4:E:44:ASP:HB3	4:E:48:VAL:HB	2.02	0.41
5:F:96:ASP:OD2	5:F:99:ARG:HB2	2.20	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
2:C:987:GLU:O	2:C:991:LYS:HG3	2.21	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.86	0.41
1:H:34:GLY:N	1:H:199:ASP:OD2	2.53	0.41
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.53	0.41
5:F:299:LYS:O	5:F:303:ILE:HG12	2.20	0.41
3:J:77:ARG:HG3	3:J:79:LYS:HB3	2.03	0.41
3:J:79:LYS:HB2	5:L:569:THR:H	1.84	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.21	0.41
1:H:61:ILE:HB	1:H:64:VAL:O	2.21	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.86	0.41
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.93	0.41
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.92	0.41
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.87	0.41
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.51	0.41
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.41
5:L:96:ASP:OD2	5:L:99:ARG:HB2	2.20	0.41
1:B:112:ALA:HB2	1:B:128:HIS:HB3	2.01	0.41
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.60	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.74	0.41
3:D:290:ILE:HD12	3:D:290:ILE:H	1.86	0.41
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.03	0.41
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.36	0.41
4:E:49:ILE:HA	4:E:52:ARG:HD3	2.02	0.41
5:F:22:LEU:H	5:F:54:GLN:CB	2.34	0.41
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.21	0.41
2:I:498:ILE:H	2:I:498:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.21	0.41
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.41
2:C:468:LEU:HA	2:C:471:VAL:HG12	2.03	0.41
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.01	0.41
5:L:250:LEU:O	5:L:254:GLU:HG2	2.21	0.41
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.53	0.41
2:I:557:ARG:HH21	2:I:607:SER:C	2.24	0.41
2:I:867:GLU:HG3	2:I:867:GLU:H	1.61	0.41
3:D:77:ARG:HG3	3:D:79:LYS:HB3	2.03	0.40
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.54	0.40
3:J:490:ILE:HD11	3:J:609:TYR:CD2	2.56	0.40
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.90	0.40
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.21	0.40
2:I:32:LEU:HA	2:I:32:LEU:HD23	1.94	0.40
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.78	0.40
2:C:60:GLN:HB3	2:C:67:GLU:HG3	2.02	0.40
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	2.03	0.40
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.02	0.40
3:J:683:ILE:HD11	3:J:754:ILE:HG12	2.02	0.40
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.03	0.40
3:J:399:LYS:HG2	3:J:403:ARG:NH2	2.36	0.40
1:H:90:VAL:HG11	1:H:146:VAL:HG11	2.02	0.40
2:I:232:ILE:HG12	2:I:237:LEU:HD13	2.03	0.40
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.56	0.40
2:I:153:PRO:O	2:I:401:GLY:HA2	2.21	0.40
2:C:516:ASP:H	2:C:526:HIS:HD1	1.69	0.40
3:J:600:ALA:O	3:J:603:LYS:HG2	2.21	0.40
3:J:290:ILE:HD12	3:J:290:ILE:H	1.86	0.40
3:D:572:THR:OG1	3:D:573:THR:N	2.54	0.40
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.85	0.40
3:D:79:LYS:HG3	3:D:80:HIS:N	2.36	0.40
5:F:569:THR:OG1	5:F:570:ASP:N	2.53	0.40
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.86	0.40
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.86	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.52	0.40
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.57	0.40
2:I:1161:LEU:HA	2:I:1161:LEU:HD12	1.81	0.40
3:J:660:GLU:O	3:J:664:ILE:HG12	2.21	0.40
3:J:697:MET:HE1	3:J:737:ILE:HG22	2.03	0.40
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.51	0.40
1:G:54:CYS:O	1:G:146:VAL:HG13	2.20	0.40
1:H:213:PRO:O	1:H:217:ILE:HG13	2.22	0.40
3:D:197:GLU:O	3:D:201:LEU:HG	2.21	0.40
5:F:250:LEU:O	5:F:254:GLU:HG2	2.21	0.40
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.40
2:C:213:LEU:HD13	2:C:422:LYS:HG2	2.03	0.40
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.77	0.40
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.88	0.40
2:C:657:THR:HG1	2:C:1187:PHE:HB2	1.84	0.40
1:B:61:ILE:HB	1:B:64:VAL:O	2.22	0.40
2:C:196:VAL:HG12	2:C:206:ALA:HA	2.04	0.40
3:D:579:LEU:HD12	3:D:582:ILE:HD12	2.03	0.40
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.62	0.40
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.85	0.40
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.81	0.40
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.52	0.40
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.20	0.40
2:I:930:ASP:HB3	2:I:1053:TYR:HB2	2.02	0.40
2:I:101:ARG:HH21	2:I:118:LYS:HE3	1.86	0.40
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	2.04	0.40
3:J:197:GLU:O	3:J:201:LEU:HG	2.21	0.40
2:I:83:GLN:O	2:I:87:ILE:HG13	2.21	0.40
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.04	0.40
3:D:600:ALA:O	3:D:603:LYS:HG2	2.21	0.40
2:C:356:THR:HG21	2:C:362:ALA:HA	2.03	0.40
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.22	0.40
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.57	0.40
2:I:69:GLN:HB3	2:I:69:GLN:HE21	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	193 (87%)	27 (12%)	2 (1%)	21	68
1	B	216/239 (90%)	190 (88%)	26 (12%)	0	100	100
1	G	226/239 (95%)	196 (87%)	27 (12%)	3 (1%)	15	61
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100	100
2	C	1338/1342 (100%)	1233 (92%)	101 (8%)	4 (0%)	46	83
2	I	1338/1342 (100%)	1234 (92%)	99 (7%)	5 (0%)	39	80
3	D	1162/1407 (83%)	1061 (91%)	97 (8%)	4 (0%)	46	83
3	J	1328/1407 (94%)	1213 (91%)	111 (8%)	4 (0%)	46	83
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	480 (90%)	52 (10%)	0	100	100
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7268/7862 (92%)	6624 (91%)	622 (9%)	22 (0%)	46	83

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	120	LEU
3	J	120	LEU
2	C	170	VAL
2	I	170	VAL
2	I	237	LEU
3	J	340	GLN
2	C	697	LYS
2	C	1136	GLN
3	D	10	ALA
3	D	710	ASP
1	G	14	VAL
2	I	697	LYS
2	I	1136	GLN
3	J	710	ASP
1	A	14	VAL
2	C	1186	VAL
1	A	167	PRO
3	D	831	VAL
1	G	167	PRO
2	I	1186	VAL
3	J	831	VAL
1	G	178	SER

5.3.2 Protein sidechains (i)

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%)	180 (94%)	11 (6%)	25	66
1	B	184/206 (89%)	168 (91%)	16 (9%)	13	50
1	G	191/206 (93%)	180 (94%)	11 (6%)	25	66
1	H	183/206 (89%)	168 (92%)	15 (8%)	14	52
2	C	1155/1157 (100%)	1063 (92%)	92 (8%)	15	54
2	I	1154/1157 (100%)	1063 (92%)	91 (8%)	15	54
3	D	975/1168 (84%)	883 (91%)	92 (9%)	11	47
3	J	1117/1168 (96%)	1015 (91%)	102 (9%)	12	48
4	E	72/75 (96%)	66 (92%)	6 (8%)	14	52
4	K	67/75 (89%)	61 (91%)	6 (9%)	12	49
5	F	426/540 (79%)	387 (91%)	39 (9%)	11	48
5	L	428/540 (79%)	391 (91%)	37 (9%)	13	51
All	All	6143/6704 (92%)	5625 (92%)	518 (8%)	14	52

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	15	ASP
1	A	35	PHE
1	A	54	CYS
1	A	61	ILE
1	A	133	LEU
1	A	145	LYS
1	A	172	LEU
1	A	186	ASN
1	A	207	THR
1	A	215	GLU
1	B	8	PHE
1	B	13	LEU
1	B	27	THR

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Mol	Chain	Res	Type
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	79	LEU
1	B	80	GLU
1	B	101	THR
1	B	105	SER
1	B	107	ILE
1	B	116	THR
1	B	124	VAL
1	B	133	LEU
1	B	160	HIS
1	B	183	ILE
2	C	11	ILE
2	C	29	SER
2	C	39	ILE
2	C	70	TYR
2	C	81	ASP
2	C	85	CYS
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	119	GLU
2	C	131	THR
2	C	179	TYR
2	C	182	SER
2	C	185	ASP
2	C	202	ARG
2	C	285	ILE
2	C	320	ASP
2	C	321	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	487	LEU
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN

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Mol	Chain	Res	Type
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	554	HIS
2	C	604	HIS
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	657	THR
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	706	ARG
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	974	ARG
2	C	990	ASP
2	C	992	LEU
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1082	ILE

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Mol	Chain	Res	Type
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1155	VAL
2	C	1156	ARG
2	C	1158	LYS
2	C	1161	LEU
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1240	ASP
2	C	1248	THR
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1313	HIS
2	C	1326	LEU
2	C	1327	LEU
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	79	LYS
3	D	92	VAL
3	D	95	THR
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	264	ASP

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Mol	Chain	Res	Type
3	D	311	ARG
3	D	324	LEU
3	D	339	ARG
3	D	356	THR
3	D	364	HIS
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	430	HIS
3	D	474	LEU
3	D	506	VAL
3	D	513	MET
3	D	545	HIS
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	641	ILE
3	D	660	GLU
3	D	678	ARG
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	740	LEU
3	D	754	ILE
3	D	757	THR
3	D	764	ARG
3	D	767	LEU
3	D	770	LEU
3	D	772	TYR
3	D	805	GLN
3	D	810	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU

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Mol	Chain	Res	Type
3	D	860	ARG
3	D	867	GLN
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	928	THR
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1173	ARG
3	D	1177	ILE
3	D	1186	TYR
3	D	1199	PHE
3	D	1202	GLU
3	D	1208	ASP
3	D	1209	VAL
3	D	1215	GLU
3	D	1244	GLN
3	D	1255	VAL
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1327	GLU
3	D	1333	THR
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP
5	F	94	THR
5	F	98	VAL
5	F	100	MET

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Mol	Chain	Res	Type
5	F	118	ASP
5	F	127	ILE
5	F	154	GLU
5	F	244	THR
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	421	TYR
5	F	429	THR
5	F	445	ASP
5	F	449	THR
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	496	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	583	THR
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
1	G	9	LEU
1	G	15	ASP
1	G	35	PHE
1	G	54	CYS
1	G	61	ILE
1	G	133	LEU
1	G	145	LYS
1	G	172	LEU
1	G	186	ASN
1	G	207	THR

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Mol	Chain	Res	Type
1	G	215	GLU
1	H	13	LEU
1	H	27	THR
1	H	54	CYS
1	H	60	GLU
1	H	65	LEU
1	H	75	GLN
1	H	79	LEU
1	H	80	GLU
1	H	101	THR
1	H	105	SER
1	H	107	ILE
1	H	116	THR
1	H	124	VAL
1	H	133	LEU
1	H	183	ILE
2	I	11	ILE
2	I	29	SER
2	I	39	ILE
2	I	70	TYR
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	119	GLU
2	I	131	THR
2	I	179	TYR
2	I	182	SER
2	I	185	ASP
2	I	202	ARG
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	493	ILE

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Mol	Chain	Res	Type
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	554	HIS
2	I	604	HIS
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	657	THR
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	706	ARG
2	I	714	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	974	ARG
2	I	990	ASP
2	I	992	LEU
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU

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Mol	Chain	Res	Type
2	I	1040	ASP
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1155	VAL
2	I	1156	ARG
2	I	1158	LYS
2	I	1161	LEU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1240	ASP
2	I	1248	THR
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1313	HIS
2	I	1326	LEU
2	I	1327	LEU
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	264	ASP

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Mol	Chain	Res	Type
3	J	311	ARG
3	J	324	LEU
3	J	339	ARG
3	J	356	THR
3	J	364	HIS
3	J	374	LEU
3	J	394	ILE
3	J	407	VAL
3	J	430	HIS
3	J	474	LEU
3	J	506	VAL
3	J	513	MET
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	641	ILE
3	J	660	GLU
3	J	678	ARG
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	740	LEU
3	J	754	ILE
3	J	757	THR
3	J	764	ARG
3	J	767	LEU
3	J	770	LEU
3	J	772	TYR
3	J	805	GLN
3	J	810	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR

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Mol	Chain	Res	Type
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP
3	J	1064	SER
3	J	1073	ASP
3	J	1115	ILE
3	J	1121	LEU
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1173	ARG
3	J	1177	ILE
3	J	1186	TYR
3	J	1199	PHE
3	J	1202	GLU
3	J	1208	ASP
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1255	VAL
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1327	GLU
3	J	1333	THR
4	K	28	ARG

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Mol	Chain	Res	Type
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET
5	L	118	ASP
5	L	154	GLU
5	L	244	THR
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	421	TYR
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	496	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	583	THR
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	343	HIS
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1257	GLN
2	C	1288	GLN
2	C	1312	ASN
3	D	340	GLN
3	D	364	HIS
3	D	419	HIS
3	D	477	GLN
3	D	560	ASN
3	D	1367	GLN
5	F	406	GLN
5	F	472	GLN
2	I	343	HIS
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1257	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	340	GLN
3	J	364	HIS
3	J	419	HIS
3	J	1268	ASN
3	J	1367	GLN
5	L	406	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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%)	-0.02	1 (0%) 93 88	57, 89, 134, 170	0
1	B	220/239 (92%)	0.21	15 (6%) 20 12	57, 121, 154, 165	0
1	G	228/239 (95%)	0.17	8 (3%) 48 32	84, 122, 155, 170	0
1	H	217/239 (90%)	0.37	21 (9%) 10 6	90, 134, 157, 166	0
2	C	1340/1342 (99%)	-0.04	25 (1%) 70 55	31, 86, 140, 175	0
2	I	1340/1342 (99%)	0.04	50 (3%) 45 30	41, 105, 151, 183	0
3	D	1166/1407 (82%)	-0.01	28 (2%) 62 46	28, 78, 140, 170	0
3	J	1334/1407 (94%)	0.28	105 (7%) 15 9	33, 99, 159, 185	0
4	E	89/91 (97%)	-0.21	0 100 100	38, 82, 122, 129	0
4	K	79/91 (86%)	-0.22	1 (1%) 79 65	60, 96, 144, 154	0
5	F	542/613 (88%)	0.18	38 (7%) 19 11	49, 127, 166, 196	0
5	L	539/613 (87%)	0.09	31 (5%) 26 16	62, 125, 165, 179	0
All	All	7318/7862 (93%)	0.09	323 (4%) 38 25	28, 102, 155, 196	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	10.1
5	F	89	SER	8.4
5	L	7	SER	8.3
5	F	167	ASP	8.2
2	C	265	LYS	7.3
2	C	251	ALA	7.3
5	L	167	ASP	6.9
3	J	1053	LEU	6.9
5	F	76	ALA	6.3
3	J	1007	ASP	6.2
5	F	88	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
2	C	252	SER	5.9
5	L	480	PRO	5.8
3	J	1088	VAL	5.7
3	J	1294	ALA	5.7
3	J	1056	LEU	5.6
2	I	998	LEU	5.5
2	I	999	GLU	5.3
2	C	266	GLY	5.2
3	J	1089	LEU	5.2
2	I	987	GLU	5.1
3	J	1295	ASN	5.1
3	J	1068	THR	5.1
1	B	146	VAL	5.0
5	L	305	LEU	4.9
3	J	1069	ALA	4.9
3	J	1055	GLY	4.7
2	I	978	VAL	4.7
3	J	991	THR	4.7
1	H	172	LEU	4.7
5	F	75	ASP	4.7
2	I	979	LEU	4.6
2	I	165	HIS	4.6
3	J	998	PRO	4.6
5	F	579	GLN	4.5
5	L	290	LEU	4.5
5	F	86	SER	4.3
3	J	340	GLN	4.2
5	F	259	PHE	4.2
1	B	66	HIS	4.2
3	J	1070	GLY	4.2
5	L	294	GLN	4.2
3	J	1103	GLY	4.2
2	I	990	ASP	4.1
3	J	1080	ILE	4.1
3	J	341	ASN	4.1
5	F	162	ILE	4.1
2	I	989	LEU	4.1
3	J	1097	ALA	4.1
3	J	1058	SER	4.0
3	J	1095	MET	4.0
3	J	1198	VAL	4.0
3	J	1093	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	147	GLN	3.9
3	J	1215	GLU	3.9
3	J	974	VAL	3.9
3	J	984	LEU	3.9
5	F	283	GLN	3.9
1	G	193	GLU	3.9
3	J	956	GLY	3.9
3	J	743	MET	3.8
3	J	1059	LEU	3.8
5	F	161	LEU	3.8
5	F	34	ASP	3.8
5	F	16	GLY	3.8
2	C	241	LEU	3.7
1	B	67	GLU	3.7
5	F	35	ILE	3.7
3	J	1030	GLU	3.7
2	I	696	ASP	3.7
3	J	1001	ALA	3.7
5	F	578	LYS	3.6
3	J	1051	ASP	3.6
5	L	610	PHE	3.6
5	F	87	VAL	3.6
3	D	756	GLU	3.5
5	L	315	TRP	3.5
5	F	85	SER	3.5
1	G	90	VAL	3.5
3	J	975	ILE	3.5
3	J	958	ILE	3.4
3	J	1044	GLN	3.4
5	L	490	PRO	3.4
3	J	1166	GLY	3.4
3	J	1006	GLY	3.3
2	C	292	ILE	3.3
2	I	976	ARG	3.3
3	J	1168	GLU	3.3
5	F	315	TRP	3.3
5	L	8	GLN	3.3
5	F	165	PHE	3.3
2	I	164	THR	3.2
1	B	59	VAL	3.2
3	J	1085	GLY	3.2
2	C	230	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
3	J	1180	VAL	3.2
1	H	146	VAL	3.2
2	I	980	VAL	3.2
3	D	743	MET	3.2
5	L	88	GLU	3.2
5	F	319	ALA	3.2
2	I	230	PHE	3.1
3	J	1161	GLY	3.1
2	I	264	GLU	3.1
2	I	169	LYS	3.1
2	I	981	ALA	3.1
1	H	97	GLU	3.1
1	H	96	ASP	3.1
3	J	957	SER	3.1
3	J	960	LEU	3.1
3	J	1090	ILE	3.1
5	F	92	GLY	3.1
5	L	165	PHE	3.0
5	F	158	LEU	3.0
3	D	1198	VAL	3.0
2	I	124	MET	3.0
2	I	1021	LEU	3.0
3	J	1181	ASP	3.0
5	F	73	ASP	3.0
5	F	575	GLU	3.0
3	J	1073	ASP	3.0
1	H	123	ILE	3.0
1	B	173	VAL	3.0
3	J	1029	THR	3.0
3	J	997	VAL	3.0
3	J	1187	GLU	3.0
3	J	955	LYS	3.0
3	D	1175	LEU	3.0
3	D	341	ASN	3.0
1	H	92	VAL	2.9
3	D	682	VAL	2.9
5	F	77	ALA	2.9
5	L	427	PHE	2.9
1	H	205	MET	2.9
5	L	286	LEU	2.9
1	H	12	ARG	2.9
5	L	289	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	2.9
3	J	987	GLU	2.9
3	J	1052	GLU	2.9
1	H	14	VAL	2.9
5	F	321	ALA	2.9
2	C	997	TRP	2.9
2	I	1010	GLN	2.9
3	J	69	GLU	2.9
2	C	282	VAL	2.8
3	J	1057	SER	2.8
3	J	1188	GLU	2.8
2	I	997	TRP	2.8
3	D	1180	VAL	2.8
1	G	54	CYS	2.8
3	D	1190	ILE	2.8
3	J	986	ASP	2.8
3	J	992	LYS	2.8
3	J	1190	ILE	2.8
3	J	1084	GLN	2.8
3	J	1082	ASP	2.8
2	I	1050	VAL	2.8
5	L	29	ASP	2.8
3	J	1091	PRO	2.8
5	F	514	ASP	2.8
1	G	88	LEU	2.7
1	H	13	LEU	2.7
1	G	209	GLY	2.7
5	L	20	GLY	2.7
1	H	133	LEU	2.7
3	J	973	LEU	2.7
1	B	158	ARG	2.7
3	D	754	ILE	2.7
5	F	74	GLU	2.7
3	D	1169	THR	2.7
1	H	144	ILE	2.7
3	J	756	GLU	2.7
2	I	988	LYS	2.7
2	C	258	ASN	2.7
2	I	246	LEU	2.7
3	J	988	PHE	2.6
2	C	206	ALA	2.6
2	I	167	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	878	ASP	2.6
1	B	144	ILE	2.6
3	J	1035	VAL	2.6
3	J	1185	PRO	2.6
5	F	78	GLU	2.6
1	G	95	LYS	2.6
3	J	1083	ALA	2.6
3	J	1062	LEU	2.6
1	A	9	LEU	2.6
2	I	745	GLU	2.6
2	I	190	PRO	2.6
3	J	218	THR	2.6
5	L	283	GLN	2.6
3	D	753	SER	2.6
2	C	257	ALA	2.5
3	J	1175	LEU	2.5
5	L	19	GLN	2.5
2	I	333	ILE	2.5
3	J	648	GLU	2.5
3	D	1200	GLU	2.5
3	J	682	VAL	2.5
2	C	319	LEU	2.5
3	J	961	SER	2.5
3	D	1376	GLY	2.5
1	H	147	GLN	2.5
3	D	1204	VAL	2.5
3	J	1114	GLN	2.5
2	I	973	SER	2.5
5	L	89	SER	2.5
5	L	569	THR	2.5
3	J	977	SER	2.5
5	L	428	SER	2.5
1	H	24	ALA	2.4
2	I	168	GLY	2.4
3	D	340	GLN	2.4
3	D	826	ILE	2.4
3	D	683	ILE	2.4
3	J	966	VAL	2.4
3	J	686	TRP	2.4
2	I	986	ALA	2.4
5	F	301	ASN	2.4
5	L	18	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	906	PHE	2.4
2	C	317	LEU	2.3
2	C	923	GLY	2.3
2	I	855	PRO	2.3
2	C	255	ILE	2.3
2	I	991	LYS	2.3
2	C	254	ASP	2.3
5	F	137	TYR	2.3
2	C	1000	LEU	2.3
3	J	670	SER	2.3
3	J	993	GLU	2.3
5	F	318	ALA	2.3
3	J	645	VAL	2.3
2	I	995	ASP	2.3
2	I	1011	LEU	2.3
3	D	1214	PRO	2.3
3	J	1079	LYS	2.3
1	B	90	VAL	2.3
5	F	15	ARG	2.3
5	L	602	SER	2.3
2	C	922	ASN	2.3
3	J	746	LEU	2.3
3	D	879	ALA	2.3
5	F	340	ALA	2.3
1	B	69	SER	2.3
3	D	674	THR	2.3
3	J	1165	PHE	2.3
3	J	683	ILE	2.3
5	F	280	VAL	2.3
1	H	90	VAL	2.2
2	I	494	ASN	2.2
3	J	664	ILE	2.2
3	D	1172	LYS	2.2
3	D	77	ARG	2.2
1	B	55	ALA	2.2
3	J	1094	ASP	2.2
3	J	1162	ILE	2.2
3	J	89	GLY	2.2
2	C	239	MET	2.2
1	H	107	ILE	2.2
2	I	725	GLN	2.2
5	F	32	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	28	LEU	2.2
1	H	67	GLU	2.2
2	I	996	ARG	2.2
5	L	287	ILE	2.2
2	I	882	ILE	2.2
2	I	1002	LEU	2.2
3	J	1047	THR	2.2
3	J	1071	GLY	2.2
1	H	106	GLY	2.2
2	I	232	ILE	2.2
3	J	1109	LEU	2.2
5	L	598	LEU	2.2
2	C	264	GLU	2.2
1	B	107	ILE	2.2
2	C	184	LEU	2.2
3	J	1106	ILE	2.2
2	C	253	PHE	2.2
3	J	1122	ALA	2.2
3	D	1171	GLY	2.1
5	L	512	GLY	2.1
2	I	265	LYS	2.1
5	L	140	ALA	2.1
2	I	100	LEU	2.1
3	J	1078	LEU	2.1
3	J	76	LYS	2.1
5	F	256	PHE	2.1
1	H	158	ARG	2.1
3	D	849	LEU	2.1
3	J	1086	ASN	2.1
3	J	857	LEU	2.1
3	J	989	GLY	2.1
1	H	132	HIS	2.1
3	J	1184	ASP	2.1
2	I	867	GLU	2.1
2	I	972	PHE	2.1
1	H	18	GLN	2.1
3	D	1203	ARG	2.1
3	D	679	TYR	2.1
2	C	183	TRP	2.1
3	D	1165	PHE	2.1
1	G	98	VAL	2.1
2	I	277	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	323	ASN	2.1
1	B	98	VAL	2.1
3	J	1031	VAL	2.1
5	L	87	VAL	2.1
5	L	337	VAL	2.1
5	L	293	GLU	2.1
3	J	712	GLN	2.1
2	I	166	SER	2.0
3	J	1043	GLY	2.0
3	J	849	LEU	2.0
2	I	420	LEU	2.0
3	J	1013	GLY	2.0
3	J	1104	LYS	2.0
4	K	58	LEU	2.0
2	I	720	ARG	2.0
1	B	97	GLU	2.0
2	I	975	ILE	2.0
2	C	164	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	D	1503	1/1	0.91	0.40	1.54	138,138,138,138	0
7	ZN	D	1502	1/1	0.97	0.12	-1.13	103,103,103,103	0
7	ZN	J	1502	1/1	0.94	0.13	-1.29	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	J	1503	1/1	0.99	0.18	-2.00	37,37,37,37	0
6	MG	D	1501	1/1	0.84	0.52	-	72,72,72,72	0
6	MG	J	1501	1/1	0.86	0.64	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.