Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 03:53 pm GMT

PDB ID	:	4AYB
Title	:	RNAP at 3.2Ang
Authors	:	Wojtas, M.N.; Mogni, M.; Millet, O.; Bell, S.D.; Abrescia, N.G.A.
Deposited on	:	2012-06-19
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

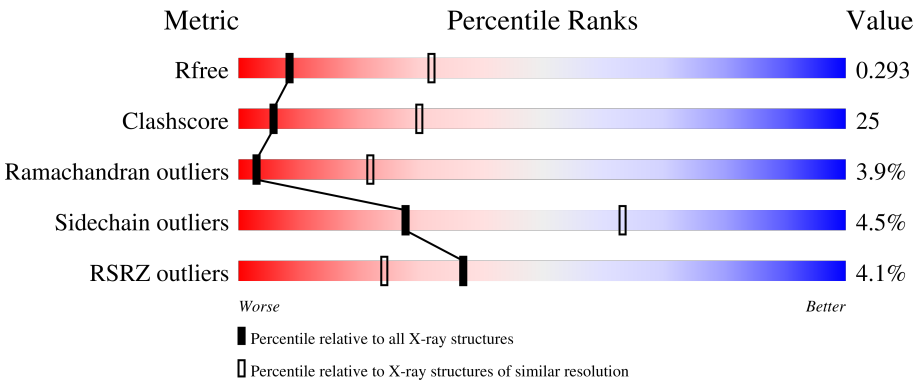
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	880	2%, 55%, 39%, 5% ••
2	B	1131	2%, 59%, 34%, • •
3	C	395	6%, 47%, 42%, 6% • 5%
4	D	265	3%, 70%, 28%, ••
5	E	180	17%, 54%, 39%, •• 5%

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Mol	Chain	Length	Quality of chain
6	F	113	21% 40% 42% 11% 7%
7	G	132	3% 36% 43% 6% 14%
8	H	84	% 57% 31% 10%
9	K	95	% 63% 22% 12%
10	L	92	72% 27%
11	N	66	50% 41% 8%
12	P	48	4% 42% 42% 8% 8%
13	Q	104	8% 17% 25% 5% 52%

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
16	SF4	D	1264	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 54890 atoms, of which 27769 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	872	13986	4424	7029	1225	1282	26	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	1103	17664	5548	8908	1552	1627	29	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	376	5974	1840	3068	493	564	9	0	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	262	4215	1339	2128	337	398	13	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	171	2772	874	1413	229	251	5	0	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	105	1666	519	839	134	171	3	0	0	0

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
7	G	113	1816	572	915	152	173	4	0	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
8	H	76	1284	405	660	111	108	0	0	0

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
9	K	84	1390	431	717	123	118	1	0	0	0

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
10	L	91	1449	454	742	114	137	2	0	0	0

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
11	N	65	1058	332	537	94	88	7	0	0	0

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
12	P	44	744	236	387	62	54	5	0	0	0

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
13	Q	50	854	270	426	74	83	1	0	0	0

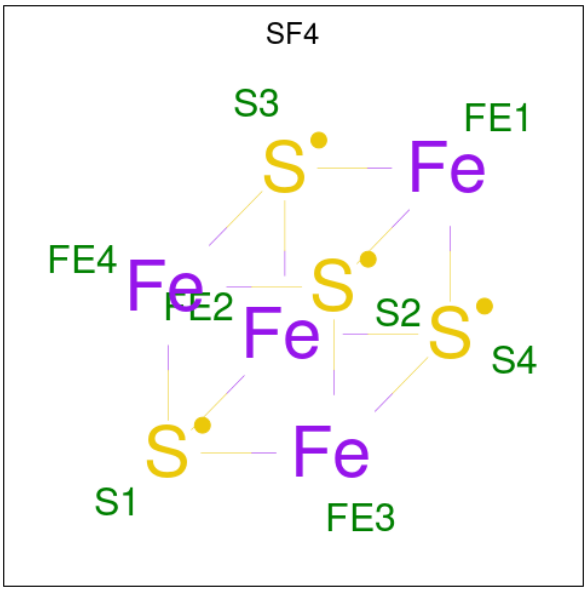
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
14	A	4	4	4	0	0
			Total	Zn		
14	B	3	3	3	0	0
			Total	Zn		
14	C	1	1	1	0	0
			Total	Zn		
14	N	1	1	1	0	0
			Total	Zn		
14	P	1	1	1	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	A	1	1	1	0	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



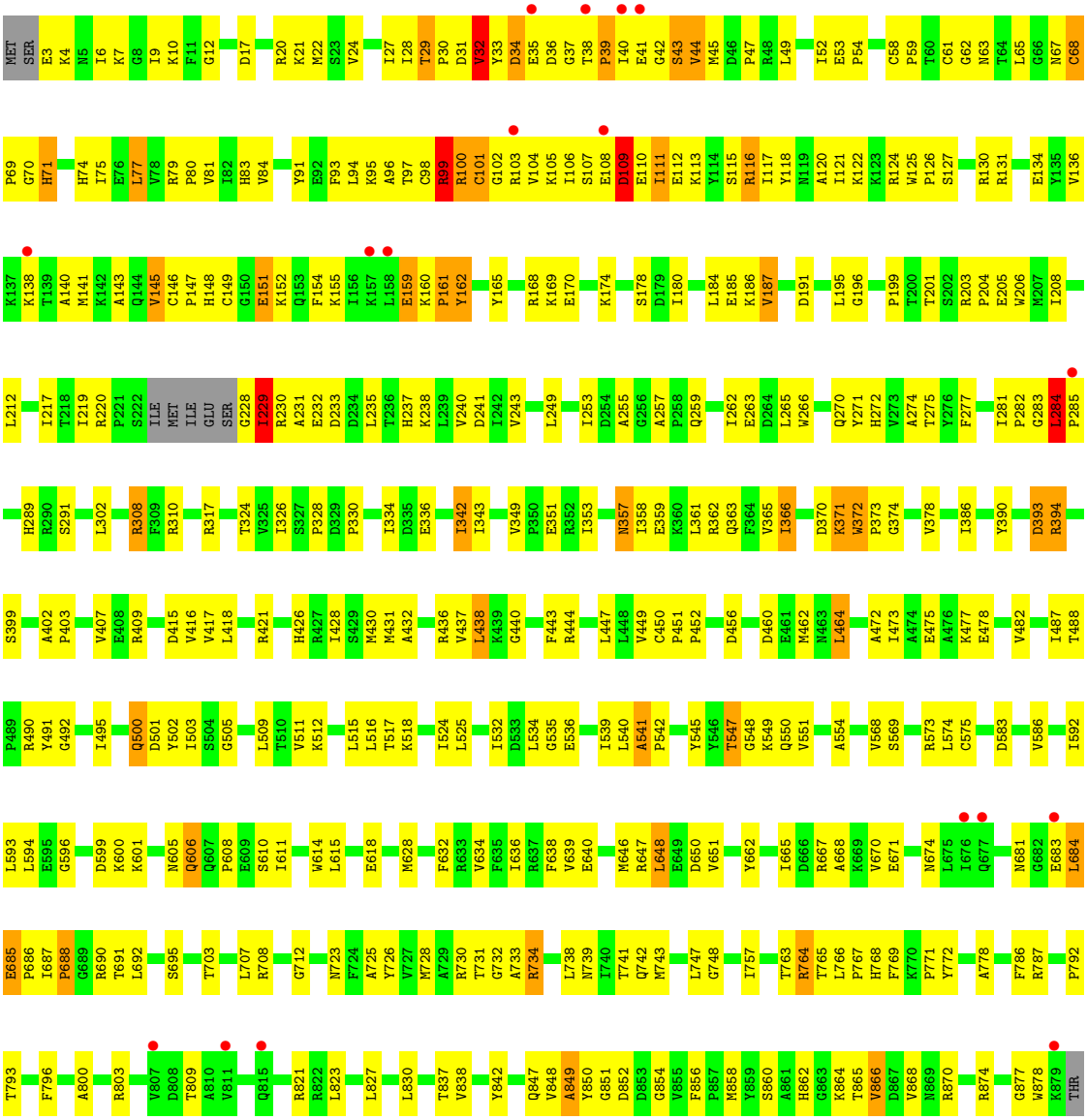
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
16	D	1	7	3	4	0	0

3 Residue-property plots (i)

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

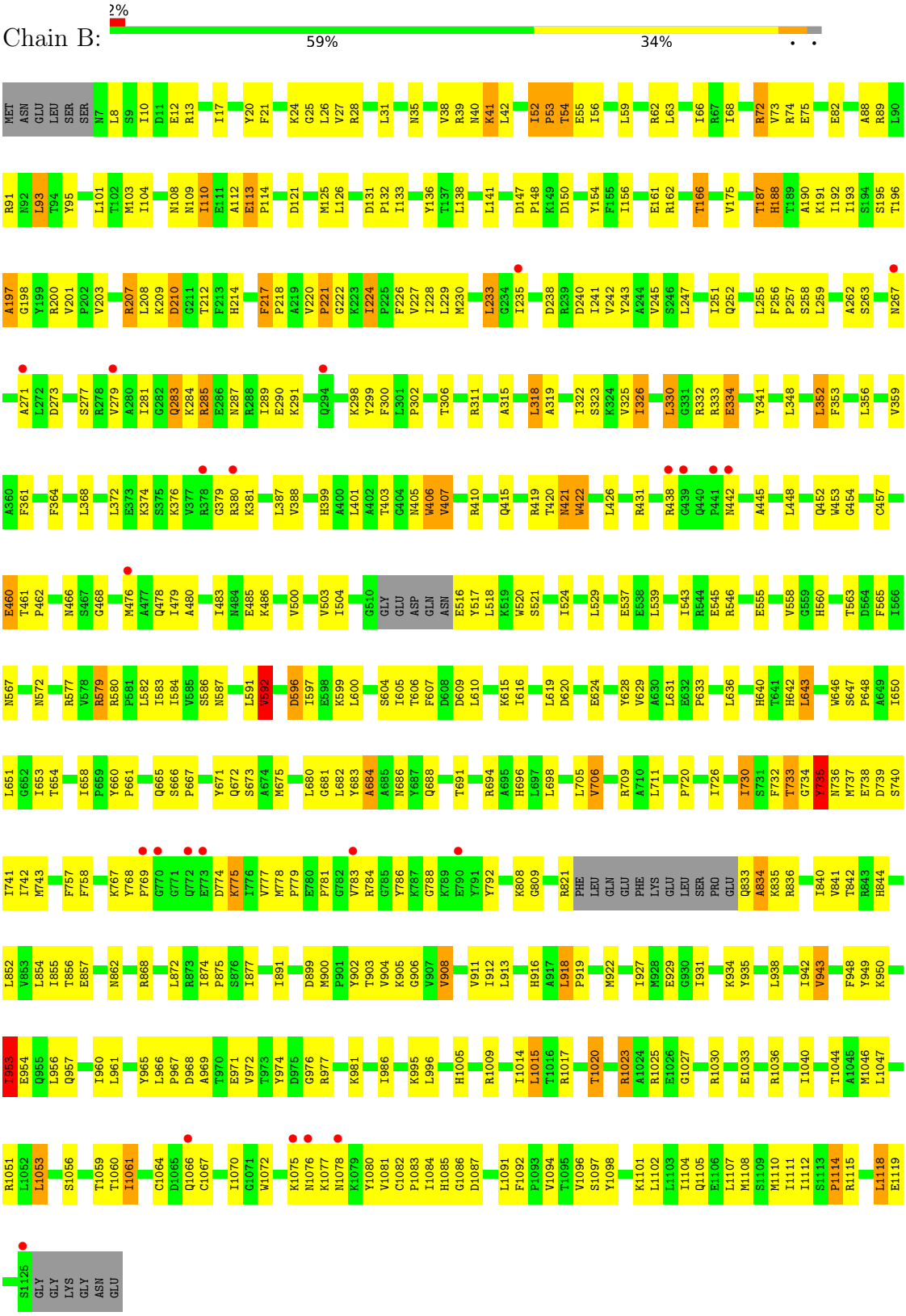
- Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain A:



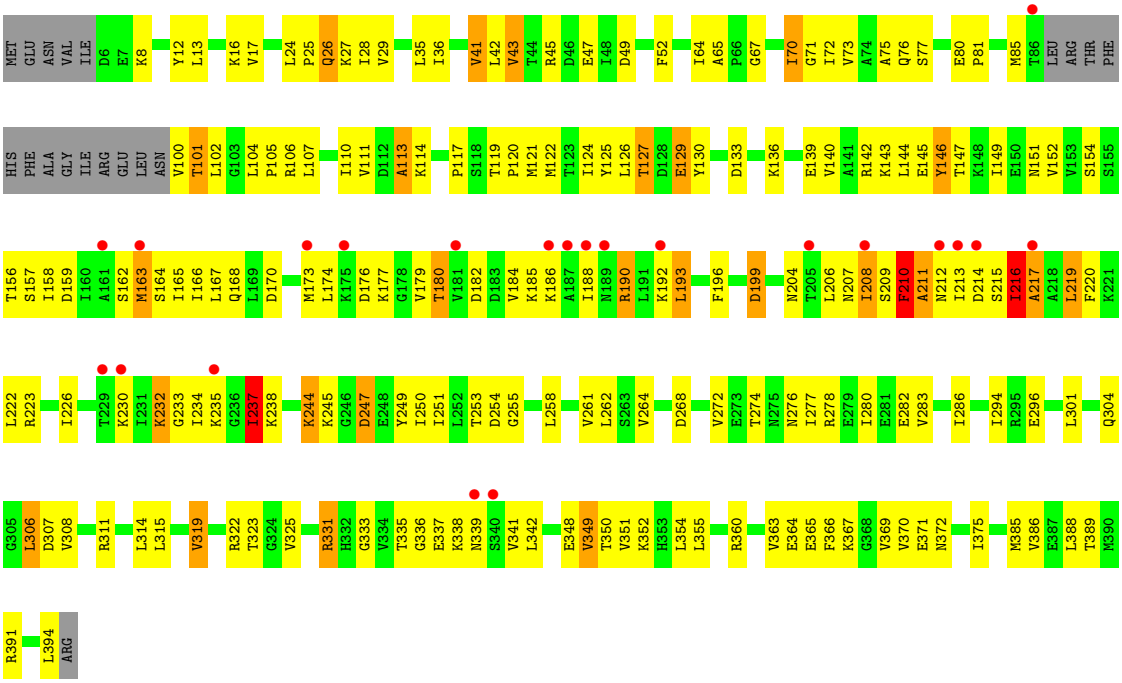
- Molecule 2: DNA-DIRECTED RNA POLYMERASE

Chain B:



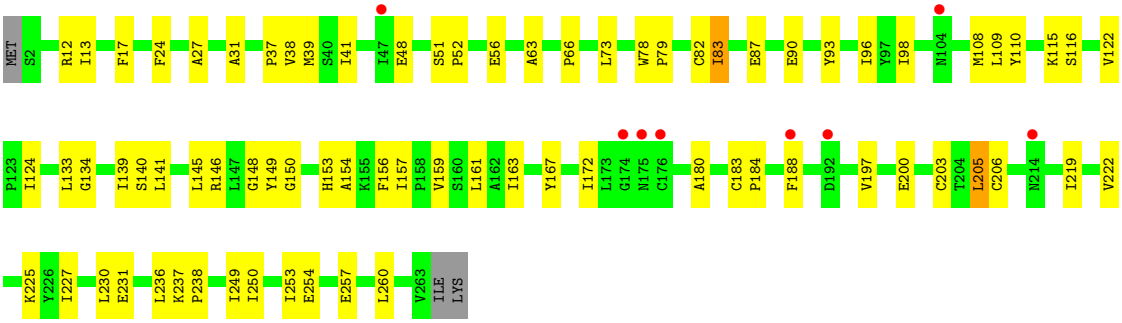
• Molecule 3: DNA-DIRECTED RNA POLYMERASE

Chain C:



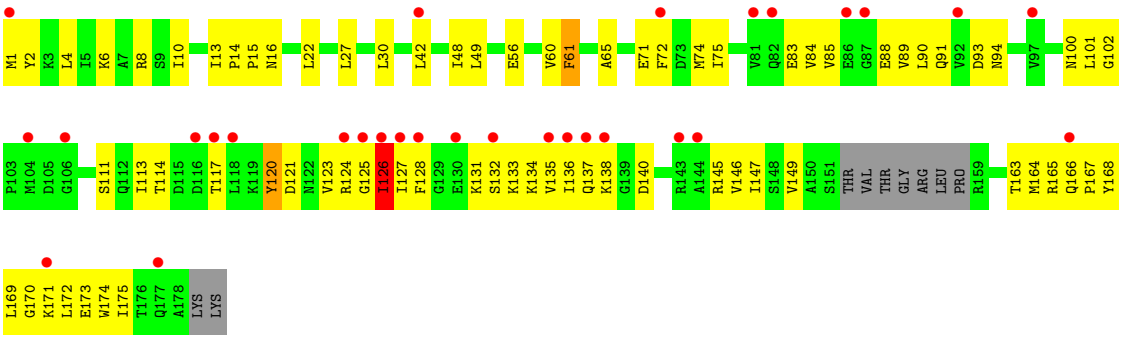
- Molecule 4: DNA-DIRECTED RNA POLYMERASE

Chain D:



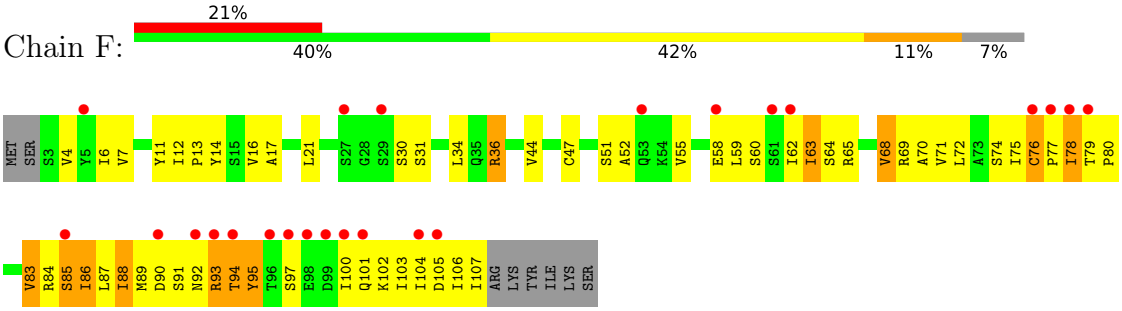
- Molecule 5: DNA-DIRECTED RNA POLYMERASE

Chain E:



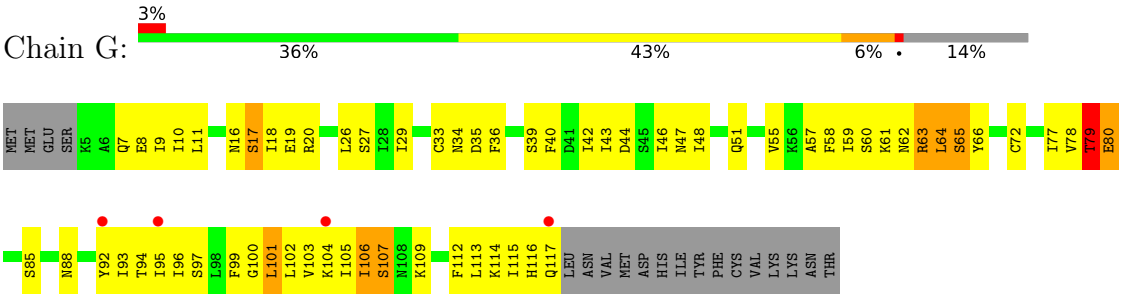
- Molecule 6: DNA-DIRECTED RNA POLYMERASE

Chain F:



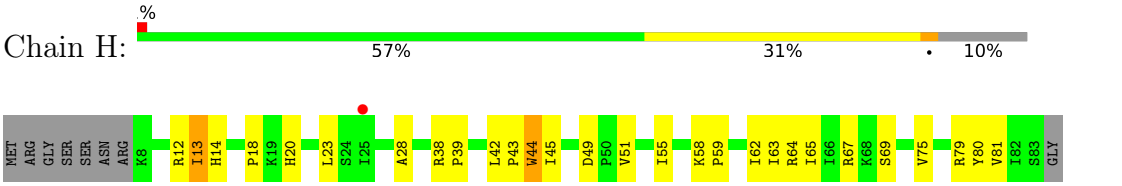
- Molecule 7: DNA-DIRECTED RNA POLYMERASE

Chain G:



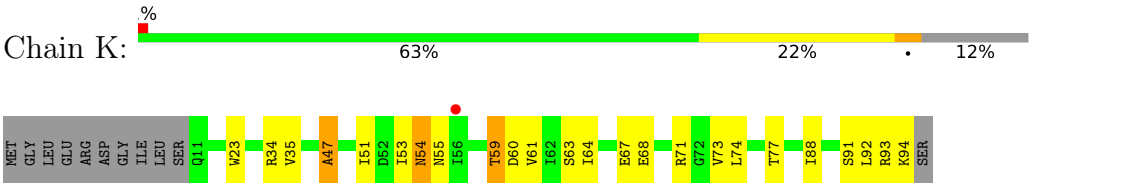
- Molecule 8: DNA-DIRECTED RNA POLYMERASE

Chain H:



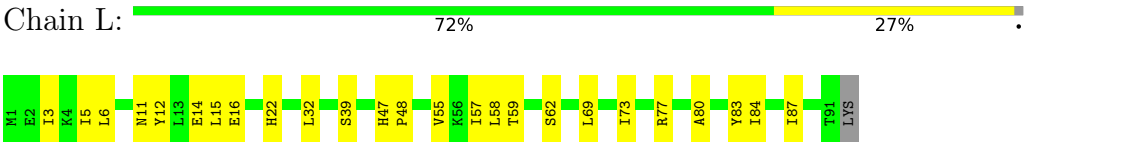
- Molecule 9: DNA-DIRECTED RNA POLYMERASE

Chain K:



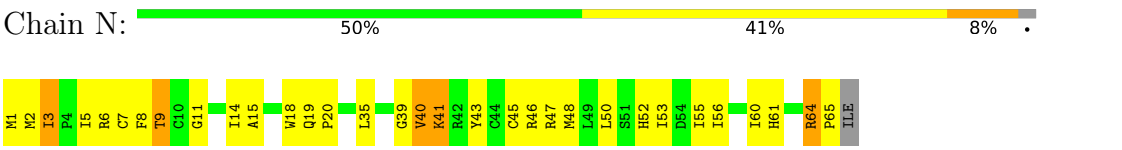
- Molecule 10: DNA-DIRECTED RNA POLYMERASE

Chain L:



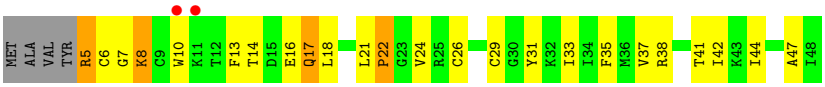
- Molecule 11: DNA-DIRECTED RNA POLYMERASE

Chain N:



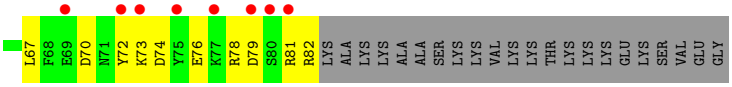
- Molecule 12: DNA-DIRECTED RNA POLYMERASE

Chain P:



• Molecule 13: DNA-DIRECTED RNA POLYMERASE

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	195.72Å 212.41Å 128.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.10 – 3.20 40.10 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.10-3.20) 99.5 (40.10-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.242 , 0.300 0.235 , 0.293	Depositor DCC
R_{free} test set	4428 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	54890	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, ZN

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	0.27	0/7108	0.45	0/9618
2	B	0.25	0/8923	0.44	0/12071
3	C	0.24	0/2930	0.46	0/3944
4	D	0.23	0/2123	0.39	0/2870
5	E	0.23	0/1379	0.40	0/1861
6	F	0.23	0/836	0.44	0/1133
7	G	0.24	0/913	0.43	0/1224
8	H	0.23	0/638	0.42	0/864
9	K	0.25	0/682	0.45	0/921
10	L	0.24	0/717	0.40	0/968
11	N	0.25	0/532	0.45	0/718
12	P	0.30	0/365	0.47	0/489
13	Q	0.23	0/434	0.41	0/580
All	All	0.25	0/27580	0.44	0/37261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6957	7029	7013	415	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8756	8908	8888	418	0
3	C	2906	3068	3063	201	0
4	D	2087	2128	2125	59	0
5	E	1359	1413	1411	75	0
6	F	827	839	839	83	0
7	G	901	915	912	87	0
8	H	624	660	658	24	0
9	K	673	717	716	20	0
10	L	707	742	739	17	0
11	N	521	537	535	38	0
12	P	357	387	387	21	0
13	Q	428	426	426	38	0
14	A	4	0	0	0	0
14	B	3	0	0	0	0
14	C	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
15	A	1	0	0	0	0
16	D	7	0	0	4	0
All	All	27121	27769	27712	1393	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 25.

All (1393) 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)
6:F:93:ARG:CB	6:F:94:THR:HA	1.87	1.05
1:A:146:CYS:SG	1:A:154:PHE:CZ	2.55	1.00
2:B:221:PRO:HB2	2:B:222:GLY:HA2	1.41	1.00
6:F:93:ARG:HB3	6:F:94:THR:HA	1.47	0.95
1:A:683:GLU:HA	1:A:684:LEU:HB3	1.51	0.93
2:B:833:GLN:N	2:B:834:ALA:HB3	1.84	0.93
7:G:65:SER:CB	7:G:66:TYR:HA	2.02	0.90
3:C:42:LEU:HA	3:C:43:VAL:HB	1.51	0.90
3:C:42:LEU:HA	3:C:43:VAL:CB	2.03	0.89
1:A:36:ASP:N	1:A:37:GLY:HA2	1.89	0.88
2:B:52:ILE:HB	2:B:53:PRO:HD3	1.54	0.87
2:B:53:PRO:HB2	2:B:54:THR:HB	1.55	0.86
2:B:53:PRO:HB2	2:B:54:THR:CA	2.07	0.85
11:N:64:ARG:HB3	11:N:65:PRO:HD3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD13	1:A:47:PRO:CG	2.08	0.84
7:G:79:THR:HB	7:G:80:GLU:HB2	1.58	0.83
2:B:53:PRO:HB2	2:B:54:THR:HA	1.61	0.82
11:N:64:ARG:CB	11:N:65:PRO:HD3	2.08	0.82
1:A:105:LYS:HZ2	1:A:140:ALA:HB3	1.43	0.82
1:A:40:ILE:HD13	1:A:47:PRO:HG3	1.62	0.81
2:B:833:GLN:HB2	2:B:834:ALA:CB	2.10	0.81
7:G:29:ILE:HB	7:G:40:PHE:HB3	1.63	0.81
13:Q:56:ASN:N	13:Q:57:GLY:HA2	1.93	0.80
1:A:283:GLY:HA3	1:A:284:LEU:HG	1.64	0.79
7:G:79:THR:CB	7:G:80:GLU:HB2	2.12	0.79
6:F:93:ARG:HB2	6:F:94:THR:HA	1.64	0.78
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.14	0.78
2:B:53:PRO:HB2	2:B:54:THR:CB	2.12	0.78
1:A:283:GLY:HA3	1:A:284:LEU:CG	2.14	0.77
1:A:372:TRP:HB3	1:A:373:PRO:HD3	1.66	0.77
1:A:47:PRO:HB2	1:A:59:PRO:HG2	1.65	0.77
6:F:78:ILE:HG23	6:F:104:ILE:HG22	1.67	0.77
1:A:283:GLY:HA3	1:A:284:LEU:CB	2.15	0.76
2:B:734:GLY:HA3	2:B:735:TYR:CG	2.21	0.76
6:F:91:SER:HB2	6:F:92:ASN:HA	1.66	0.76
2:B:380:ARG:HB3	2:B:381:LYS:HA	1.66	0.75
1:A:103:ARG:HB2	1:A:186:LYS:HB2	1.69	0.74
1:A:97:THR:HG22	1:A:99:ARG:H	1.51	0.74
7:G:65:SER:HB2	7:G:66:TYR:HA	1.69	0.74
3:C:42:LEU:HA	3:C:43:VAL:CG2	2.16	0.74
3:C:211:ALA:HA	3:C:212:ASN:HB2	1.69	0.73
6:F:93:ARG:CB	6:F:94:THR:CA	2.66	0.73
3:C:176:ASP:H	3:C:177:LYS:HB2	1.54	0.72
1:A:541:ALA:CB	1:A:542:PRO:CD	2.68	0.72
2:B:833:GLN:HB2	2:B:834:ALA:HB2	1.71	0.72
7:G:65:SER:HB3	7:G:66:TYR:HA	1.70	0.72
3:C:176:ASP:HB2	3:C:177:LYS:HB2	1.71	0.72
2:B:734:GLY:HA3	2:B:735:TYR:CB	2.18	0.72
3:C:211:ALA:CA	3:C:212:ASN:HB2	2.20	0.71
2:B:52:ILE:CB	2:B:53:PRO:HD3	2.20	0.71
1:A:33:TYR:H	1:A:34:ASP:HB2	1.55	0.71
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.25	0.71
2:B:734:GLY:CA	2:B:735:TYR:HB2	2.22	0.70
2:B:732:PHE:O	2:B:733:THR:HG22	1.91	0.70
5:E:1:MET:HE3	5:E:85:VAL:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LYS:HA	1:A:865:THR:CB	2.21	0.70
1:A:146:CYS:SG	1:A:154:PHE:CE2	2.85	0.69
1:A:103:ARG:CG	1:A:187:VAL:HG13	2.23	0.69
1:A:547:THR:HG23	1:A:550:GLN:HB2	1.73	0.69
1:A:668:ALA:CB	1:A:707:LEU:HD13	2.23	0.69
6:F:76:CYS:CB	6:F:104:ILE:HG23	2.22	0.69
2:B:112:ALA:O	2:B:113:GLU:CB	2.41	0.69
1:A:651:VAL:HG11	1:A:743:MET:HB3	1.75	0.68
1:A:33:TYR:N	1:A:34:ASP:HB2	2.08	0.68
5:E:170:GLY:N	5:E:175:ILE:HD11	2.08	0.68
1:A:40:ILE:CD1	1:A:47:PRO:HG3	2.23	0.68
1:A:47:PRO:HB2	1:A:59:PRO:CG	2.24	0.68
1:A:864:LYS:HA	1:A:865:THR:HB	1.75	0.68
1:A:541:ALA:CB	1:A:542:PRO:HD3	2.24	0.68
5:E:113:ILE:HG22	5:E:114:THR:HG23	1.76	0.67
1:A:103:ARG:CB	1:A:186:LYS:HB2	2.24	0.67
3:C:211:ALA:HB1	3:C:212:ASN:C	2.14	0.67
1:A:108:GLU:HG3	1:A:147:PRO:HG2	1.77	0.67
2:B:953:ILE:HD13	2:B:953:ILE:N	2.09	0.67
2:B:833:GLN:HB2	2:B:834:ALA:HB3	1.76	0.67
3:C:211:ALA:CB	3:C:212:ASN:HB2	2.24	0.67
1:A:101:CYS:SG	1:A:152:LYS:CG	2.82	0.67
7:G:101:LEU:HD22	7:G:102:LEU:N	2.10	0.67
11:N:3:ILE:HG22	11:N:52:HIS:CG	2.29	0.67
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.77	0.66
2:B:406:TRP:HA	2:B:407:VAL:HB	1.76	0.66
2:B:112:ALA:O	2:B:113:GLU:HB2	1.95	0.66
6:F:79:THR:OG1	6:F:80:PRO:HD3	1.96	0.66
1:A:40:ILE:HG21	1:A:47:PRO:HD3	1.78	0.66
7:G:65:SER:CB	7:G:66:TYR:CA	2.73	0.66
1:A:739:ASN:HB2	2:B:922:MET:SD	2.36	0.66
1:A:29:THR:OG1	1:A:30:PRO:HD3	1.96	0.65
2:B:833:GLN:CA	2:B:834:ALA:HB3	2.26	0.65
12:P:17:GLN:HG3	12:P:18:LEU:H	1.61	0.65
13:Q:33:PHE:HB3	13:Q:34:PRO:HD2	1.78	0.65
1:A:220:ARG:HD3	1:A:235:LEU:HB3	1.78	0.65
3:C:211:ALA:HB1	3:C:212:ASN:HB2	1.78	0.65
13:Q:78:ARG:HD3	13:Q:78:ARG:C	2.17	0.65
2:B:256:PHE:N	2:B:257:PRO:HD2	2.12	0.65
2:B:53:PRO:CB	2:B:54:THR:HB	2.28	0.64
1:A:101:CYS:SG	1:A:152:LYS:HG3	2.36	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:HA	2:B:319:ALA:HB1	1.79	0.64
1:A:417:VAL:HG11	1:A:464:LEU:HD21	1.80	0.64
1:A:668:ALA:HB1	1:A:707:LEU:HD13	1.78	0.64
2:B:56:ILE:HG23	2:B:59:LEU:HB2	1.78	0.64
2:B:808:LYS:HD2	2:B:809:GLY:N	2.11	0.64
1:A:160:LYS:HB3	1:A:161:PRO:HD2	1.78	0.64
6:F:76:CYS:HB2	6:F:104:ILE:HG23	1.78	0.64
3:C:176:ASP:CB	3:C:177:LYS:HB2	2.27	0.64
6:F:88:ILE:HG23	6:F:88:ILE:O	1.96	0.64
7:G:99:PHE:O	7:G:103:VAL:HG12	1.98	0.64
1:A:125:TRP:CZ2	13:Q:48:THR:HG21	2.33	0.64
3:C:211:ALA:HB3	3:C:213:ILE:HG12	1.79	0.64
1:A:842:TYR:CZ	3:C:339:ASN:O	2.50	0.64
2:B:1082:CYS:HB2	2:B:1083:PRO:HD2	1.78	0.64
1:A:33:TYR:HB3	1:A:34:ASP:CA	2.28	0.63
2:B:658:ILE:HG12	2:B:672:GLN:HG2	1.81	0.63
3:C:146:TYR:HA	3:C:233:GLY:HA3	1.79	0.63
1:A:487:ILE:HD12	1:A:858:MET:O	1.98	0.63
3:C:42:LEU:HA	3:C:43:VAL:HG23	1.79	0.63
5:E:102:GLY:O	6:F:36:ARG:HD3	1.99	0.63
1:A:106:ILE:CG2	1:A:143:ALA:HB3	2.29	0.63
1:A:606:GLN:O	1:A:608:PRO:HD3	1.99	0.63
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.78	0.63
1:A:535:GLY:O	1:A:536:GLU:C	2.36	0.63
2:B:781:PRO:HA	2:B:786:TYR:CE2	2.34	0.62
5:E:85:VAL:HG11	5:E:101:LEU:HD22	1.81	0.62
13:Q:57:GLY:O	13:Q:59:ILE:N	2.32	0.62
1:A:185:GLU:HA	1:A:205:GLU:HG2	1.82	0.62
1:A:600:LYS:O	1:A:600:LYS:HG2	1.99	0.62
1:A:830:LEU:HD11	3:C:319:VAL:HG21	1.81	0.62
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.35	0.62
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.81	0.62
1:A:33:TYR:HB3	1:A:34:ASP:HA	1.81	0.62
1:A:681:ASN:HB2	1:A:683:GLU:HG2	1.82	0.62
13:Q:78:ARG:HH22	13:Q:82:ARG:HD3	1.63	0.62
1:A:79:ARG:HB3	1:A:266:TRP:CZ3	2.35	0.62
1:A:363:GLN:O	1:A:366:ILE:HG22	1.98	0.62
2:B:1014:ILE:O	2:B:1015:LEU:CB	2.47	0.62
4:D:188:PHE:CE2	16:D:1264:SF4:S3	2.93	0.62
2:B:406:TRP:CA	2:B:407:VAL:HB	2.30	0.61
7:G:106:ILE:O	7:G:107:SER:CB	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:HA	1:A:205:GLU:CG	2.31	0.61
1:A:796:PHE:CZ	2:B:448:LEU:HD22	2.35	0.61
3:C:213:ILE:HB	3:C:214:ASP:C	2.21	0.61
7:G:78:VAL:O	7:G:79:THR:HG23	2.00	0.61
13:Q:54:LEU:HA	13:Q:59:ILE:HG22	1.82	0.61
3:C:213:ILE:HB	3:C:214:ASP:O	2.00	0.61
1:A:687:ILE:HG21	1:A:690:ARG:HB2	1.82	0.61
1:A:110:GLU:OE2	1:A:148:HIS:CE1	2.53	0.61
2:B:1111:ILE:HD12	2:B:1111:ILE:N	2.16	0.61
6:F:58:GLU:HB3	6:F:103:ILE:HG21	1.82	0.61
1:A:848:VAL:O	1:A:849:ALA:HB3	2.00	0.61
12:P:5:ARG:HA	12:P:6:CYS:SG	2.41	0.61
7:G:79:THR:CG2	7:G:80:GLU:HB2	2.30	0.61
1:A:763:THR:O	1:A:764:ARG:HB3	2.01	0.61
11:N:2:MET:O	11:N:3:ILE:O	2.19	0.61
13:Q:44:LEU:O	13:Q:48:THR:HG23	1.99	0.61
1:A:431:MET:HE2	1:A:482:VAL:HG13	1.83	0.60
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.83	0.60
3:C:42:LEU:CA	3:C:43:VAL:HB	2.25	0.60
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.82	0.60
2:B:196:THR:O	2:B:197:ALA:CB	2.48	0.60
7:G:36:PHE:CD1	7:G:96:ILE:HD13	2.36	0.60
12:P:17:GLN:HG3	12:P:18:LEU:N	2.16	0.60
1:A:107:SER:HB2	1:A:108:GLU:HB2	1.83	0.60
13:Q:46:LYS:HE2	13:Q:46:LYS:HA	1.81	0.60
1:A:33:TYR:HB3	1:A:34:ASP:CB	2.31	0.60
1:A:75:ILE:HD12	1:A:243:VAL:HG22	1.82	0.60
1:A:646:MET:HE2	1:A:725:ALA:HB2	1.82	0.60
1:A:796:PHE:CZ	2:B:448:LEU:CD2	2.84	0.60
6:F:78:ILE:HD13	6:F:78:ILE:H	1.64	0.60
1:A:146:CYS:SG	1:A:154:PHE:HZ	2.21	0.60
2:B:108:ASN:O	2:B:109:ASN:HB2	2.02	0.60
6:F:93:ARG:HB2	6:F:94:THR:CA	2.29	0.60
11:N:64:ARG:CB	11:N:65:PRO:CD	2.79	0.60
1:A:103:ARG:HG3	1:A:187:VAL:HG13	1.83	0.60
2:B:1064:CYS:HA	2:B:1091:LEU:CD2	2.32	0.60
3:C:349:VAL:HG13	3:C:352:LYS:HE2	1.84	0.60
1:A:70:GLY:O	1:A:71:HIS:HB2	2.02	0.60
3:C:176:ASP:N	3:C:177:LYS:O	2.35	0.60
7:G:65:SER:HB2	7:G:66:TYR:CA	2.32	0.60
1:A:283:GLY:CA	1:A:284:LEU:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HD21	1:A:551:VAL:HG23	1.83	0.59
2:B:660:TYR:N	2:B:661:PRO:HD3	2.16	0.59
2:B:323:SER:HA	2:B:326:ILE:HD11	1.83	0.59
3:C:213:ILE:H	3:C:214:ASP:HA	1.66	0.59
1:A:284:LEU:HD22	1:A:285:PRO:CD	2.32	0.59
2:B:39:ARG:HG3	2:B:40:ASN:N	2.17	0.59
4:D:153:HIS:CG	4:D:153:HIS:O	2.55	0.59
5:E:114:THR:HG21	5:E:134:LYS:HD3	1.84	0.59
2:B:162:ARG:HG2	2:B:401:LEU:O	2.02	0.59
3:C:81:PRO:HB3	3:C:306:LEU:HG	1.85	0.59
2:B:196:THR:HG21	2:B:302:PRO:HB2	1.83	0.59
2:B:600:LEU:HD11	2:B:610:LEU:HD11	1.85	0.59
2:B:696:HIS:CE1	2:B:757:PHE:HD1	2.21	0.59
2:B:1064:CYS:HB3	2:B:1067:CYS:HB2	1.85	0.59
1:A:33:TYR:HB3	1:A:34:ASP:HB2	1.85	0.59
1:A:283:GLY:CA	1:A:284:LEU:CB	2.80	0.59
5:E:15:PRO:HD3	5:E:65:ALA:HB2	1.84	0.59
3:C:192:LYS:HB3	3:C:193:LEU:HB2	1.84	0.58
3:C:192:LYS:CB	3:C:193:LEU:HB2	2.33	0.58
8:H:43:PRO:HB2	8:H:79:ARG:HG2	1.83	0.58
1:A:99:ARG:O	1:A:100:ARG:HB3	2.02	0.58
1:A:324:THR:HG22	1:A:443:PHE:CD2	2.39	0.58
6:F:65:ARG:O	6:F:69:ARG:HG3	2.03	0.58
3:C:213:ILE:N	3:C:214:ASP:HA	2.18	0.58
4:D:63:ALA:HB2	12:P:47:ALA:HB1	1.84	0.58
11:N:1:MET:O	11:N:2:MET:HB2	2.02	0.58
1:A:334:ILE:HD11	1:A:628:MET:HB3	1.83	0.58
1:A:431:MET:CE	1:A:482:VAL:HA	2.33	0.58
8:H:43:PRO:O	8:H:44:TRP:CB	2.51	0.58
1:A:532:ILE:HD13	1:A:554:ALA:HB1	1.84	0.58
2:B:480:ALA:HB2	2:B:579:ARG:CD	2.33	0.58
3:C:325:VAL:HG11	13:Q:33:PHE:CZ	2.38	0.58
11:N:14:ILE:HD11	11:N:45:CYS:HB3	1.85	0.58
1:A:105:LYS:CE	1:A:195:LEU:HD21	2.33	0.58
3:C:176:ASP:N	3:C:177:LYS:HB2	2.16	0.58
5:E:102:GLY:O	6:F:36:ARG:CD	2.52	0.58
5:E:145:ARG:NH2	6:F:86:ILE:HD11	2.18	0.58
1:A:84:VAL:HG11	1:A:274:ALA:HB1	1.84	0.58
1:A:105:LYS:HE2	1:A:136:VAL:HG12	1.85	0.58
1:A:107:SER:HA	1:A:108:GLU:HG3	1.86	0.58
2:B:233:LEU:HD11	2:B:311:ARG:C	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:THR:CG2	2:B:734:GLY:N	2.67	0.58
1:A:372:TRP:CB	1:A:373:PRO:HD3	2.34	0.58
1:A:501:ASP:HB2	2:B:737:MET:SD	2.44	0.58
3:C:185:LYS:HA	3:C:188:ILE:HD12	1.84	0.58
12:P:5:ARG:N	12:P:6:CYS:HA	2.18	0.58
1:A:147:PRO:O	1:A:148:HIS:HB2	2.04	0.58
2:B:453:TRP:CE2	2:B:650:ILE:HD11	2.39	0.58
2:B:628:TYR:CE2	2:B:640:HIS:CE1	2.91	0.58
3:C:80:GLU:HB3	3:C:81:PRO:HD3	1.85	0.58
2:B:380:ARG:CB	2:B:381:LYS:HA	2.31	0.58
7:G:72:CYS:SG	7:G:114:LYS:HD2	2.44	0.58
11:N:8:PHE:O	11:N:9:THR:CB	2.51	0.58
13:Q:58:LYS:O	13:Q:59:ILE:HB	2.03	0.57
1:A:733:ALA:O	1:A:734:ARG:C	2.43	0.57
3:C:154:SER:HB3	3:C:170:ASP:HB2	1.85	0.57
11:N:48:MET:HA	11:N:48:MET:HE2	1.86	0.57
1:A:687:ILE:HG13	1:A:688:PRO:HD2	1.85	0.57
11:N:3:ILE:CG2	11:N:52:HIS:CD2	2.87	0.57
5:E:126:ILE:HG13	5:E:127:ILE:N	2.19	0.57
1:A:97:THR:HG23	1:A:103:ARG:CD	2.34	0.57
1:A:101:CYS:SG	1:A:152:LYS:HG2	2.44	0.57
3:C:211:ALA:HB1	3:C:212:ASN:CA	2.34	0.57
2:B:1014:ILE:O	2:B:1015:LEU:HB3	2.05	0.57
6:F:91:SER:HB2	6:F:92:ASN:CA	2.35	0.57
7:G:20:ARG:HA	7:G:27:SER:HA	1.87	0.57
1:A:764:ARG:HD2	1:A:769:PHE:O	2.04	0.57
2:B:196:THR:O	2:B:197:ALA:HB3	2.05	0.57
2:B:379:GLY:O	2:B:380:ARG:HB2	2.05	0.57
3:C:211:ALA:CB	3:C:213:ILE:HG12	2.35	0.57
6:F:91:SER:CB	6:F:92:ASN:CA	2.82	0.57
5:E:164:MET:HB3	5:E:170:GLY:HA2	1.87	0.57
6:F:60:SER:HA	6:F:69:ARG:CZ	2.35	0.57
2:B:101:LEU:HD12	2:B:103:MET:HE3	1.86	0.57
2:B:190:ALA:HB2	2:B:325:VAL:HG22	1.86	0.57
2:B:406:TRP:HA	2:B:407:VAL:CB	2.35	0.57
5:E:94:ASN:HB3	5:E:120:TYR:CD2	2.40	0.57
1:A:219:ILE:O	1:A:220:ARG:HD2	2.05	0.56
2:B:364:PHE:CE1	2:B:388:VAL:HG13	2.40	0.56
2:B:209:LYS:O	2:B:210:ASP:CB	2.53	0.56
3:C:211:ALA:HB1	3:C:212:ASN:CB	2.35	0.56
7:G:57:ALA:HA	7:G:115:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HG3	1:A:178:SER:HA	1.88	0.56
1:A:33:TYR:CA	1:A:34:ASP:HB2	2.35	0.56
1:A:108:GLU:CG	1:A:147:PRO:HG2	2.34	0.56
2:B:406:TRP:CB	2:B:407:VAL:HB	2.35	0.56
1:A:28:ILE:HD12	1:A:44:VAL:HA	1.88	0.56
2:B:592:VAL:CG2	2:B:596:ASP:CG	2.73	0.56
2:B:833:GLN:CB	2:B:834:ALA:HB3	2.35	0.56
2:B:1064:CYS:SG	2:B:1067:CYS:HB2	2.45	0.56
3:C:366:PHE:O	3:C:367:LYS:HB2	2.06	0.56
7:G:16:ASN:O	7:G:17:SER:CB	2.53	0.56
1:A:17:ASP:HA	1:A:20:ARG:HG2	1.88	0.56
1:A:33:TYR:CB	1:A:34:ASP:HB2	2.36	0.56
1:A:40:ILE:HG22	1:A:41:GLU:N	2.19	0.56
1:A:277:PHE:CZ	2:B:1111:ILE:HD13	2.40	0.56
4:D:197:VAL:HG11	4:D:200:GLU:HB2	1.88	0.56
9:K:51:ILE:HG21	9:K:71:ARG:NH2	2.21	0.56
1:A:97:THR:HG23	1:A:103:ARG:HD3	1.88	0.56
2:B:665:GLN:HG2	2:B:667:PRO:HD2	1.88	0.56
4:D:78:TRP:HB3	4:D:79:PRO:HD2	1.88	0.56
12:P:6:CYS:HB2	12:P:37:VAL:HG12	1.88	0.56
1:A:503:ILE:HB	1:A:733:ALA:HB2	1.88	0.55
2:B:242:VAL:CG1	2:B:252:GLN:HG3	2.36	0.55
5:E:168:TYR:CD2	6:F:83:VAL:HG11	2.40	0.55
1:A:108:GLU:O	1:A:112:GLU:HB2	2.06	0.55
2:B:918:LEU:HD13	2:B:927:ILE:HD11	1.88	0.55
2:B:1067:CYS:SG	2:B:1085:HIS:HE1	2.27	0.55
7:G:101:LEU:O	7:G:105:ILE:HG12	2.06	0.55
13:Q:39:GLN:OE1	13:Q:78:ARG:CZ	2.54	0.55
2:B:372:LEU:HD23	2:B:387:LEU:HD13	1.89	0.55
3:C:294:ILE:HD13	3:C:314:LEU:HD23	1.89	0.55
3:C:210:PHE:CE1	3:C:214:ASP:O	2.59	0.55
6:F:62:ILE:CD1	6:F:100:ILE:HG12	2.36	0.55
2:B:406:TRP:HB3	2:B:407:VAL:O	2.06	0.55
1:A:651:VAL:HG12	1:A:651:VAL:O	2.07	0.55
2:B:736:ASN:HB3	2:B:742:ILE:HG13	1.88	0.55
1:A:187:VAL:HG21	1:A:204:PRO:HG3	1.88	0.55
1:A:238:LYS:HE2	1:A:275:THR:HB	1.87	0.55
2:B:833:GLN:CB	2:B:834:ALA:CB	2.84	0.55
2:B:406:TRP:HB3	2:B:407:VAL:C	2.27	0.55
6:F:78:ILE:HG12	6:F:79:THR:N	2.22	0.55
6:F:91:SER:CB	6:F:92:ASN:HA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:HB3	1:A:272:HIS:NE2	2.22	0.55
1:A:160:LYS:HB3	1:A:161:PRO:CD	2.36	0.54
1:A:683:GLU:CA	1:A:684:LEU:HB3	2.31	0.54
2:B:734:GLY:HA3	2:B:735:TYR:HB2	1.83	0.54
2:B:1017:ARG:HD3	2:B:1098:TYR:CG	2.42	0.54
3:C:144:LEU:O	3:C:237:ILE:HD11	2.07	0.54
3:C:157:SER:HB3	3:C:166:ILE:HB	1.88	0.54
3:C:176:ASP:HB2	3:C:177:LYS:HD2	1.87	0.54
6:F:88:ILE:O	6:F:88:ILE:CG2	2.54	0.54
8:H:43:PRO:O	8:H:44:TRP:CG	2.60	0.54
11:N:8:PHE:O	11:N:9:THR:HB	2.06	0.54
1:A:98:CYS:O	1:A:101:CYS:SG	2.65	0.54
3:C:184:VAL:HG12	3:C:188:ILE:HD11	1.88	0.54
7:G:16:ASN:O	7:G:17:SER:HB3	2.07	0.54
7:G:79:THR:HG22	7:G:80:GLU:HB2	1.89	0.54
11:N:35:LEU:HD13	11:N:46:ARG:HG3	1.89	0.54
1:A:691:THR:HG22	1:A:692:LEU:N	2.23	0.54
1:A:703:THR:HG22	1:A:707:LEU:HD12	1.90	0.54
1:A:848:VAL:O	1:A:849:ALA:CB	2.55	0.54
2:B:227:VAL:CG1	2:B:262:ALA:HB3	2.37	0.54
5:E:126:ILE:CG2	5:E:137:GLN:HG2	2.38	0.54
6:F:62:ILE:O	6:F:63:ILE:HB	2.07	0.54
12:P:5:ARG:N	12:P:17:GLN:HA	2.22	0.54
1:A:21:LYS:O	1:A:24:VAL:HG13	2.08	0.54
1:A:370:ASP:O	1:A:371:LYS:HB3	2.07	0.54
1:A:763:THR:O	1:A:764:ARG:CB	2.55	0.54
4:D:203:CYS:HA	16:D:1264:SF4:S1	2.47	0.54
8:H:43:PRO:O	8:H:44:TRP:HB2	2.07	0.54
11:N:40:VAL:O	11:N:41:LYS:HB2	2.08	0.54
3:C:348:GLU:O	3:C:349:VAL:HB	2.08	0.54
13:Q:78:ARG:NH2	13:Q:82:ARG:HD3	2.22	0.54
1:A:447:LEU:HD13	2:B:737:MET:SD	2.48	0.54
1:A:574:LEU:HD23	1:A:575:CYS:N	2.23	0.54
3:C:101:THR:C	3:C:102:LEU:HD22	2.27	0.54
3:C:176:ASP:CA	3:C:177:LYS:HB2	2.37	0.54
1:A:203:ARG:HB2	1:A:206:TRP:CD2	2.42	0.54
2:B:902:TYR:CE1	2:B:974:TYR:HB2	2.43	0.54
3:C:146:TYR:HB3	3:C:237:ILE:CD1	2.38	0.54
4:D:222:VAL:HG11	4:D:225:LYS:HD3	1.88	0.54
1:A:42:GLY:O	1:A:43:SER:CB	2.56	0.54
1:A:67:ASN:O	1:A:69:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:HB3	1:A:272:HIS:CD2	2.42	0.54
2:B:734:GLY:HA3	2:B:735:TYR:CD2	2.42	0.54
2:B:734:GLY:CA	2:B:735:TYR:CB	2.81	0.54
3:C:13:LEU:HD23	3:C:13:LEU:C	2.28	0.54
10:L:83:TYR:CZ	10:L:87:ILE:HD11	2.43	0.54
1:A:650:ASP:OD2	1:A:723:ASN:HB2	2.08	0.54
1:A:692:LEU:N	1:A:692:LEU:HD12	2.23	0.54
11:N:64:ARG:HB2	11:N:65:PRO:HD3	1.88	0.54
1:A:393:ASP:O	1:A:394:ARG:HB3	2.08	0.54
1:A:541:ALA:HB2	7:G:72:CYS:N	2.22	0.54
2:B:356:LEU:HA	2:B:407:VAL:HG11	1.90	0.54
6:F:100:ILE:O	6:F:104:ILE:HG13	2.08	0.54
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.89	0.53
2:B:918:LEU:H	2:B:919:PRO:HD2	1.73	0.53
3:C:124:ILE:HB	3:C:251:ILE:HB	1.91	0.53
1:A:282:PRO:O	1:A:284:LEU:HG	2.08	0.53
1:A:436:ARG:O	1:A:438:LEU:HD22	2.09	0.53
2:B:906:GLY:HA2	4:D:163:ILE:HD11	1.90	0.53
1:A:851:GLY:O	1:A:852:ASP:HB2	2.08	0.53
2:B:778:MET:HE3	2:B:779:PRO:HD2	1.90	0.53
3:C:244:LYS:HB3	3:C:249:TYR:CD1	2.43	0.53
3:C:277:ILE:O	3:C:278:ARG:HB3	2.09	0.53
7:G:102:LEU:HA	7:G:105:ILE:HG12	1.90	0.53
1:A:451:PRO:N	1:A:452:PRO:HD2	2.24	0.53
2:B:52:ILE:HB	2:B:53:PRO:CD	2.32	0.53
2:B:52:ILE:CB	2:B:53:PRO:CD	2.87	0.53
1:A:475:GLU:OE1	2:B:1046:MET:HB2	2.09	0.53
2:B:66:ILE:HG13	2:B:101:LEU:HD23	1.91	0.53
4:D:154:ALA:HA	4:D:157:ILE:HG13	1.91	0.53
13:Q:78:ARG:HD3	13:Q:79:ASP:N	2.23	0.53
1:A:281:ILE:HG13	1:A:284:LEU:HD12	1.91	0.53
4:D:96:ILE:HG12	4:D:145:LEU:HD11	1.91	0.53
1:A:184:LEU:O	1:A:187:VAL:CG2	2.56	0.53
1:A:324:THR:HG22	1:A:443:PHE:CE2	2.44	0.53
1:A:402:ALA:HB1	1:A:403:PRO:HD2	1.90	0.53
2:B:1017:ARG:HD3	2:B:1098:TYR:CD2	2.44	0.53
1:A:95:LYS:HD3	1:A:141:MET:CE	2.39	0.53
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.39	0.53
1:A:703:THR:HG22	1:A:707:LEU:CD1	2.39	0.53
2:B:210:ASP:HA	3:C:220:PHE:CD2	2.44	0.53
2:B:212:THR:HG21	2:B:214:HIS:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:TRP:CZ3	2:B:426:LEU:HD11	2.43	0.53
3:C:70:ILE:HD13	3:C:70:ILE:H	1.74	0.53
3:C:102:LEU:HB2	3:C:106:ARG:HB2	1.91	0.53
3:C:144:LEU:HD22	3:C:235:LYS:NZ	2.24	0.53
3:C:322:ARG:O	3:C:323:THR:HB	2.08	0.53
5:E:125:GLY:C	5:E:126:ILE:HG23	2.29	0.53
5:E:136:ILE:HG12	5:E:171:LYS:HB2	1.91	0.53
1:A:284:LEU:HD22	1:A:285:PRO:HD2	1.90	0.52
2:B:696:HIS:CE1	2:B:757:PHE:CD1	2.96	0.52
5:E:113:ILE:CG2	5:E:136:ILE:HD12	2.39	0.52
1:A:548:GLY:HA2	1:A:551:VAL:HG12	1.91	0.52
2:B:953:ILE:HD13	2:B:953:ILE:H	1.72	0.52
4:D:161:LEU:HD12	4:D:163:ILE:HD13	1.90	0.52
1:A:488:THR:O	1:A:491:TYR:O	2.27	0.52
2:B:138:LEU:HG	2:B:148:PRO:HB3	1.91	0.52
2:B:953:ILE:HG12	2:B:954:GLU:H	1.75	0.52
3:C:216:ILE:O	3:C:217:ALA:HB2	2.08	0.52
4:D:13:ILE:HG21	4:D:238:PRO:HB2	1.90	0.52
1:A:456:ASP:OD1	1:A:460:ASP:CG	2.37	0.52
3:C:41:VAL:O	3:C:42:LEU:C	2.48	0.52
3:C:100:VAL:HG12	3:C:100:VAL:O	2.10	0.52
7:G:106:ILE:O	7:G:107:SER:HB2	2.09	0.52
1:A:65:LEU:HD23	1:A:65:LEU:C	2.29	0.52
1:A:94:LEU:HD21	1:A:180:ILE:HG23	1.91	0.52
2:B:26:LEU:H	2:B:26:LEU:HD23	1.74	0.52
2:B:854:LEU:C	2:B:854:LEU:HD23	2.30	0.52
2:B:968:ASP:O	2:B:969:ALA:HB3	2.09	0.52
8:H:42:LEU:HB3	8:H:43:PRO:HD2	1.91	0.52
1:A:747:LEU:HD22	1:A:786:PHE:CE2	2.44	0.52
2:B:235:ILE:HD12	2:B:235:ILE:N	2.23	0.52
2:B:521:SER:HB3	2:B:567:ASN:ND2	2.24	0.52
1:A:118:TYR:O	1:A:121:ILE:HG22	2.10	0.52
1:A:130:ARG:O	1:A:134:GLU:HG2	2.10	0.52
2:B:166:THR:HB	2:B:348:LEU:HD23	1.91	0.52
2:B:233:LEU:HD11	2:B:311:ARG:O	2.10	0.52
3:C:80:GLU:N	3:C:81:PRO:CD	2.72	0.52
3:C:104:LEU:N	3:C:105:PRO:CD	2.73	0.52
11:N:35:LEU:HD11	11:N:50:LEU:HG	1.91	0.52
1:A:106:ILE:O	1:A:147:PRO:HD2	2.09	0.52
3:C:140:VAL:O	3:C:144:LEU:HG	2.10	0.52
3:C:162:SER:O	3:C:163:MET:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:ILE:HG21	6:F:21:LEU:HD11	1.91	0.52
5:E:91:GLN:HA	5:E:138:LYS:HE2	1.92	0.52
11:N:43:TYR:HA	11:N:46:ARG:HB3	1.91	0.52
13:Q:34:PRO:O	13:Q:35:LYS:CB	2.57	0.52
1:A:91:TYR:CE1	1:A:95:LYS:HD2	2.45	0.52
1:A:431:MET:CE	1:A:482:VAL:HG13	2.40	0.52
2:B:52:ILE:HG22	2:B:53:PRO:N	2.25	0.52
3:C:301:LEU:HD13	3:C:308:VAL:CG1	2.39	0.52
1:A:27:ILE:HG22	1:A:74:HIS:CE1	2.45	0.51
2:B:255:LEU:C	2:B:257:PRO:HD2	2.30	0.51
4:D:183:CYS:SG	16:D:1264:SF4:S3	3.00	0.51
4:D:219:ILE:HD12	4:D:219:ILE:N	2.25	0.51
11:N:3:ILE:HG22	11:N:52:HIS:CD2	2.44	0.51
1:A:12:GLY:HA3	1:A:201:THR:HG22	1.92	0.51
1:A:349:VAL:HG21	1:A:409:ARG:NH2	2.24	0.51
2:B:454:GLY:HA3	2:B:580:ARG:HD3	1.93	0.51
3:C:322:ARG:O	3:C:323:THR:CB	2.58	0.51
4:D:134:GLY:N	11:N:60:ILE:HD11	2.25	0.51
4:D:180:ALA:HA	4:D:188:PHE:HB2	1.92	0.51
7:G:78:VAL:HG12	7:G:79:THR:OG1	2.10	0.51
2:B:688:GLN:HG3	11:N:64:ARG:HG2	1.91	0.51
3:C:67:GLY:HA3	3:C:385:MET:HE2	1.93	0.51
3:C:176:ASP:HB3	3:C:177:LYS:HG3	1.93	0.51
5:E:100:ASN:ND2	6:F:36:ARG:HH11	2.08	0.51
6:F:6:ILE:N	6:F:6:ILE:HD12	2.25	0.51
7:G:96:ILE:HD12	7:G:99:PHE:HB2	1.93	0.51
1:A:509:LEU:O	1:A:548:GLY:HA3	2.11	0.51
2:B:406:TRP:CA	2:B:407:VAL:CB	2.89	0.51
2:B:730:ILE:HG23	2:B:986:ILE:HD12	1.92	0.51
3:C:24:LEU:HB3	3:C:25:PRO:HD2	1.91	0.51
7:G:96:ILE:CD1	7:G:99:PHE:HB2	2.40	0.51
7:G:99:PHE:O	7:G:99:PHE:CD2	2.64	0.51
1:A:7:LYS:HB2	2:B:1119:GLU:HB2	1.92	0.51
1:A:860:SER:HB2	1:A:864:LYS:O	2.10	0.51
2:B:72:ARG:NH1	2:B:74:ARG:CG	2.74	0.51
3:C:245:LYS:HE2	3:C:250:ILE:HD11	1.92	0.51
5:E:121:ASP:C	5:E:125:GLY:HA2	2.30	0.51
5:E:126:ILE:HD11	5:E:128:PHE:CD1	2.46	0.51
6:F:52:ALA:O	6:F:55:VAL:HG12	2.11	0.51
13:Q:54:LEU:HA	13:Q:59:ILE:CG2	2.40	0.51
1:A:160:LYS:HD3	1:A:165:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ILE:HD13	2:B:136:TYR:CE2	2.45	0.51
2:B:636:LEU:HD21	2:B:643:LEU:HD12	1.92	0.51
2:B:786:TYR:CE1	2:B:792:TYR:CE1	2.99	0.51
2:B:833:GLN:CA	2:B:834:ALA:CB	2.89	0.51
9:K:91:SER:O	9:K:92:LEU:HB2	2.11	0.51
1:A:372:TRP:O	1:A:374:GLY:N	2.44	0.51
3:C:119:THR:HG22	3:C:121:MET:HE2	1.92	0.51
3:C:274:THR:HG22	3:C:276:ASN:H	1.75	0.51
4:D:37:PRO:HG3	4:D:78:TRP:CZ3	2.45	0.51
6:F:95:TYR:CE1	6:F:97:SER:HB2	2.46	0.51
7:G:34:ASN:O	7:G:35:ASP:HB2	2.10	0.51
1:A:284:LEU:HD22	1:A:285:PRO:HD3	1.92	0.51
2:B:647:SER:N	2:B:648:PRO:CD	2.73	0.51
2:B:734:GLY:N	2:B:735:TYR:HB2	2.26	0.51
3:C:235:LYS:HE2	3:C:261:VAL:HA	1.92	0.51
8:H:63:ILE:HD13	8:H:81:VAL:CG2	2.41	0.51
1:A:6:ILE:HD12	3:C:375:ILE:HD11	1.93	0.51
1:A:237:HIS:O	1:A:240:VAL:HB	2.11	0.51
2:B:208:LEU:HD11	2:B:214:HIS:CD2	2.46	0.51
2:B:743:MET:HE1	2:B:875:PRO:HB2	1.92	0.51
2:B:775:LYS:HG3	2:B:777:VAL:HG23	1.93	0.51
2:B:1086:GLY:O	2:B:1087:ASP:HB2	2.11	0.51
3:C:143:LYS:O	3:C:234:ILE:HB	2.10	0.51
4:D:250:ILE:O	4:D:253:ILE:HG22	2.09	0.51
1:A:111:ILE:HG22	1:A:112:GLU:N	2.26	0.51
1:A:302:LEU:HD23	1:A:308:ARG:HG3	1.92	0.51
2:B:583:ILE:HD13	2:B:616:ILE:HG12	1.93	0.51
2:B:726:ILE:CD1	11:N:47:ARG:NH1	2.73	0.51
2:B:1112:ILE:O	2:B:1114:PRO:HD3	2.11	0.51
3:C:192:LYS:CA	3:C:193:LEU:HB2	2.40	0.51
1:A:105:LYS:HG3	1:A:107:SER:O	2.11	0.50
1:A:122:LYS:O	1:A:122:LYS:HG2	2.11	0.50
1:A:334:ILE:CG2	1:A:482:VAL:CG1	2.88	0.50
1:A:336:GLU:OE2	1:A:436:ARG:HD2	2.11	0.50
2:B:52:ILE:HG22	2:B:53:PRO:CD	2.41	0.50
2:B:88:ALA:HA	2:B:93:LEU:HB2	1.92	0.50
2:B:136:TYR:HB2	2:B:141:LEU:CD1	2.41	0.50
2:B:1051:ARG:NE	2:B:1051:ARG:HA	2.26	0.50
2:B:1080:TYR:HB3	2:B:1091:LEU:HD12	1.93	0.50
5:E:30:LEU:HD22	5:E:72:PHE:CE2	2.46	0.50
7:G:93:ILE:HG22	7:G:94:THR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ALA:HB1	1:A:542:PRO:HD3	1.93	0.50
1:A:765:THR:HG22	1:A:766:LEU:HD22	1.91	0.50
3:C:152:VAL:HG23	3:C:174:LEU:HG	1.94	0.50
3:C:214:ASP:HB2	3:C:215:SER:HA	1.92	0.50
2:B:247:LEU:HD11	2:B:503:VAL:HG12	1.93	0.50
2:B:399:HIS:O	2:B:403:THR:HG22	2.12	0.50
3:C:237:ILE:HG12	3:C:238:LYS:N	2.25	0.50
1:A:98:CYS:HB2	1:A:104:VAL:H	1.75	0.50
2:B:52:ILE:CG2	2:B:53:PRO:HD3	2.41	0.50
2:B:733:THR:HG23	2:B:734:GLY:N	2.24	0.50
2:B:768:TYR:HB3	2:B:769:PRO:HD2	1.94	0.50
3:C:158:ILE:HD11	3:C:223:ARG:NH2	2.27	0.50
7:G:10:ILE:CD1	7:G:58:PHE:CD2	2.94	0.50
1:A:231:ALA:CB	2:B:821:ARG:NH2	2.75	0.50
3:C:209:SER:O	3:C:210:PHE:HB2	2.10	0.50
7:G:96:ILE:HG22	7:G:97:SER:N	2.27	0.50
13:Q:70:ASP:O	13:Q:73:LYS:HG2	2.12	0.50
1:A:49:LEU:HB2	1:A:217:ILE:HG13	1.94	0.50
1:A:599:ASP:HB2	1:A:731:THR:O	2.12	0.50
2:B:72:ARG:HB3	2:B:82:GLU:HA	1.94	0.50
2:B:323:SER:HA	2:B:326:ILE:CG1	2.42	0.50
2:B:680:LEU:HD22	2:B:696:HIS:CB	2.40	0.50
2:B:720:PRO:HD2	11:N:53:ILE:CD1	2.42	0.50
2:B:1066:GLN:HG3	2:B:1085:HIS:CE1	2.47	0.50
6:F:69:ARG:NH1	6:F:69:ARG:HG2	2.26	0.50
1:A:77:LEU:N	1:A:77:LEU:CD2	2.75	0.50
1:A:106:ILE:HG12	1:A:154:PHE:CZ	2.46	0.50
1:A:440:GLY:HA3	1:A:444:ARG:NH2	2.27	0.50
1:A:792:PRO:HA	2:B:948:PHE:CZ	2.47	0.50
2:B:10:ILE:HA	2:B:13:ARG:HD3	1.92	0.50
2:B:221:PRO:HB2	2:B:222:GLY:CA	2.27	0.50
3:C:151:ASN:O	3:C:173:MET:HG2	2.12	0.50
4:D:183:CYS:SG	16:D:1264:SF4:S1	3.09	0.50
7:G:112:PHE:HB3	7:G:114:LYS:HE2	1.92	0.50
1:A:77:LEU:N	1:A:77:LEU:HD23	2.27	0.50
1:A:231:ALA:HB2	2:B:821:ARG:NH2	2.26	0.50
2:B:500:VAL:O	2:B:504:ILE:HG12	2.12	0.50
2:B:545:GLU:HG3	2:B:546:ARG:N	2.26	0.50
2:B:596:ASP:HA	2:B:599:LYS:HG2	1.92	0.50
2:B:856:THR:HG23	2:B:857:GLU:N	2.27	0.50
1:A:70:GLY:O	1:A:71:HIS:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HG22	1:A:208:ILE:HD11	1.94	0.50
1:A:362:ARG:O	1:A:365:VAL:HG12	2.12	0.50
1:A:372:TRP:CZ2	1:A:437:VAL:HB	2.47	0.50
1:A:541:ALA:CB	7:G:72:CYS:N	2.75	0.50
2:B:54:THR:OG1	2:B:55:GLU:N	2.45	0.50
2:B:605:ILE:HG22	2:B:609:ASP:HB2	1.93	0.50
2:B:877:ILE:HD12	2:B:877:ILE:H	1.76	0.50
2:B:900:MET:SD	2:B:912:ILE:HD11	2.52	0.50
3:C:170:ASP:O	3:C:174:LEU:HD12	2.12	0.50
8:H:69:SER:HB2	8:H:75:VAL:HG23	1.93	0.50
9:K:93:ARG:O	9:K:94:LYS:HB2	2.12	0.50
11:N:6:ARG:HD3	11:N:11:GLY:O	2.12	0.50
1:A:541:ALA:HB2	7:G:72:CYS:HB2	1.94	0.49
2:B:352:LEU:HD12	2:B:406:TRP:NE1	2.27	0.49
2:B:855:ILE:HD12	2:B:855:ILE:N	2.27	0.49
10:L:15:LEU:HB3	10:L:55:VAL:CG2	2.41	0.49
1:A:618:GLU:OE2	1:A:874:ARG:HD3	2.11	0.49
2:B:17:ILE:O	2:B:20:TYR:HB3	2.12	0.49
2:B:453:TRP:CE2	2:B:650:ILE:CD1	2.95	0.49
3:C:211:ALA:CA	3:C:212:ASN:CB	2.88	0.49
3:C:306:LEU:HD13	3:C:306:LEU:H	1.77	0.49
2:B:284:LYS:O	2:B:285:ARG:C	2.51	0.49
1:A:509:LEU:HA	1:A:638:PHE:CE2	2.46	0.49
2:B:136:TYR:HB2	2:B:141:LEU:HD11	1.94	0.49
2:B:221:PRO:CB	2:B:222:GLY:HA2	2.26	0.49
1:A:228:GLY:C	1:A:229:ILE:HG23	2.33	0.49
1:A:742:GLN:HG2	1:A:747:LEU:HA	1.94	0.49
4:D:41:ILE:HB	4:D:63:ALA:HA	1.94	0.49
5:E:13:ILE:CD1	5:E:22:LEU:HG	2.42	0.49
7:G:100:GLY:O	7:G:104:LYS:HB2	2.12	0.49
2:B:20:TYR:HB2	2:B:607:PHE:CE2	2.48	0.49
2:B:201:VAL:HG23	2:B:218:PRO:HG2	1.94	0.49
6:F:69:ARG:HG2	6:F:69:ARG:HH11	1.78	0.49
2:B:235:ILE:HG22	2:B:241:ILE:HG13	1.95	0.49
4:D:133:LEU:HD21	4:D:139:ILE:HG12	1.94	0.49
7:G:77:ILE:CD1	7:G:106:ILE:HG21	2.43	0.49
1:A:27:ILE:CG2	1:A:74:HIS:CE1	2.95	0.49
1:A:618:GLU:CD	1:A:874:ARG:HD3	2.33	0.49
2:B:403:THR:HG23	2:B:405:ASN:N	2.28	0.49
2:B:591:LEU:O	2:B:592:VAL:HG12	2.13	0.49
2:B:1053:LEU:HD23	2:B:1053:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:394:LEU:N	3:C:394:LEU:HD22	2.27	0.49
7:G:8:GLU:CB	7:G:60:SER:HB2	2.42	0.49
13:Q:63:GLU:O	13:Q:67:LEU:HD13	2.13	0.49
1:A:328:PRO:HB3	1:A:447:LEU:HD21	1.95	0.49
1:A:349:VAL:HG21	1:A:409:ARG:CZ	2.42	0.49
2:B:666:SER:N	2:B:667:PRO:HD2	2.28	0.49
3:C:85:MET:HE2	3:C:104:LEU:HD12	1.95	0.49
3:C:126:LEU:HB3	3:C:130:TYR:HB2	1.94	0.49
13:Q:35:LYS:O	13:Q:36:LEU:C	2.50	0.49
1:A:83:HIS:CD2	1:A:277:PHE:CE2	3.01	0.49
1:A:105:LYS:NZ	1:A:140:ALA:HB3	2.23	0.49
1:A:228:GLY:O	1:A:229:ILE:HG12	2.13	0.49
1:A:505:GLY:CA	1:A:639:VAL:CG2	2.91	0.49
2:B:682:LEU:HD22	11:N:55:ILE:HD12	1.93	0.49
2:B:1061:ILE:HG23	2:B:1070:ILE:HD13	1.95	0.49
3:C:29:VAL:HG23	3:C:52:PHE:HE1	1.78	0.49
4:D:98:ILE:HB	4:D:141:LEU:HG	1.94	0.49
1:A:145:VAL:O	1:A:147:PRO:HD3	2.12	0.48
1:A:431:MET:HE3	1:A:482:VAL:HA	1.95	0.48
1:A:490:ARG:HG2	3:C:77:SER:HB2	1.94	0.48
1:A:549:LYS:HD2	1:A:593:LEU:HD22	1.93	0.48
1:A:691:THR:HG22	1:A:692:LEU:H	1.78	0.48
2:B:8:LEU:N	2:B:8:LEU:HD22	2.28	0.48
2:B:516:GLU:O	2:B:517:TYR:HB2	2.13	0.48
2:B:1005:HIS:HB3	2:B:1023:ARG:HD3	1.95	0.48
5:E:166:GLN:HB3	5:E:167:PRO:HD2	1.95	0.48
9:K:67:GLU:O	9:K:71:ARG:HG2	2.13	0.48
1:A:823:LEU:HD13	3:C:75:ALA:HA	1.95	0.48
2:B:162:ARG:NH1	2:B:415:GLN:C	2.66	0.48
2:B:242:VAL:HG13	2:B:252:GLN:HG3	1.95	0.48
2:B:633:PRO:HA	2:B:636:LEU:CD2	2.43	0.48
3:C:8:LYS:HD2	3:C:8:LYS:N	2.28	0.48
3:C:211:ALA:HB1	3:C:213:ILE:N	2.28	0.48
3:C:235:LYS:CE	3:C:264:VAL:HG21	2.43	0.48
4:D:79:PRO:HG2	4:D:149:TYR:CD2	2.48	0.48
8:H:18:PRO:HB3	8:H:67:ARG:HB3	1.94	0.48
2:B:53:PRO:CB	2:B:54:THR:CA	2.83	0.48
2:B:406:TRP:HB2	2:B:410:ARG:HG3	1.95	0.48
3:C:188:ILE:HG12	3:C:230:LYS:NZ	2.28	0.48
5:E:100:ASN:ND2	6:F:36:ARG:NH1	2.61	0.48
2:B:1064:CYS:CB	2:B:1067:CYS:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:GLU:C	3:C:237:ILE:HD11	2.33	0.48
3:C:209:SER:O	3:C:210:PHE:CB	2.61	0.48
6:F:11:TYR:HB3	6:F:70:ALA:HB1	1.94	0.48
6:F:102:LYS:O	6:F:106:ILE:HG13	2.13	0.48
1:A:277:PHE:CZ	2:B:1111:ILE:CD1	2.96	0.48
2:B:217:PHE:HZ	2:B:300:PHE:CA	2.26	0.48
2:B:478:GLN:HG2	2:B:479:ILE:N	2.27	0.48
2:B:1044:THR:HG23	2:B:1044:THR:O	2.13	0.48
3:C:211:ALA:HA	3:C:212:ASN:CB	2.42	0.48
5:E:147:ILE:HD11	5:E:163:THR:HG21	1.94	0.48
8:H:59:PRO:HB3	13:Q:44:LEU:HD21	1.95	0.48
1:A:58:CYS:HB3	1:A:62:GLY:H	1.78	0.48
1:A:105:LYS:CE	1:A:136:VAL:HG12	2.43	0.48
1:A:196:GLY:O	3:C:360:ARG:HD3	2.13	0.48
1:A:667:ARG:O	1:A:670:VAL:HG22	2.14	0.48
2:B:217:PHE:CB	2:B:221:PRO:O	2.62	0.48
3:C:129:GLU:HG3	3:C:130:TYR:H	1.79	0.48
6:F:76:CYS:HB2	6:F:104:ILE:CG2	2.42	0.48
1:A:105:LYS:NZ	1:A:195:LEU:HD21	2.29	0.48
2:B:101:LEU:HD12	2:B:103:MET:CE	2.44	0.48
2:B:187:THR:HG22	2:B:188:HIS:ND1	2.29	0.48
2:B:359:VAL:HG11	2:B:407:VAL:HG13	1.94	0.48
2:B:461:THR:CG2	2:B:468:GLY:H	2.26	0.48
3:C:36:ILE:HG23	3:C:43:VAL:HG11	1.95	0.48
3:C:165:ILE:HD13	3:C:223:ARG:HB2	1.95	0.48
7:G:64:LEU:HD23	7:G:64:LEU:N	2.28	0.48
10:L:3:ILE:N	10:L:3:ILE:HD12	2.29	0.48
1:A:40:ILE:CG2	1:A:41:GLU:N	2.76	0.48
2:B:784:ARG:HG2	2:B:835:LYS:O	2.14	0.48
4:D:260:LEU:HD11	10:L:69:LEU:HD23	1.95	0.48
5:E:134:LYS:CE	5:E:171:LYS:HB3	2.43	0.48
7:G:95:ILE:C	7:G:96:ILE:HG13	2.33	0.48
7:G:101:LEU:HD13	7:G:102:LEU:H	1.79	0.48
13:Q:35:LYS:O	13:Q:37:SER:N	2.47	0.48
1:A:687:ILE:CG1	1:A:688:PRO:HD2	2.43	0.48
1:A:856:PHE:HB2	3:C:64:ILE:HA	1.95	0.48
2:B:256:PHE:N	2:B:257:PRO:CD	2.77	0.48
3:C:127:THR:H	3:C:268:ASP:HB2	1.78	0.48
5:E:117:THR:HG23	5:E:131:LYS:NZ	2.29	0.48
12:P:33:ILE:HD12	12:P:33:ILE:N	2.29	0.48
1:A:104:VAL:HA	1:A:191:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:CYS:SG	2:B:460:GLU:HB2	2.53	0.48
5:E:126:ILE:HG12	5:E:128:PHE:CE2	2.49	0.48
6:F:11:TYR:HB3	6:F:70:ALA:CB	2.44	0.48
7:G:63:ARG:C	7:G:64:LEU:HD23	2.34	0.48
1:A:30:PRO:O	1:A:243:VAL:HG11	2.14	0.47
1:A:349:VAL:CG2	1:A:409:ARG:CZ	2.91	0.47
1:A:684:LEU:O	1:A:685:GLU:C	2.53	0.47
2:B:767:LYS:HE2	2:B:862:ASN:OD1	2.14	0.47
3:C:365:GLU:O	3:C:366:PHE:HB2	2.14	0.47
4:D:12:ARG:HA	4:D:231:GLU:HA	1.96	0.47
5:E:42:LEU:HD12	5:E:42:LEU:N	2.28	0.47
7:G:61:LYS:O	7:G:62:ASN:HB2	2.14	0.47
1:A:417:VAL:HG11	1:A:464:LEU:CD2	2.44	0.47
2:B:461:THR:HG22	2:B:462:PRO:HD2	1.96	0.47
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.96	0.47
3:C:386:VAL:HG11	9:K:34:ARG:HB2	1.96	0.47
6:F:88:ILE:O	6:F:90:ASP:N	2.47	0.47
7:G:8:GLU:HB2	7:G:60:SER:HB2	1.96	0.47
11:N:64:ARG:HB3	11:N:65:PRO:CD	2.37	0.47
12:P:7:GLY:HA2	12:P:35:PHE:O	2.14	0.47
1:A:91:TYR:CZ	1:A:95:LYS:HD2	2.50	0.47
1:A:541:ALA:CB	7:G:72:CYS:H	2.28	0.47
1:A:864:LYS:CA	1:A:865:THR:CB	2.91	0.47
2:B:584:ILE:HB	2:B:591:LEU:HD12	1.96	0.47
2:B:592:VAL:HG23	2:B:615:LYS:HD3	1.95	0.47
2:B:935:TYR:CD2	2:B:956:LEU:HD22	2.50	0.47
2:B:1096:VAL:CG1	2:B:1097:SER:N	2.77	0.47
2:B:1104:ILE:HG23	2:B:1114:PRO:HG2	1.96	0.47
2:B:1111:ILE:O	2:B:1111:ILE:HG22	2.14	0.47
3:C:144:LEU:HD22	3:C:235:LYS:HE3	1.97	0.47
3:C:235:LYS:CE	3:C:261:VAL:HA	2.44	0.47
8:H:45:ILE:HG13	8:H:79:ARG:HB3	1.96	0.47
10:L:11:ASN:HB3	10:L:59:THR:HG23	1.95	0.47
1:A:416:VAL:HG21	1:A:477:LYS:HB2	1.95	0.47
2:B:39:ARG:HG3	2:B:40:ASN:H	1.79	0.47
2:B:904:VAL:HG23	2:B:972:VAL:HG13	1.95	0.47
9:K:88:ILE:N	9:K:88:ILE:HD12	2.29	0.47
13:Q:56:ASN:N	13:Q:57:GLY:CA	2.73	0.47
2:B:483:ILE:HG13	2:B:555:GLU:HB2	1.96	0.47
2:B:599:LYS:CD	2:B:605:ILE:HG13	2.44	0.47
3:C:139:GLU:O	3:C:142:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:GLN:O	6:F:105:ASP:N	2.47	0.47
7:G:85:SER:O	7:G:92:TYR:N	2.48	0.47
1:A:353:ILE:HD11	1:A:407:VAL:HG23	1.97	0.47
1:A:614:TRP:O	1:A:618:GLU:HG2	2.15	0.47
1:A:793:THR:HG23	2:B:631:LEU:HD11	1.97	0.47
2:B:287:ASN:O	2:B:291:LYS:N	2.48	0.47
2:B:572:ASN:HB3	2:B:577:ARG:HD3	1.95	0.47
3:C:120:PRO:HG2	3:C:255:GLY:HA2	1.97	0.47
4:D:237:LYS:HA	4:D:237:LYS:HE2	1.96	0.47
5:E:8:ARG:HG2	5:E:71:GLU:HG2	1.95	0.47
6:F:14:TYR:CD2	6:F:44:VAL:HG21	2.48	0.47
6:F:64:SER:HB2	6:F:69:ARG:CZ	2.45	0.47
12:P:44:ILE:N	12:P:44:ILE:HD12	2.28	0.47
1:A:113:LYS:O	1:A:117:ILE:HG13	2.14	0.47
1:A:683:GLU:HG3	1:A:683:GLU:O	2.15	0.47
2:B:683:TYR:O	2:B:684:ALA:HB2	2.14	0.47
4:D:172:ILE:HD11	4:D:188:PHE:CE1	2.49	0.47
5:E:100:ASN:HD21	6:F:36:ARG:HH11	1.62	0.47
5:E:134:LYS:HE3	5:E:171:LYS:HB3	1.97	0.47
5:E:134:LYS:HD2	5:E:174:TRP:CG	2.50	0.47
1:A:511:VAL:O	1:A:512:LYS:C	2.53	0.47
2:B:228:ILE:HG23	2:B:271:ALA:HB1	1.97	0.47
2:B:539:LEU:HD11	2:B:543:ILE:HD11	1.97	0.47
2:B:1081:VAL:C	2:B:1091:LEU:HD11	2.35	0.47
5:E:88:GLU:HG2	5:E:89:VAL:N	2.30	0.47
12:P:26:CYS:SG	12:P:29:CYS:HB2	2.54	0.47
1:A:36:ASP:N	1:A:37:GLY:CA	2.69	0.47
1:A:516:LEU:N	1:A:516:LEU:HD12	2.30	0.47
1:A:864:LYS:CA	1:A:865:THR:HB	2.44	0.47
2:B:41:LYS:O	2:B:42:LEU:HB3	2.14	0.47
2:B:220:VAL:O	2:B:221:PRO:C	2.53	0.47
2:B:1061:ILE:HD11	2:B:1101:LYS:HD2	1.97	0.47
3:C:65:ALA:HA	9:K:23:TRP:CZ2	2.50	0.47
3:C:278:ARG:O	3:C:282:GLU:HG3	2.15	0.47
7:G:18:ILE:HG22	7:G:29:ILE:HG23	1.95	0.47
1:A:103:ARG:HB3	1:A:186:LYS:CB	2.46	0.46
1:A:220:ARG:CD	1:A:235:LEU:HB3	2.45	0.46
1:A:517:THR:O	1:A:518:LYS:C	2.54	0.46
2:B:421:ASN:OD1	2:B:421:ASN:C	2.53	0.46
2:B:524:ILE:HD12	2:B:524:ILE:N	2.31	0.46
2:B:592:VAL:CG2	2:B:615:LYS:HD3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:GLN:NE2	3:C:204:ASN:OD1	2.47	0.46
4:D:73:LEU:HD11	4:D:236:LEU:CD2	2.45	0.46
4:D:159:VAL:HG21	4:D:230:LEU:HD22	1.97	0.46
1:A:35:GLU:O	1:A:39:PRO:HD2	2.15	0.46
1:A:106:ILE:HD11	1:A:154:PHE:CE1	2.50	0.46
1:A:106:ILE:HG22	1:A:143:ALA:HB3	1.96	0.46
1:A:492:GLY:HA3	1:A:862:HIS:HA	1.96	0.46
2:B:874:ILE:HG23	2:B:875:PRO:HD2	1.97	0.46
5:E:172:LEU:HD23	5:E:173:GLU:N	2.30	0.46
6:F:78:ILE:HG23	6:F:104:ILE:CG2	2.42	0.46
1:A:146:CYS:HB3	1:A:149:CYS:HB2	1.64	0.46
2:B:406:TRP:HA	2:B:407:VAL:CG2	2.45	0.46
2:B:646:TRP:CE2	2:B:648:PRO:HG2	2.51	0.46
2:B:726:ILE:HD12	11:N:47:ARG:NH1	2.30	0.46
2:B:1096:VAL:HG12	2:B:1097:SER:N	2.30	0.46
3:C:164:SER:HB3	3:C:208:ILE:HA	1.98	0.46
4:D:236:LEU:HD12	4:D:236:LEU:N	2.31	0.46
6:F:62:ILE:O	6:F:63:ILE:CB	2.62	0.46
13:Q:38:ILE:HD12	13:Q:38:ILE:H	1.80	0.46
1:A:22:MET:HA	2:B:1084:ILE:HD12	1.98	0.46
1:A:539:ILE:HG21	7:G:46:ILE:HD11	1.98	0.46
6:F:76:CYS:N	6:F:77:PRO:HD3	2.30	0.46
7:G:100:GLY:O	7:G:104:LYS:CB	2.64	0.46
1:A:418:LEU:HD23	1:A:430:MET:CE	2.46	0.46
1:A:541:ALA:O	1:A:542:PRO:C	2.54	0.46
1:A:856:PHE:CD2	1:A:858:MET:HB3	2.50	0.46
3:C:331:ARG:O	3:C:336:GLY:HA3	2.14	0.46
4:D:141:LEU:HD12	4:D:141:LEU:C	2.36	0.46
5:E:1:MET:HE3	5:E:85:VAL:CG2	2.42	0.46
5:E:60:VAL:HG22	5:E:61:PHE:N	2.30	0.46
1:A:10:LYS:HB2	2:B:1115:ARG:HB2	1.96	0.46
1:A:492:GLY:CA	1:A:862:HIS:HA	2.45	0.46
1:A:592:ILE:O	1:A:594:LEU:HD22	2.16	0.46
1:A:877:GLY:O	1:A:878:TRP:CD1	2.69	0.46
2:B:251:ILE:CG2	2:B:326:ILE:HD12	2.45	0.46
2:B:586:SER:O	2:B:587:ASN:HB2	2.15	0.46
2:B:606:THR:HG22	2:B:609:ASP:OD2	2.16	0.46
3:C:176:ASP:CB	3:C:177:LYS:CB	2.94	0.46
4:D:93:TYR:CE1	4:D:146:ARG:HG2	2.50	0.46
9:K:93:ARG:O	9:K:94:LYS:CB	2.64	0.46
11:N:2:MET:HG2	11:N:56:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:OG1	1:A:30:PRO:CD	2.63	0.46
1:A:229:ILE:O	1:A:230:ARG:HB2	2.14	0.46
1:A:393:ASP:O	1:A:394:ARG:CB	2.63	0.46
2:B:147:ASP:OD1	2:B:150:ASP:HB2	2.16	0.46
2:B:235:ILE:HG23	2:B:240:ASP:HB3	1.98	0.46
2:B:323:SER:HA	2:B:326:ILE:CD1	2.46	0.46
2:B:420:THR:O	2:B:421:ASN:CG	2.53	0.46
3:C:168:GLN:CD	3:C:204:ASN:OD1	2.53	0.46
4:D:17:PHE:O	4:D:225:LYS:HA	2.16	0.46
1:A:370:ASP:O	1:A:371:LYS:CB	2.64	0.46
2:B:931:ILE:HG12	2:B:969:ALA:HB2	1.98	0.46
2:B:1040:ILE:HG22	3:C:72:ILE:HG13	1.98	0.46
3:C:152:VAL:CG2	3:C:174:LEU:HG	2.45	0.46
4:D:115:LYS:O	4:D:116:SER:HB2	2.16	0.46
5:E:132:SER:O	5:E:133:LYS:HG2	2.15	0.46
6:F:78:ILE:HD13	6:F:78:ILE:N	2.31	0.46
8:H:20:HIS:CE1	8:H:51:VAL:HG11	2.51	0.46
1:A:512:LYS:HE3	1:A:583:ASP:HB2	1.97	0.46
1:A:541:ALA:HB3	1:A:542:PRO:HD2	1.94	0.46
3:C:277:ILE:HG22	3:C:278:ARG:N	2.31	0.46
11:N:3:ILE:HG23	11:N:52:HIS:NE2	2.31	0.46
12:P:8:LYS:HA	12:P:14:THR:O	2.16	0.46
1:A:109:ASP:N	1:A:109:ASP:OD1	2.49	0.46
1:A:162:TYR:O	1:A:162:TYR:CD1	2.69	0.46
1:A:866:VAL:HB	3:C:28:ILE:HD13	1.98	0.46
2:B:68:ILE:HD12	2:B:68:ILE:N	2.31	0.46
2:B:691:THR:HG23	2:B:691:THR:O	2.15	0.46
2:B:741:ILE:HG23	2:B:911:VAL:HG13	1.98	0.46
6:F:88:ILE:C	6:F:90:ASP:N	2.69	0.46
1:A:61:CYS:HB2	1:A:68:CYS:SG	2.55	0.45
1:A:452:PRO:HA	1:A:495:ILE:HD13	1.98	0.45
1:A:665:ILE:O	1:A:668:ALA:HB3	2.17	0.45
2:B:341:TYR:CE1	2:B:452:GLN:HG2	2.51	0.45
2:B:520:TRP:N	2:B:520:TRP:CD1	2.84	0.45
3:C:113:ALA:O	3:C:114:LYS:HB3	2.16	0.45
4:D:82:CYS:O	4:D:83:ILE:HG13	2.15	0.45
8:H:45:ILE:HG13	8:H:79:ARG:CB	2.46	0.45
1:A:97:THR:O	1:A:106:ILE:HD11	2.17	0.45
1:A:127:SER:O	1:A:131:ARG:HG3	2.16	0.45
1:A:259:GLN:HA	1:A:262:ILE:HG22	1.97	0.45
1:A:440:GLY:HA3	1:A:444:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:TRP:CZ2	2:B:709:ARG:HD2	2.51	0.45
3:C:348:GLU:O	3:C:349:VAL:CB	2.65	0.45
5:E:49:LEU:HD12	5:E:49:LEU:N	2.31	0.45
7:G:101:LEU:HD22	7:G:101:LEU:C	2.36	0.45
9:K:59:THR:CG2	9:K:63:SER:HB3	2.46	0.45
1:A:145:VAL:HG13	1:A:151:GLU:HG2	1.97	0.45
1:A:505:GLY:HA3	1:A:639:VAL:HG23	1.97	0.45
1:A:747:LEU:HD21	1:A:786:PHE:CD2	2.51	0.45
2:B:12:GLU:HB3	2:B:597:ILE:HG12	1.99	0.45
2:B:448:LEU:C	2:B:448:LEU:HD23	2.37	0.45
2:B:680:LEU:HD22	2:B:696:HIS:CG	2.51	0.45
2:B:774:ASP:O	2:B:775:LYS:HB3	2.17	0.45
3:C:184:VAL:O	3:C:188:ILE:HG13	2.17	0.45
3:C:333:GLY:O	3:C:337:GLU:HG2	2.16	0.45
6:F:106:ILE:O	6:F:107:ILE:C	2.54	0.45
1:A:38:THR:H	1:A:39:PRO:HD2	1.81	0.45
1:A:95:LYS:HE2	1:A:141:MET:HE2	1.98	0.45
1:A:568:VAL:HG13	1:A:730:ARG:NH1	2.32	0.45
1:A:662:TYR:O	1:A:665:ILE:HG12	2.16	0.45
2:B:694:ARG:HA	2:B:758:PHE:O	2.15	0.45
2:B:733:THR:CG2	2:B:735:TYR:HB2	2.44	0.45
2:B:781:PRO:HA	2:B:786:TYR:CZ	2.52	0.45
3:C:237:ILE:C	3:C:237:ILE:HD13	2.37	0.45
3:C:244:LYS:HB3	3:C:249:TYR:HD1	1.82	0.45
3:C:253:THR:HG22	3:C:254:ASP:N	2.31	0.45
8:H:23:LEU:HD21	8:H:64:ARG:HD2	1.98	0.45
8:H:38:ARG:HB3	8:H:39:PRO:HD2	1.98	0.45
1:A:112:GLU:O	1:A:116:ARG:HD3	2.16	0.45
1:A:648:LEU:HD21	1:A:787:ARG:NE	2.32	0.45
2:B:406:TRP:CG	2:B:407:VAL:HB	2.52	0.45
2:B:543:ILE:HD12	2:B:558:VAL:HG21	1.99	0.45
3:C:262:LEU:HD11	3:C:283:VAL:HG11	1.99	0.45
13:Q:42:GLU:O	13:Q:45:MET:HB3	2.17	0.45
13:Q:81:ARG:HA	13:Q:81:ARG:HD3	1.85	0.45
1:A:27:ILE:HG22	1:A:74:HIS:NE2	2.32	0.45
3:C:16:LYS:HE2	3:C:49:ASP:HA	1.99	0.45
3:C:219:LEU:HA	3:C:222:LEU:HD23	1.99	0.45
3:C:363:VAL:HG12	3:C:364:GLU:N	2.32	0.45
6:F:13:PRO:HG2	6:F:16:VAL:HG12	1.99	0.45
7:G:39:SER:HB3	7:G:93:ILE:HB	1.99	0.45
7:G:95:ILE:HD12	7:G:95:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:19:GLN:HB3	11:N:20:PRO:CD	2.47	0.45
1:A:47:PRO:O	1:A:59:PRO:HD2	2.16	0.45
1:A:84:VAL:CG1	1:A:274:ALA:HB1	2.47	0.45
1:A:263:GLU:O	1:A:266:TRP:HB3	2.16	0.45
2:B:166:THR:CG2	2:B:431:ARG:O	2.65	0.45
2:B:591:LEU:O	2:B:592:VAL:CB	2.64	0.45
3:C:67:GLY:CA	3:C:385:MET:HE2	2.46	0.45
3:C:107:LEU:O	3:C:110:ILE:HG22	2.17	0.45
3:C:117:PRO:HG2	3:C:120:PRO:HB3	1.98	0.45
3:C:165:ILE:HG22	3:C:167:LEU:CD1	2.46	0.45
5:E:166:GLN:HB2	5:E:169:LEU:HD12	1.98	0.45
10:L:3:ILE:CG2	10:L:15:LEU:HD11	2.47	0.45
12:P:10:TRP:HB2	12:P:31:TYR:CE2	2.51	0.45
1:A:44:VAL:HG13	1:A:45:MET:N	2.31	0.45
1:A:117:ILE:O	1:A:120:ALA:HB3	2.16	0.45
1:A:417:VAL:O	1:A:432:ALA:HA	2.16	0.45
1:A:547:THR:HG21	7:G:88:ASN:CB	2.46	0.45
1:A:636:ILE:O	1:A:640:GLU:HG3	2.17	0.45
1:A:827:LEU:O	3:C:71:GLY:HA3	2.17	0.45
2:B:938:LEU:HD23	11:N:43:TYR:HB3	1.97	0.45
3:C:41:VAL:O	3:C:41:VAL:HG22	2.17	0.45
5:E:2:TYR:HB2	6:F:12:ILE:HB	1.97	0.45
12:P:17:GLN:CG	12:P:18:LEU:H	2.25	0.45
1:A:97:THR:HA	1:A:103:ARG:CZ	2.47	0.45
1:A:767:PRO:HG2	1:A:768:HIS:CE1	2.52	0.45
2:B:35:ASN:O	2:B:38:VAL:HG12	2.17	0.45
2:B:243:TYR:O	2:B:504:ILE:HD12	2.17	0.45
2:B:259:LEU:O	2:B:263:SER:HB3	2.16	0.45
2:B:322:ILE:O	2:B:326:ILE:HG12	2.16	0.45
2:B:742:ILE:HB	2:B:912:ILE:HB	1.99	0.45
2:B:908:VAL:O	11:N:9:THR:HG23	2.17	0.45
2:B:974:TYR:CZ	2:B:981:LYS:HB3	2.52	0.45
6:F:13:PRO:CA	6:F:74:SER:HB3	2.47	0.45
7:G:58:PHE:HB2	7:G:114:LYS:HB2	1.98	0.45
10:L:32:LEU:HD13	10:L:57:ILE:HG12	1.99	0.45
12:P:24:VAL:HG13	12:P:24:VAL:O	2.17	0.45
1:A:81:VAL:HA	1:A:270:GLN:OE1	2.16	0.45
1:A:103:ARG:HG2	1:A:187:VAL:HG13	1.99	0.45
1:A:366:ILE:HD13	1:A:366:ILE:O	2.16	0.45
2:B:89:ARG:HG3	2:B:156:ILE:HD13	1.99	0.45
2:B:217:PHE:O	2:B:221:PRO:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:GLN:O	2:B:283:GLN:HG3	2.17	0.45
3:C:130:TYR:CD2	3:C:136:LYS:HB3	2.51	0.45
5:E:48:ILE:CD1	5:E:74:MET:HG2	2.47	0.45
5:E:164:MET:SD	5:E:170:GLY:HA2	2.57	0.45
7:G:101:LEU:O	7:G:104:LYS:HB3	2.17	0.45
1:A:160:LYS:O	1:A:162:TYR:N	2.50	0.44
1:A:238:LYS:CE	1:A:275:THR:HB	2.47	0.44
1:A:500:GLN:HB2	2:B:916:HIS:CD2	2.51	0.44
2:B:191:LYS:HE2	2:B:193:ILE:HD11	1.99	0.44
2:B:942:ILE:O	2:B:943:VAL:HB	2.18	0.44
3:C:214:ASP:N	3:C:215:SER:HA	2.31	0.44
4:D:116:SER:CB	4:D:122:VAL:HG12	2.47	0.44
5:E:30:LEU:HD22	5:E:72:PHE:CZ	2.52	0.44
7:G:65:SER:HB2	7:G:66:TYR:HB3	1.99	0.44
7:G:92:TYR:CE2	7:G:113:LEU:CD2	3.00	0.44
1:A:515:LEU:HD23	1:A:545:TYR:CD2	2.52	0.44
1:A:601:LYS:O	1:A:610:SER:HB2	2.16	0.44
1:A:687:ILE:HG22	1:A:695:SER:HB2	1.99	0.44
2:B:63:LEU:HD22	2:B:101:LEU:HD11	1.99	0.44
2:B:195:SER:HB3	2:B:200:ARG:HD3	1.99	0.44
2:B:518:LEU:HG	2:B:520:TRP:HE1	1.83	0.44
2:B:833:GLN:N	2:B:834:ALA:CB	2.71	0.44
2:B:966:LEU:CD2	4:D:184:PRO:HG3	2.47	0.44
3:C:186:LYS:O	3:C:190:ARG:CD	2.65	0.44
3:C:237:ILE:CD1	3:C:237:ILE:H	2.30	0.44
4:D:66:PRO:HG2	4:D:124:ILE:HG12	1.99	0.44
8:H:58:LYS:HE2	13:Q:72:TYR:CZ	2.52	0.44
12:P:37:VAL:HG22	12:P:38:ARG:N	2.32	0.44
1:A:4:LYS:HG3	2:B:1092:PHE:CD2	2.53	0.44
1:A:351:GLU:HB3	1:A:361:LEU:HD21	2.00	0.44
1:A:357:ASN:ND2	1:A:361:LEU:HD22	2.32	0.44
1:A:472:ALA:HB1	2:B:1047:LEU:HD12	1.99	0.44
2:B:35:ASN:HA	2:B:38:VAL:HG12	1.98	0.44
2:B:196:THR:HG22	2:B:302:PRO:C	2.37	0.44
2:B:902:TYR:HE2	2:B:976:GLY:HA2	1.82	0.44
3:C:25:PRO:O	3:C:26:GLN:CB	2.65	0.44
3:C:304:GLN:O	3:C:306:LEU:HD13	2.16	0.44
7:G:55:VAL:HB	7:G:116:HIS:O	2.17	0.44
1:A:212:LEU:C	1:A:212:LEU:HD23	2.38	0.44
2:B:72:ARG:NH2	2:B:121:ASP:OD1	2.50	0.44
2:B:104:ILE:HD13	2:B:114:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ILE:HD13	2:B:110:ILE:N	2.33	0.44
2:B:604:SER:C	2:B:605:ILE:HD13	2.38	0.44
2:B:681:GLY:HA2	2:B:698:LEU:HB3	1.98	0.44
3:C:76:GLN:O	3:C:80:GLU:N	2.51	0.44
3:C:104:LEU:C	3:C:104:LEU:HD23	2.37	0.44
4:D:145:LEU:N	4:D:145:LEU:HD12	2.32	0.44
5:E:126:ILE:HG22	5:E:137:GLN:HG2	1.98	0.44
11:N:19:GLN:HB3	11:N:20:PRO:HD3	2.00	0.44
1:A:334:ILE:CD1	1:A:628:MET:HB3	2.47	0.44
1:A:728:MET:O	1:A:731:THR:HG22	2.17	0.44
2:B:31:LEU:HD23	2:B:125:MET:SD	2.56	0.44
2:B:72:ARG:HD2	2:B:72:ARG:C	2.38	0.44
2:B:273:ASP:HB2	2:B:289:ILE:HD11	1.99	0.44
2:B:774:ASP:O	2:B:775:LYS:CB	2.65	0.44
2:B:841:VAL:HG12	2:B:842:THR:N	2.32	0.44
2:B:1118:LEU:H	2:B:1118:LEU:HD23	1.83	0.44
4:D:79:PRO:HG3	4:D:148:GLY:HA2	2.00	0.44
1:A:40:ILE:HD13	1:A:47:PRO:HG2	1.97	0.44
1:A:96:ALA:HB1	1:A:105:LYS:HZ3	1.83	0.44
1:A:103:ARG:HB3	1:A:186:LYS:HB2	1.99	0.44
1:A:249:LEU:HD21	1:A:265:LEU:HB2	2.00	0.44
1:A:334:ILE:CG2	1:A:482:VAL:HG11	2.47	0.44
1:A:830:LEU:HD11	3:C:319:VAL:CG2	2.47	0.44
2:B:224:ILE:CD1	2:B:229:LEU:HG	2.48	0.44
2:B:333:ARG:O	2:B:334:GLU:HB3	2.18	0.44
2:B:403:THR:HG23	2:B:405:ASN:H	1.83	0.44
2:B:783:VAL:HB	2:B:784:ARG:HA	1.98	0.44
3:C:149:ILE:HD13	3:C:230:LYS:HB2	1.98	0.44
5:E:126:ILE:CD1	5:E:135:VAL:HG13	2.47	0.44
7:G:58:PHE:HB3	7:G:64:LEU:CD1	2.47	0.44
10:L:12:TYR:CE2	10:L:14:GLU:HG3	2.52	0.44
1:A:281:ILE:CD1	1:A:284:LEU:HD12	2.48	0.44
2:B:1059:THR:HG22	2:B:1060:THR:N	2.33	0.44
5:E:94:ASN:HB3	5:E:120:TYR:CE2	2.52	0.44
5:E:140:ASP:CG	5:E:171:LYS:HE2	2.37	0.44
1:A:79:ARG:CB	1:A:266:TRP:CZ3	3.01	0.44
1:A:856:PHE:CE2	1:A:858:MET:HB3	2.53	0.44
1:A:870:ARG:HA	1:A:870:ARG:HD2	1.85	0.44
2:B:73:VAL:HG11	2:B:93:LEU:HD23	2.00	0.44
6:F:75:ILE:HG22	6:F:77:PRO:HG3	1.99	0.44
1:A:219:ILE:HD11	2:B:1105:GLN:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TRP:CB	1:A:373:PRO:CD	2.96	0.44
1:A:850:TYR:O	1:A:854:GLY:HA2	2.18	0.44
3:C:101:THR:O	3:C:102:LEU:HD13	2.17	0.44
3:C:110:ILE:HD12	3:C:296:GLU:HB3	2.00	0.44
6:F:51:SER:O	6:F:55:VAL:N	2.51	0.44
9:K:68:GLU:HG3	9:K:74:LEU:HD21	2.00	0.44
1:A:33:TYR:O	1:A:41:GLU:HB2	2.18	0.43
1:A:42:GLY:O	1:A:43:SER:HB3	2.18	0.43
1:A:837:THR:HG22	1:A:838:VAL:N	2.32	0.43
1:A:838:VAL:HB	1:A:847:GLN:HB2	1.99	0.43
2:B:56:ILE:CG2	2:B:59:LEU:HB2	2.45	0.43
2:B:348:LEU:HD21	2:B:479:ILE:HD12	2.00	0.43
2:B:654:THR:HG21	2:B:673:SER:O	2.18	0.43
3:C:268:ASP:O	3:C:272:VAL:HG23	2.18	0.43
3:C:286:ILE:HG12	8:H:49:ASP:OD1	2.18	0.43
1:A:180:ILE:CG2	1:A:208:ILE:HD11	2.48	0.43
1:A:769:PHE:CE2	1:A:778:ALA:HA	2.53	0.43
2:B:131:ASP:OD1	2:B:132:PRO:HD2	2.18	0.43
4:D:31:ALA:HB2	4:D:249:ILE:HD11	2.00	0.43
5:E:30:LEU:HD13	5:E:72:PHE:CZ	2.53	0.43
7:G:43:ILE:HG22	7:G:44:ASP:N	2.33	0.43
7:G:64:LEU:HD12	7:G:114:LYS:HG3	2.00	0.43
1:A:9:ILE:HA	2:B:1115:ARG:O	2.19	0.43
1:A:502:TYR:CD1	1:A:632:PHE:HB3	2.54	0.43
1:A:505:GLY:CA	1:A:639:VAL:HG23	2.48	0.43
2:B:91:ARG:HB2	2:B:93:LEU:HD13	1.99	0.43
2:B:251:ILE:HG23	2:B:326:ILE:HD12	2.00	0.43
2:B:957:GLN:HA	2:B:960:ILE:HG12	2.00	0.43
3:C:43:VAL:HA	3:C:47:GLU:OE1	2.19	0.43
5:E:123:VAL:O	5:E:124:ARG:HB2	2.18	0.43
6:F:76:CYS:HB3	6:F:104:ILE:HG23	2.00	0.43
7:G:18:ILE:O	7:G:19:GLU:HG3	2.18	0.43
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.99	0.43
1:A:449:VAL:HG12	1:A:449:VAL:O	2.19	0.43
2:B:209:LYS:O	2:B:210:ASP:HB2	2.17	0.43
2:B:996:LEU:N	2:B:996:LEU:HD12	2.34	0.43
3:C:156:THR:HG22	3:C:157:SER:N	2.33	0.43
3:C:182:ASP:HA	3:C:185:LYS:HB2	1.99	0.43
3:C:351:VAL:HG23	3:C:352:LYS:H	1.82	0.43
1:A:31:ASP:OD2	1:A:240:VAL:HG13	2.18	0.43
1:A:33:TYR:C	1:A:41:GLU:HB2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD11	1:A:628:MET:CB	2.48	0.43
1:A:365:VAL:O	1:A:394:ARG:HD3	2.18	0.43
2:B:592:VAL:HG22	2:B:596:ASP:HB2	2.00	0.43
2:B:646:TRP:NE1	2:B:648:PRO:HB2	2.33	0.43
5:E:167:PRO:O	5:E:168:TYR:HB2	2.19	0.43
7:G:65:SER:HB2	7:G:66:TYR:CB	2.49	0.43
7:G:99:PHE:CE2	7:G:103:VAL:HB	2.53	0.43
10:L:15:LEU:HB3	10:L:55:VAL:HG22	2.00	0.43
1:A:131:ARG:HH22	13:Q:33:PHE:HB2	1.84	0.43
1:A:271:TYR:HE1	1:A:285:PRO:HG2	1.83	0.43
1:A:378:VAL:HG22	1:A:386:ILE:HB	2.01	0.43
1:A:614:TRP:O	1:A:615:LEU:C	2.57	0.43
2:B:809:GLY:O	2:B:842:THR:HB	2.18	0.43
3:C:188:ILE:HA	3:C:230:LYS:HE2	1.99	0.43
5:E:1:MET:HE2	5:E:83:GLU:HG2	2.01	0.43
5:E:30:LEU:CD2	5:E:72:PHE:CE2	3.02	0.43
6:F:84:ARG:HB3	6:F:88:ILE:HD13	2.00	0.43
9:K:68:GLU:HB2	9:K:73:VAL:CG2	2.48	0.43
11:N:5:ILE:HA	11:N:15:ALA:HB2	2.00	0.43
2:B:671:TYR:O	2:B:675:MET:HB2	2.18	0.43
3:C:234:ILE:O	3:C:235:LYS:HB2	2.19	0.43
4:D:48:GLU:HB3	4:D:140:SER:HB3	1.99	0.43
4:D:150:GLY:HA2	4:D:156:PHE:HB2	2.00	0.43
6:F:84:ARG:O	6:F:85:SER:C	2.57	0.43
7:G:96:ILE:HD13	7:G:99:PHE:CD1	2.53	0.43
9:K:53:ILE:O	9:K:54:ASN:C	2.56	0.43
1:A:35:GLU:O	1:A:39:PRO:CD	2.66	0.43
1:A:105:LYS:HE3	1:A:140:ALA:CB	2.49	0.43
2:B:361:PHE:O	2:B:364:PHE:HB3	2.19	0.43
2:B:582:LEU:HD12	2:B:619:LEU:HD12	2.00	0.43
2:B:628:TYR:CD2	2:B:640:HIS:ND1	2.87	0.43
2:B:961:LEU:O	2:B:961:LEU:HD23	2.17	0.43
3:C:235:LYS:HZ3	3:C:261:VAL:HA	1.84	0.43
4:D:257:GLU:HB2	10:L:73:ILE:HG21	2.00	0.43
6:F:60:SER:HA	6:F:69:ARG:NE	2.34	0.43
6:F:84:ARG:O	6:F:86:ILE:N	2.51	0.43
7:G:42:ILE:HG12	7:G:43:ILE:N	2.33	0.43
11:N:3:ILE:HD13	11:N:18:TRP:CB	2.49	0.43
13:Q:56:ASN:H	13:Q:57:GLY:HA2	1.80	0.43
1:A:63:ASN:HB3	1:A:67:ASN:HB2	2.00	0.43
1:A:317:ARG:HA	2:B:1030:ARG:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:SER:HA	1:A:573:ARG:O	2.18	0.43
1:A:734:ARG:HG3	2:B:916:HIS:O	2.19	0.43
1:A:738:LEU:C	1:A:738:LEU:HD12	2.38	0.43
4:D:78:TRP:HB3	4:D:79:PRO:CD	2.48	0.43
2:B:233:LEU:CD1	2:B:315:ALA:HB2	2.48	0.43
2:B:238:ASP:CG	2:B:259:LEU:HD11	2.39	0.43
2:B:543:ILE:HG21	2:B:558:VAL:CG2	2.49	0.43
3:C:364:GLU:OE2	3:C:371:GLU:HG2	2.19	0.43
5:E:169:LEU:C	5:E:175:ILE:HD11	2.39	0.43
5:E:171:LYS:HG3	5:E:172:LEU:N	2.33	0.43
8:H:39:PRO:HB2	8:H:80:TYR:CE1	2.54	0.43
13:Q:57:GLY:O	13:Q:59:ILE:HG22	2.18	0.43
13:Q:72:TYR:CE1	13:Q:76:GLU:HG2	2.54	0.43
1:A:159:GLU:HG2	1:A:160:LYS:O	2.18	0.42
1:A:342:ILE:HD13	1:A:342:ILE:O	2.18	0.42
2:B:226:PHE:CZ	2:B:230:MET:HG3	2.54	0.42
2:B:332:ARG:HB3	2:B:565:PHE:HB3	2.01	0.42
2:B:981:LYS:NZ	4:D:205:LEU:HD13	2.34	0.42
3:C:104:LEU:N	3:C:105:PRO:HD2	2.34	0.42
5:E:10:ILE:N	5:E:10:ILE:HD12	2.34	0.42
8:H:45:ILE:HG12	8:H:79:ARG:CD	2.49	0.42
13:Q:39:GLN:HG2	13:Q:40:ASP:H	1.84	0.42
1:A:95:LYS:HD3	1:A:141:MET:HE3	2.00	0.42
1:A:220:ARG:HD3	1:A:235:LEU:CD2	2.49	0.42
2:B:190:ALA:HB2	2:B:325:VAL:CG2	2.49	0.42
2:B:480:ALA:HB2	2:B:579:ARG:HD3	2.01	0.42
2:B:743:MET:HE1	2:B:891:ILE:HD11	2.00	0.42
2:B:840:ILE:HD12	2:B:840:ILE:N	2.33	0.42
2:B:1033:GLU:O	2:B:1036:ARG:HB3	2.19	0.42
3:C:12:TYR:HB2	3:C:45:ARG:NH2	2.34	0.42
7:G:26:LEU:HD22	7:G:42:ILE:O	2.19	0.42
7:G:61:LYS:O	7:G:62:ASN:CB	2.66	0.42
10:L:5:ILE:O	10:L:5:ILE:HG13	2.19	0.42
10:L:47:HIS:HA	10:L:48:PRO:HD3	1.87	0.42
1:A:107:SER:HA	1:A:108:GLU:CB	2.49	0.42
1:A:310:ARG:HD3	1:A:821:ARG:NH2	2.34	0.42
2:B:961:LEU:HG	2:B:967:PRO:HD3	2.01	0.42
6:F:59:LEU:HB3	6:F:69:ARG:NH1	2.34	0.42
7:G:18:ILE:CG2	7:G:29:ILE:HG12	2.49	0.42
1:A:684:LEU:HD12	1:A:686:PRO:HD3	2.01	0.42
4:D:73:LEU:HD11	4:D:236:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PRO:HB3	9:K:47:ALA:HB2	2.01	0.42
5:E:84:VAL:HG21	6:F:84:ARG:NH1	2.34	0.42
5:E:100:ASN:OD1	6:F:36:ARG:NH1	2.52	0.42
6:F:68:VAL:HA	6:F:71:VAL:HG12	2.02	0.42
13:Q:73:LYS:HG3	13:Q:74:ASP:N	2.35	0.42
1:A:33:TYR:O	1:A:41:GLU:CB	2.67	0.42
1:A:107:SER:HB3	1:A:140:ALA:HA	2.02	0.42
2:B:212:THR:O	2:B:258:SER:HB2	2.20	0.42
2:B:226:PHE:CE1	2:B:230:MET:CG	3.03	0.42
6:F:68:VAL:O	6:F:71:VAL:HG12	2.19	0.42
7:G:10:ILE:C	7:G:11:LEU:HD12	2.39	0.42
7:G:26:LEU:HD23	7:G:43:ILE:HD13	2.01	0.42
1:A:107:SER:CB	1:A:108:GLU:HB2	2.49	0.42
1:A:115:SER:HA	1:A:118:TYR:HD2	1.84	0.42
1:A:127:SER:O	1:A:131:ARG:HD2	2.20	0.42
1:A:868:VAL:HG12	3:C:35:LEU:HD12	2.01	0.42
3:C:144:LEU:HD22	3:C:235:LYS:CE	2.49	0.42
4:D:108:MET:HG3	4:D:110:TYR:CE2	2.55	0.42
5:E:145:ARG:CZ	6:F:86:ILE:CD1	2.98	0.42
10:L:80:ALA:O	10:L:84:ILE:HG12	2.19	0.42
12:P:41:THR:HG22	12:P:42:ILE:N	2.34	0.42
1:A:101:CYS:SG	1:A:152:LYS:HE2	2.59	0.42
1:A:105:LYS:HE3	1:A:140:ALA:HB2	2.01	0.42
1:A:122:LYS:HE2	13:Q:45:MET:HA	2.00	0.42
1:A:219:ILE:O	1:A:219:ILE:HG22	2.19	0.42
1:A:342:ILE:CG2	1:A:343:ILE:N	2.82	0.42
1:A:692:LEU:N	1:A:692:LEU:CD1	2.83	0.42
1:A:712:GLY:HA2	1:A:741:THR:HG23	2.00	0.42
2:B:27:VAL:HG11	2:B:426:LEU:HD22	2.01	0.42
3:C:199:ASP:HB2	3:C:206:LEU:HB3	2.02	0.42
3:C:389:THR:HG23	9:K:77:THR:HB	2.02	0.42
4:D:167:TYR:CD2	4:D:227:ILE:HD11	2.55	0.42
6:F:91:SER:CB	6:F:93:ARG:HG3	2.49	0.42
7:G:43:ILE:O	7:G:46:ILE:HG22	2.19	0.42
7:G:55:VAL:HG12	7:G:117:GLN:HA	2.00	0.42
7:G:94:THR:HG22	7:G:96:ILE:HD11	2.00	0.42
10:L:6:LEU:HD11	10:L:16:GLU:HB2	2.02	0.42
1:A:185:GLU:CA	1:A:205:GLU:HG2	2.49	0.42
1:A:228:GLY:N	2:B:768:TYR:HH	2.17	0.42
1:A:671:GLU:O	1:A:674:ASN:OD1	2.37	0.42
1:A:757:ILE:HD13	1:A:800:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:PHE:HZ	2:B:300:PHE:HB2	1.85	0.42
2:B:330:LEU:HD13	2:B:332:ARG:CZ	2.50	0.42
2:B:650:ILE:HD13	2:B:650:ILE:HA	1.90	0.42
2:B:1020:THR:O	2:B:1027:GLY:HA3	2.20	0.42
6:F:103:ILE:HA	6:F:106:ILE:HD12	2.01	0.42
7:G:79:THR:HB	7:G:80:GLU:CB	2.41	0.42
7:G:99:PHE:O	7:G:99:PHE:CG	2.72	0.42
1:A:102:GLY:O	1:A:103:ARG:C	2.58	0.42
1:A:837:THR:HG23	1:A:847:GLN:O	2.20	0.42
2:B:73:VAL:HG23	2:B:75:GLU:HG3	2.02	0.42
2:B:1107:LEU:HD21	3:C:354:LEU:HD13	2.02	0.42
3:C:144:LEU:O	3:C:237:ILE:CD1	2.68	0.42
3:C:258:LEU:HD22	3:C:280:ILE:HD13	2.02	0.42
3:C:349:VAL:HG12	3:C:352:LYS:HB2	2.01	0.42
6:F:11:TYR:CB	6:F:70:ALA:CB	2.98	0.42
9:K:59:THR:OG1	9:K:63:SER:HB3	2.20	0.42
1:A:162:TYR:OH	1:A:270:GLN:HB3	2.20	0.42
1:A:165:TYR:CE1	1:A:174:LYS:HB2	2.54	0.42
1:A:229:ILE:O	1:A:230:ARG:CB	2.67	0.42
1:A:431:MET:HE2	1:A:482:VAL:HG22	2.02	0.42
2:B:874:ILE:CG2	2:B:875:PRO:HD2	2.50	0.42
2:B:957:GLN:O	2:B:960:ILE:HG12	2.20	0.42
3:C:81:PRO:CB	3:C:306:LEU:HG	2.49	0.42
3:C:211:ALA:CB	3:C:213:ILE:N	2.83	0.42
5:E:1:MET:CE	5:E:85:VAL:HG22	2.48	0.42
5:E:111:SER:HA	5:E:165:ARG:NH2	2.35	0.42
1:A:67:ASN:C	1:A:69:PRO:HD3	2.40	0.41
1:A:146:CYS:HB2	1:A:151:GLU:HA	2.00	0.41
1:A:450:CYS:HB2	1:A:451:PRO:HD3	2.01	0.41
1:A:796:PHE:CZ	2:B:448:LEU:HD21	2.55	0.41
2:B:25:GLY:HA3	2:B:28:ARG:HG2	2.02	0.41
2:B:175:VAL:HA	2:B:192:ILE:HG12	2.02	0.41
2:B:197:ALA:HA	2:B:198:GLY:HA2	1.73	0.41
2:B:579:ARG:HG3	2:B:620:ASP:HB3	2.01	0.41
2:B:592:VAL:HG22	2:B:596:ASP:CG	2.41	0.41
2:B:736:ASN:HA	2:B:740:SER:HB3	2.02	0.41
2:B:903:THR:HG21	2:B:971:GLU:OE1	2.20	0.41
2:B:1005:HIS:HB3	2:B:1023:ARG:CD	2.50	0.41
4:D:41:ILE:HD13	4:D:145:LEU:HG	2.02	0.41
6:F:59:LEU:C	6:F:69:ARG:NH1	2.73	0.41
8:H:13:ILE:HG23	8:H:13:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:68:GLU:O	9:K:73:VAL:HG22	2.20	0.41
12:P:37:VAL:HG22	12:P:38:ARG:H	1.85	0.41
1:A:99:ARG:HB3	1:A:154:PHE:CE1	2.55	0.41
1:A:110:GLU:OE2	1:A:148:HIS:NE2	2.52	0.41
1:A:358:ILE:HG23	1:A:359:GLU:N	2.34	0.41
1:A:767:PRO:HG3	2:B:624:GLU:OE2	2.19	0.41
2:B:72:ARG:HD2	2:B:73:VAL:N	2.35	0.41
2:B:209:LYS:O	2:B:210:ASP:CG	2.58	0.41
2:B:233:LEU:HD13	2:B:233:LEU:O	2.19	0.41
2:B:406:TRP:HA	2:B:407:VAL:HG23	2.02	0.41
2:B:454:GLY:HA3	2:B:580:ARG:CD	2.49	0.41
2:B:457:CYS:HB3	2:B:460:GLU:HB2	2.02	0.41
2:B:485:GLU:O	2:B:486:LYS:C	2.58	0.41
2:B:660:TYR:N	2:B:661:PRO:CD	2.83	0.41
2:B:680:LEU:HG	2:B:995:LYS:O	2.20	0.41
2:B:905:LYS:HG3	2:B:965:TYR:CE2	2.55	0.41
2:B:931:ILE:O	2:B:934:LYS:HB3	2.19	0.41
2:B:996:LEU:N	2:B:996:LEU:CD1	2.83	0.41
2:B:1072:TRP:NE1	2:B:1081:VAL:HG13	2.35	0.41
2:B:1110:MET:O	2:B:1110:MET:HG2	2.20	0.41
3:C:147:THR:O	3:C:232:LYS:HB2	2.20	0.41
3:C:226:ILE:HG23	3:C:230:LYS:NZ	2.34	0.41
5:E:4:LEU:HB2	6:F:12:ILE:HD11	2.03	0.41
5:E:146:VAL:CG1	5:E:149:VAL:HG23	2.50	0.41
6:F:76:CYS:CB	6:F:104:ILE:CG2	2.96	0.41
9:K:64:ILE:O	9:K:68:GLU:HG2	2.21	0.41
13:Q:35:LYS:O	13:Q:36:LEU:HD12	2.20	0.41
1:A:31:ASP:C	1:A:32:VAL:CG2	2.89	0.41
1:A:107:SER:CA	1:A:108:GLU:CB	2.98	0.41
1:A:155:LYS:HG3	1:A:168:ARG:CD	2.50	0.41
1:A:308:ARG:HD3	1:A:308:ARG:HA	1.88	0.41
1:A:708:ARG:CD	1:A:748:GLY:HA3	2.50	0.41
2:B:356:LEU:O	2:B:359:VAL:HG12	2.21	0.41
2:B:537:GLU:HG3	2:B:560:HIS:CE1	2.55	0.41
2:B:903:THR:HG22	2:B:904:VAL:N	2.35	0.41
2:B:1064:CYS:HA	2:B:1091:LEU:HD22	2.02	0.41
3:C:85:MET:SD	3:C:304:GLN:HG3	2.61	0.41
3:C:388:LEU:CD1	9:K:35:VAL:HG12	2.50	0.41
4:D:38:VAL:HG12	4:D:39:MET:N	2.35	0.41
6:F:13:PRO:CB	6:F:74:SER:HB3	2.50	0.41
6:F:104:ILE:HG22	6:F:104:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:ILE:HB	7:G:46:ILE:HG22	2.01	0.41
8:H:28:ALA:CB	8:H:62:ILE:HD11	2.51	0.41
10:L:11:ASN:O	10:L:58:LEU:HD12	2.20	0.41
11:N:2:MET:O	11:N:3:ILE:CG1	2.68	0.41
1:A:600:LYS:CB	1:A:732:GLY:HA3	2.50	0.41
2:B:91:ARG:CB	2:B:93:LEU:HD13	2.50	0.41
2:B:233:LEU:HG	2:B:315:ALA:HB2	2.02	0.41
2:B:306:THR:O	2:B:306:THR:HG22	2.19	0.41
3:C:111:VAL:HG22	3:C:111:VAL:O	2.21	0.41
5:E:6:LYS:O	6:F:7:VAL:HB	2.20	0.41
5:E:133:LYS:O	5:E:133:LYS:HG3	2.20	0.41
7:G:46:ILE:O	7:G:46:ILE:HG12	2.20	0.41
7:G:99:PHE:CD2	7:G:103:VAL:HB	2.56	0.41
13:Q:40:ASP:O	13:Q:43:LEU:N	2.54	0.41
13:Q:59:ILE:HG12	13:Q:60:SER:N	2.35	0.41
1:A:417:VAL:HG11	1:A:464:LEU:HD11	2.03	0.41
1:A:769:PHE:CD2	1:A:778:ALA:HA	2.55	0.41
2:B:287:ASN:HA	2:B:290:GLU:HB2	2.03	0.41
2:B:629:VAL:HG22	2:B:642:HIS:HB2	2.03	0.41
3:C:331:ARG:H	3:C:335:THR:HB	1.85	0.41
1:A:134:GLU:O	1:A:138:LYS:HG2	2.20	0.41
1:A:823:LEU:CD1	3:C:75:ALA:HB1	2.51	0.41
2:B:53:PRO:CG	2:B:54:THR:HB	2.50	0.41
2:B:230:MET:CE	2:B:230:MET:HA	2.51	0.41
2:B:235:ILE:HG23	2:B:240:ASP:CB	2.49	0.41
2:B:298:LYS:HG3	2:B:299:TYR:CD2	2.55	0.41
2:B:1094:VAL:HG12	2:B:1096:VAL:HG23	2.02	0.41
3:C:186:LYS:O	3:C:190:ARG:HG2	2.20	0.41
3:C:391:ARG:HG3	5:E:56:GLU:HG2	2.02	0.41
5:E:102:GLY:O	6:F:36:ARG:HD2	2.20	0.41
6:F:104:ILE:O	6:F:107:ILE:HG13	2.20	0.41
12:P:10:TRP:CB	12:P:31:TYR:CE2	3.03	0.41
1:A:53:GLU:HA	1:A:54:PRO:HD3	1.94	0.41
1:A:63:ASN:HA	2:B:1075:LYS:CD	2.51	0.41
1:A:428:ILE:HG22	1:A:428:ILE:O	2.20	0.41
2:B:17:ILE:HG13	2:B:476:MET:SD	2.61	0.41
2:B:675:MET:HB2	2:B:675:MET:HE3	1.93	0.41
2:B:1112:ILE:HD11	3:C:355:LEU:HD23	2.02	0.41
3:C:104:LEU:HB3	3:C:105:PRO:HD3	2.03	0.41
3:C:164:SER:HB2	3:C:207:ASN:O	2.21	0.41
3:C:247:ASP:OD1	3:C:247:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:ASN:HA	3:C:375:ILE:HG22	2.01	0.41
9:K:51:ILE:HG21	9:K:71:ARG:HH22	1.85	0.41
13:Q:39:GLN:OE1	13:Q:78:ARG:NE	2.54	0.41
1:A:63:ASN:HA	2:B:1075:LYS:HD3	2.03	0.41
1:A:220:ARG:HD3	1:A:235:LEU:CB	2.47	0.41
1:A:728:MET:CE	2:B:919:PRO:HG3	2.50	0.41
2:B:52:ILE:CD1	2:B:368:LEU:HD23	2.51	0.41
2:B:273:ASP:O	2:B:277:SER:N	2.52	0.41
2:B:279:VAL:HG12	2:B:291:LYS:HE2	2.03	0.41
2:B:438:ARG:NH2	2:B:466:ASN:OD1	2.53	0.41
2:B:606:THR:O	2:B:609:ASP:HB2	2.20	0.41
2:B:768:TYR:CE2	2:B:774:ASP:OD1	2.74	0.41
2:B:808:LYS:O	2:B:809:GLY:C	2.59	0.41
3:C:104:LEU:HD23	3:C:104:LEU:O	2.21	0.41
3:C:146:TYR:HB3	3:C:237:ILE:HD11	2.02	0.41
3:C:214:ASP:HB2	3:C:215:SER:CA	2.50	0.41
3:C:369:VAL:HG23	3:C:370:VAL:N	2.36	0.41
6:F:72:LEU:HG	6:F:84:ARG:NH2	2.35	0.41
1:A:326:ILE:HA	1:A:443:PHE:O	2.21	0.41
1:A:421:ARG:HB2	1:A:462:MET:HE3	2.02	0.41
1:A:547:THR:HG21	7:G:88:ASN:O	2.21	0.41
1:A:743:MET:HG3	2:B:922:MET:HG2	2.01	0.41
2:B:10:ILE:HD13	2:B:949:TYR:HB3	2.02	0.41
2:B:442:ASN:HB3	2:B:445:ALA:HB3	2.03	0.41
2:B:647:SER:HB2	2:B:648:PRO:HD3	2.03	0.41
3:C:133:ASP:HB3	3:C:136:LYS:HG2	2.02	0.41
3:C:237:ILE:CD1	3:C:237:ILE:N	2.83	0.41
3:C:341:VAL:HG13	3:C:342:LEU:N	2.36	0.41
3:C:391:ARG:CG	5:E:56:GLU:HG2	2.50	0.41
4:D:197:VAL:CG1	4:D:200:GLU:HB2	2.50	0.41
4:D:254:GLU:OE1	10:L:77:ARG:HD3	2.21	0.41
6:F:62:ILE:O	6:F:62:ILE:HG22	2.20	0.41
7:G:9:ILE:HG22	7:G:11:LEU:HD11	2.02	0.41
7:G:36:PHE:HA	7:G:96:ILE:HG12	2.03	0.41
8:H:63:ILE:HG22	8:H:65:ILE:HD12	2.03	0.41
8:H:65:ILE:HD12	8:H:65:ILE:N	2.36	0.41
9:K:59:THR:OG1	9:K:60:ASP:N	2.54	0.41
1:A:22:MET:HE1	2:B:1108:MET:HE3	2.02	0.41
1:A:145:VAL:HG13	1:A:146:CYS:N	2.36	0.41
1:A:416:VAL:HB	1:A:473:ILE:HG23	2.03	0.41
1:A:495:ILE:O	1:A:605:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LEU:HD22	2:B:154:TYR:CE1	2.56	0.41
2:B:453:TRP:NE1	2:B:650:ILE:HD11	2.35	0.41
2:B:461:THR:HG21	2:B:468:GLY:N	2.36	0.41
2:B:633:PRO:HA	2:B:636:LEU:HD21	2.03	0.41
2:B:977:ARG:HD2	10:L:22:HIS:CE1	2.56	0.41
3:C:125:TYR:CE1	3:C:250:ILE:HD13	2.56	0.41
11:N:3:ILE:O	11:N:3:ILE:HG13	2.21	0.41
11:N:40:VAL:HG12	11:N:41:LYS:N	2.36	0.41
1:A:747:LEU:CD2	1:A:786:PHE:CE2	3.04	0.40
1:A:771:PRO:O	1:A:772:TYR:HB2	2.22	0.40
2:B:226:PHE:CE1	2:B:318:LEU:HD22	2.56	0.40
2:B:599:LYS:HB2	2:B:604:SER:HB2	2.03	0.40
2:B:653:ILE:HG23	2:B:654:THR:N	2.36	0.40
2:B:705:LEU:O	2:B:706:VAL:CG1	2.69	0.40
8:H:28:ALA:HB1	8:H:62:ILE:HD11	2.02	0.40
1:A:284:LEU:CB	1:A:285:PRO:HD2	2.51	0.40
1:A:353:ILE:HD12	1:A:353:ILE:N	2.36	0.40
2:B:17:ILE:HG12	2:B:21:PHE:CE2	2.57	0.40
2:B:161:GLU:OE1	2:B:419:ARG:NH1	2.53	0.40
2:B:220:VAL:O	2:B:222:GLY:N	2.54	0.40
2:B:480:ALA:HB2	2:B:579:ARG:NE	2.36	0.40
2:B:733:THR:HG23	2:B:735:TYR:CB	2.49	0.40
3:C:27:LYS:HD2	3:C:27:LYS:N	2.37	0.40
3:C:277:ILE:O	3:C:278:ARG:CB	2.69	0.40
4:D:56:GLU:CD	4:D:56:GLU:H	2.25	0.40
5:E:14:PRO:HA	5:E:65:ALA:HB2	2.03	0.40
8:H:55:ILE:HG13	8:H:55:ILE:O	2.21	0.40
1:A:253:ILE:HG12	1:A:262:ILE:HD11	2.04	0.40
1:A:362:ARG:HE	1:A:399:SER:HA	1.87	0.40
1:A:586:VAL:HG11	1:A:611:ILE:HD11	2.04	0.40
2:B:733:THR:HG23	2:B:735:TYR:HD2	1.86	0.40
3:C:179:VAL:HG12	3:C:180:THR:O	2.22	0.40
3:C:350:THR:HG22	3:C:351:VAL:N	2.36	0.40
4:D:109:LEU:C	4:D:109:LEU:HD23	2.42	0.40
4:D:159:VAL:HG22	4:D:161:LEU:H	1.86	0.40
5:E:100:ASN:CG	6:F:36:ARG:HH11	2.25	0.40
1:A:108:GLU:O	1:A:109:ASP:HB2	2.21	0.40
1:A:547:THR:HG21	7:G:88:ASN:HB3	2.04	0.40
1:A:731:THR:HG23	1:A:733:ALA:H	1.86	0.40
1:A:823:LEU:C	1:A:823:LEU:HD12	2.42	0.40
2:B:62:ARG:HB2	2:B:104:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ARG:O	2:B:207:ARG:CG	2.70	0.40
2:B:720:PRO:CD	11:N:53:ILE:HD13	2.51	0.40
2:B:1082:CYS:CB	2:B:1083:PRO:HD2	2.51	0.40
3:C:235:LYS:HZ3	3:C:261:VAL:HG13	1.86	0.40
3:C:311:ARG:HA	3:C:314:LEU:HD12	2.02	0.40
4:D:24:PHE:O	4:D:27:ALA:HB3	2.21	0.40
4:D:108:MET:CG	4:D:110:TYR:CE2	3.05	0.40
5:E:125:GLY:O	5:E:126:ILE:HG12	2.21	0.40
5:E:164:MET:HB3	5:E:170:GLY:CA	2.51	0.40
6:F:12:ILE:HG21	6:F:17:ALA:HB2	2.04	0.40
6:F:30:SER:HB2	6:F:34:LEU:HD22	2.04	0.40
7:G:33:CYS:HB2	7:G:36:PHE:O	2.21	0.40
12:P:21:LEU:HA	12:P:22:PRO:HA	1.89	0.40
1:A:170:GLU:O	1:A:170:GLU:HG2	2.21	0.40
1:A:703:THR:O	1:A:707:LEU:HD12	2.22	0.40
2:B:726:ILE:HD12	2:B:726:ILE:N	2.36	0.40
2:B:738:GLU:O	2:B:739:ASP:HB2	2.21	0.40
2:B:857:GLU:HG3	12:P:24:VAL:CG1	2.52	0.40
3:C:17:VAL:HG13	3:C:29:VAL:CG2	2.52	0.40
3:C:122:MET:SD	3:C:261:VAL:HG21	2.62	0.40
6:F:6:ILE:HG22	6:F:7:VAL:N	2.36	0.40
7:G:40:PHE:CE1	7:G:115:ILE:HG13	2.57	0.40
7:G:59:ILE:N	7:G:59:ILE:HD12	2.37	0.40
7:G:96:ILE:HD12	7:G:99:PHE:CB	2.51	0.40
11:N:40:VAL:HG11	11:N:46:ARG:CZ	2.50	0.40
13:Q:46:LYS:O	13:Q:50:ILE:HG13	2.22	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	868/880 (99%)	712 (82%)	124 (14%)	32 (4%)	3	22
2	B	1097/1131 (97%)	928 (85%)	133 (12%)	36 (3%)	4	25
3	C	372/395 (94%)	304 (82%)	49 (13%)	19 (5%)	2	15
4	D	260/265 (98%)	218 (84%)	37 (14%)	5 (2%)	8	39
5	E	167/180 (93%)	150 (90%)	16 (10%)	1 (1%)	25	64
6	F	103/113 (91%)	78 (76%)	17 (16%)	8 (8%)	1	6
7	G	111/132 (84%)	83 (75%)	20 (18%)	8 (7%)	1	7
8	H	74/84 (88%)	63 (85%)	8 (11%)	3 (4%)	3	21
9	K	82/95 (86%)	69 (84%)	9 (11%)	4 (5%)	2	17
10	L	89/92 (97%)	83 (93%)	4 (4%)	2 (2%)	6	35
11	N	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	0	3
12	P	42/48 (88%)	29 (69%)	9 (21%)	4 (10%)	0	3
13	Q	48/104 (46%)	38 (79%)	5 (10%)	5 (10%)	0	3
All	All	3376/3585 (94%)	2802 (83%)	441 (13%)	133 (4%)	3	22

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	43	SER
1	A	44	VAL
1	A	229	ILE
1	A	291	SER
1	A	372	TRP
1	A	541	ALA
1	A	764	ARG
2	B	52	ILE
2	B	113	GLU
2	B	221	PRO
2	B	285	ARG
2	B	953	ILE
2	B	1015	LEU
3	C	41	VAL
3	C	43	VAL
3	C	163	MET
3	C	210	PHE
4	D	87	GLU
5	E	126	ILE

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Mol	Chain	Res	Type
7	G	17	SER
7	G	65	SER
7	G	107	SER
8	H	13	ILE
8	H	44	TRP
9	K	55	ASN
11	N	3	ILE
11	N	9	THR
11	N	64	ARG
12	P	17	GLN
12	P	22	PRO
13	Q	35	LYS
13	Q	36	LEU
13	Q	58	LYS
1	A	32	VAL
1	A	71	HIS
1	A	161	PRO
1	A	684	LEU
1	A	734	ARG
1	A	849	ALA
2	B	41	LYS
2	B	95	TYR
2	B	197	ALA
2	B	283	GLN
2	B	407	VAL
2	B	592	VAL
2	B	706	VAL
2	B	735	TYR
3	C	127	THR
3	C	146	TYR
3	C	180	THR
3	C	193	LEU
3	C	211	ALA
7	G	106	ILE
9	K	54	ASN
9	K	61	VAL
11	N	40	VAL
12	P	8	LYS
13	Q	34	PRO
13	Q	59	ILE
1	A	99	ARG
2	B	24	LYS

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Mol	Chain	Res	Type
2	B	53	PRO
2	B	267	ASN
2	B	563	THR
2	B	684	ALA
2	B	844	HIS
2	B	943	VAL
2	B	1053	LEU
2	B	1056	SER
2	B	1078	ASN
3	C	101	THR
3	C	129	GLU
3	C	331	ARG
3	C	338	LYS
4	D	206	CYS
6	F	4	VAL
6	F	63	ILE
6	F	68	VAL
6	F	83	VAL
6	F	89	MET
7	G	51	GLN
7	G	79	THR
9	K	47	ALA
11	N	39	GLY
1	A	29	THR
1	A	101	CYS
1	A	151	GLU
1	A	257	ALA
1	A	308	ARG
1	A	393	ASP
1	A	685	GLU
1	A	866	VAL
2	B	187	THR
2	B	203	VAL
2	B	334	GLU
2	B	775	LYS
2	B	834	ALA
2	B	1009	ARG
2	B	1076	ASN
3	C	113	ALA
3	C	217	ALA
3	C	349	VAL
4	D	83	ILE

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Mol	Chain	Res	Type
4	D	90	GLU
6	F	85	SER
7	G	80	GLU
11	N	41	LYS
1	A	109	ASP
1	A	255	ALA
1	A	284	LEU
1	A	371	LYS
1	A	394	ARG
1	A	688	PRO
2	B	281	ILE
3	C	26	GLN
4	D	205	LEU
6	F	31	SER
6	F	93	ARG
7	G	47	ASN
10	L	62	SER
2	B	210	ASP
2	B	836	ARG
2	B	1114	PRO
8	H	12	ARG
10	L	39	SER
12	P	16	GLU
1	A	126	PRO
2	B	918	LEU
3	C	237	ILE
3	C	216	ILE
1	A	39	PRO
1	A	199	PRO

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	758/766 (99%)	717 (95%)	41 (5%)	22	58
2	B	951/975 (98%)	905 (95%)	46 (5%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	324/341 (95%)	307 (95%)	17 (5%)	23	59
4	D	235/238 (99%)	235 (100%)	0	100	100
5	E	150/158 (95%)	143 (95%)	7 (5%)	26	62
6	F	99/107 (92%)	90 (91%)	9 (9%)	9	34
7	G	106/125 (85%)	99 (93%)	7 (7%)	16	51
8	H	69/75 (92%)	68 (99%)	1 (1%)	67	86
9	K	74/83 (89%)	73 (99%)	1 (1%)	67	86
10	L	79/80 (99%)	79 (100%)	0	100	100
11	N	59/60 (98%)	57 (97%)	2 (3%)	37	70
12	P	40/43 (93%)	38 (95%)	2 (5%)	24	60
13	Q	48/96 (50%)	46 (96%)	2 (4%)	30	65
All	All	2992/3147 (95%)	2857 (96%)	135 (4%)	27	63

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	32	VAL
1	A	52	ILE
1	A	68	CYS
1	A	77	LEU
1	A	93	PHE
1	A	99	ARG
1	A	100	ARG
1	A	109	ASP
1	A	111	ILE
1	A	116	ARG
1	A	124	ARG
1	A	145	VAL
1	A	159	GLU
1	A	162	TYR
1	A	169	LYS
1	A	187	VAL
1	A	229	ILE
1	A	232	GLU
1	A	233	ASP
1	A	284	LEU
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	342	ILE
1	A	357	ASN
1	A	366	ILE
1	A	390	TYR
1	A	415	ASP
1	A	426	HIS
1	A	438	LEU
1	A	464	LEU
1	A	478	GLU
1	A	500	GLN
1	A	534	LEU
1	A	540	LEU
1	A	547	THR
1	A	606	GLN
1	A	647	ARG
1	A	648	LEU
1	A	726	TYR
1	A	803	ARG
1	A	809	THR
2	B	54	THR
2	B	72	ARG
2	B	93	LEU
2	B	110	ILE
2	B	166	THR
2	B	188	HIS
2	B	207	ARG
2	B	217	PHE
2	B	224	ILE
2	B	233	LEU
2	B	318	LEU
2	B	326	ILE
2	B	330	LEU
2	B	352	LEU
2	B	353	PHE
2	B	374	LYS
2	B	376	LYS
2	B	406	TRP
2	B	421	ASN
2	B	422	TRP
2	B	460	GLU
2	B	529	LEU
2	B	579	ARG

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Mol	Chain	Res	Type
2	B	592	VAL
2	B	596	ASP
2	B	643	LEU
2	B	651	LEU
2	B	686	ASN
2	B	711	LEU
2	B	730	ILE
2	B	733	THR
2	B	735	TYR
2	B	872	LEU
2	B	899	ASP
2	B	908	VAL
2	B	913	LEU
2	B	929	GLU
2	B	950	LYS
2	B	953	ILE
2	B	1020	THR
2	B	1023	ARG
2	B	1025	ARG
2	B	1061	ILE
2	B	1077	LYS
2	B	1102	LEU
2	B	1118	LEU
3	C	70	ILE
3	C	159	ASP
3	C	190	ARG
3	C	196	PHE
3	C	199	ASP
3	C	208	ILE
3	C	210	PHE
3	C	216	ILE
3	C	219	LEU
3	C	232	LYS
3	C	237	ILE
3	C	244	LYS
3	C	247	ASP
3	C	306	LEU
3	C	307	ASP
3	C	315	LEU
3	C	319	VAL
5	E	16	ASN
5	E	27	LEU

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Mol	Chain	Res	Type
5	E	61	PHE
5	E	90	LEU
5	E	93	ASP
5	E	120	TYR
5	E	126	ILE
6	F	36	ARG
6	F	47	CYS
6	F	76	CYS
6	F	78	ILE
6	F	86	ILE
6	F	87	LEU
6	F	88	ILE
6	F	94	THR
6	F	95	TYR
7	G	7	GLN
7	G	48	ILE
7	G	63	ARG
7	G	64	LEU
7	G	79	THR
7	G	101	LEU
7	G	109	LYS
8	H	14	HIS
9	K	59	THR
11	N	7	CYS
11	N	61	HIS
12	P	5	ARG
12	P	13	PHE
13	Q	36	LEU
13	Q	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
2	B	640	HIS
2	B	686	ASN
2	B	696	HIS
2	B	926	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	SF4	D	1264	4	0,9,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	D	1264	4	-	-	0/3/3/5

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	1264	SF4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	872/880 (99%)	0.05	17 (1%)	66	53	21, 75, 161, 226	0
2	B	1103/1131 (97%)	0.07	23 (2%)	63	49	26, 73, 154, 281	0
3	C	376/395 (95%)	0.38	22 (5%)	22	13	30, 89, 170, 288	0
4	D	262/265 (98%)	0.20	8 (3%)	49	32	54, 92, 150, 180	0
5	E	171/180 (95%)	1.03	30 (17%)	1	1	49, 169, 233, 275	0
6	F	105/113 (92%)	1.14	24 (22%)	0	0	103, 197, 244, 281	0
7	G	113/132 (85%)	0.56	4 (3%)	44	28	60, 123, 170, 266	0
8	H	76/84 (90%)	0.05	1 (1%)	77	65	49, 77, 132, 176	0
9	K	84/95 (88%)	-0.03	1 (1%)	79	67	35, 58, 149, 195	0
10	L	91/92 (98%)	0.05	0	100	100	48, 86, 132, 218	0
11	N	65/66 (98%)	0.08	0	100	100	36, 81, 119, 143	0
12	P	44/48 (91%)	0.27	2 (4%)	33	21	52, 94, 153, 227	0
13	Q	50/104 (48%)	0.90	8 (16%)	1	1	98, 154, 195, 204	0
All	All	3412/3585 (95%)	0.22	140 (4%)	37	24	21, 85, 188, 288	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	229	THR	7.3
6	F	78	ILE	6.4
1	A	40	ILE	5.9
6	F	79	THR	5.6
5	E	117	THR	5.4
2	B	380	ARG	5.3
6	F	77	PRO	5.1
5	E	143	ARG	4.8
2	B	267	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
6	F	61	SER	4.6
5	E	137	GLN	4.4
3	C	192	LYS	4.3
5	E	92	VAL	4.2
3	C	189	ASN	4.1
12	P	11	LYS	4.1
6	F	104	ILE	4.0
5	E	136	ILE	4.0
6	F	98	GLU	3.9
6	F	99	ASP	3.9
1	A	38	THR	3.9
5	E	82	GLN	3.8
1	A	103	ARG	3.8
13	Q	80	SER	3.7
5	E	87	GLY	3.7
6	F	94	THR	3.7
3	C	214	ASP	3.7
6	F	90	ASP	3.7
3	C	212	ASN	3.7
3	C	86	THR	3.6
1	A	676	ILE	3.6
3	C	340	SER	3.6
3	C	161	ALA	3.6
5	E	124	ARG	3.4
13	Q	79	ASP	3.4
6	F	100	ILE	3.4
1	A	815	GLN	3.3
5	E	171	LYS	3.3
2	B	769	PRO	3.3
6	F	53	GLN	3.3
1	A	108	GLU	3.3
6	F	27	SER	3.3
13	Q	75	TYR	3.3
4	D	214	ASN	3.2
3	C	230	LYS	3.2
6	F	105	ASP	3.2
3	C	181	VAL	3.2
5	E	128	PHE	3.2
2	B	378	ARG	3.2
5	E	81	VAL	3.2
3	C	213	ILE	3.1
1	A	35	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	175	ASN	3.1
4	D	192	ASP	3.1
7	G	95	ILE	3.1
6	F	58	GLU	3.1
3	C	339	ASN	3.0
2	B	438	ARG	3.0
5	E	144	ALA	3.0
1	A	41	GLU	3.0
6	F	76	CYS	3.0
5	E	86	GLU	2.9
5	E	177	GLN	2.9
3	C	208	ILE	2.9
13	Q	77	LYS	2.8
1	A	285	PRO	2.8
1	A	811	VAL	2.8
5	E	72	PHE	2.8
5	E	127	ILE	2.8
4	D	104	ASN	2.8
2	B	790	GLU	2.7
13	Q	81	ARG	2.7
4	D	174	GLY	2.7
13	Q	69	GLU	2.7
6	F	85	SER	2.7
9	K	56	ILE	2.7
7	G	104	LYS	2.7
3	C	217	ALA	2.7
5	E	106	GLY	2.6
3	C	205	THR	2.6
4	D	176	CYS	2.6
7	G	92	TYR	2.5
2	B	1076	ASN	2.5
5	E	42	LEU	2.5
6	F	101	GLN	2.5
6	F	62	ILE	2.5
2	B	294	GLN	2.5
2	B	1125	SER	2.5
5	E	118	LEU	2.4
8	H	25	ILE	2.4
1	A	158	LEU	2.4
4	D	47	ILE	2.4
5	E	132	SER	2.4
5	E	130	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	96	THR	2.4
5	E	126	ILE	2.4
2	B	772	GLN	2.4
7	G	117	GLN	2.4
5	E	97	VAL	2.3
3	C	163	MET	2.3
13	Q	73	LYS	2.3
2	B	442	ASN	2.3
2	B	773	GLU	2.3
1	A	807	VAL	2.3
5	E	166	GLN	2.3
2	B	1075	LYS	2.3
3	C	187	ALA	2.3
6	F	29	SER	2.3
5	E	1	MET	2.2
5	E	116	ASP	2.2
2	B	271	ALA	2.2
5	E	125	GLY	2.2
1	A	138	LYS	2.2
2	B	235	ILE	2.2
2	B	476	MET	2.2
3	C	175	LYS	2.2
2	B	1078	ASN	2.2
2	B	441	PRO	2.2
1	A	683	GLU	2.2
3	C	186	LYS	2.2
3	C	173	MET	2.2
5	E	104	MET	2.2
1	A	677	GLN	2.1
6	F	5	TYR	2.1
2	B	783	VAL	2.1
3	C	188	ILE	2.1
2	B	439	GLY	2.1
12	P	10	TRP	2.1
13	Q	72	TYR	2.1
6	F	92	ASN	2.1
3	C	235	LYS	2.1
5	E	135	VAL	2.1
2	B	770	GLY	2.1
6	F	97	SER	2.1
5	E	138	LYS	2.0
2	B	1066	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	188	PHE	2.0
1	A	157	LYS	2.0
1	A	879	LYS	2.0
6	F	93	ARG	2.0
2	B	279	VAL	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	B	2128	1/1	0.83	0.29	81,81,81,81	0
14	ZN	A	1880	1/1	0.89	0.08	81,81,81,81	0
15	MG	A	1884	1/1	0.89	0.23	81,81,81,81	0
14	ZN	A	1882	1/1	0.92	0.34	81,81,81,81	0
14	ZN	A	1883	1/1	0.92	0.16	81,81,81,81	0
14	ZN	B	2127	1/1	0.93	0.34	81,81,81,81	0
14	ZN	C	1395	1/1	0.94	0.06	81,81,81,81	0
14	ZN	N	1066	1/1	0.94	0.21	88,88,88,88	0
14	ZN	A	1881	1/1	0.94	0.10	81,81,81,81	0
16	SF4	D	1264	7/8	0.95	0.21	81,81,81,81	0
14	ZN	B	2126	1/1	0.97	0.11	81,81,81,81	0
14	ZN	P	1049	1/1	0.98	0.10	118,118,118,118	0

6.5 Other polymers (i)

There are no such residues in this entry.