



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 PM UTC

PDB ID : 4AYB / pdb_00004ayb
Title : RNAP at 3.2Ång
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

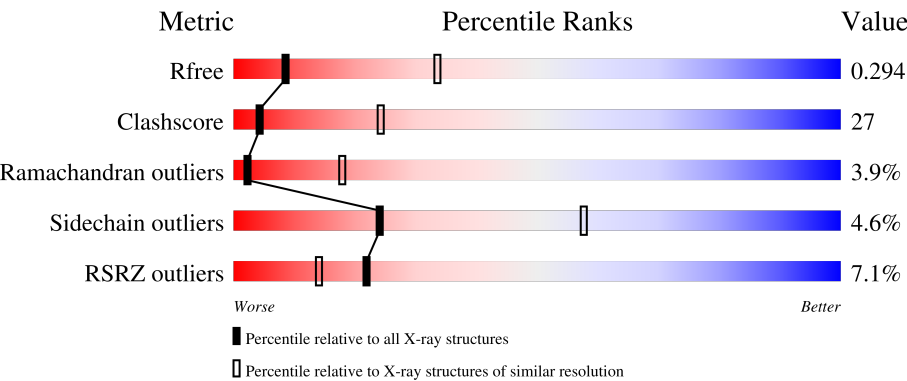
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	880	7% 55% 39% 5% ..
2	B	1131	5% 56% 37% 5% .
3	C	395	8% 45% 43% 6% 5%
4	D	265	4% 67% 31% ..
5	E	180	14% 52% 41% .. 5%

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Mol	Chain	Length	Quality of chain
6	F	113	
7	G	132	
8	H	84	
9	K	95	
10	L	92	
11	N	66	
12	P	48	
13	Q	104	

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
1	A	872	Total	C	H	N	O	S	0	0	0
			13986	4424	7029	1225	1282	26			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

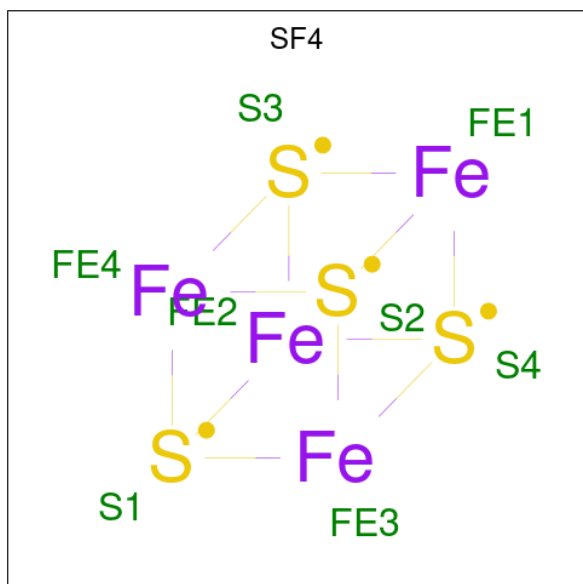
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

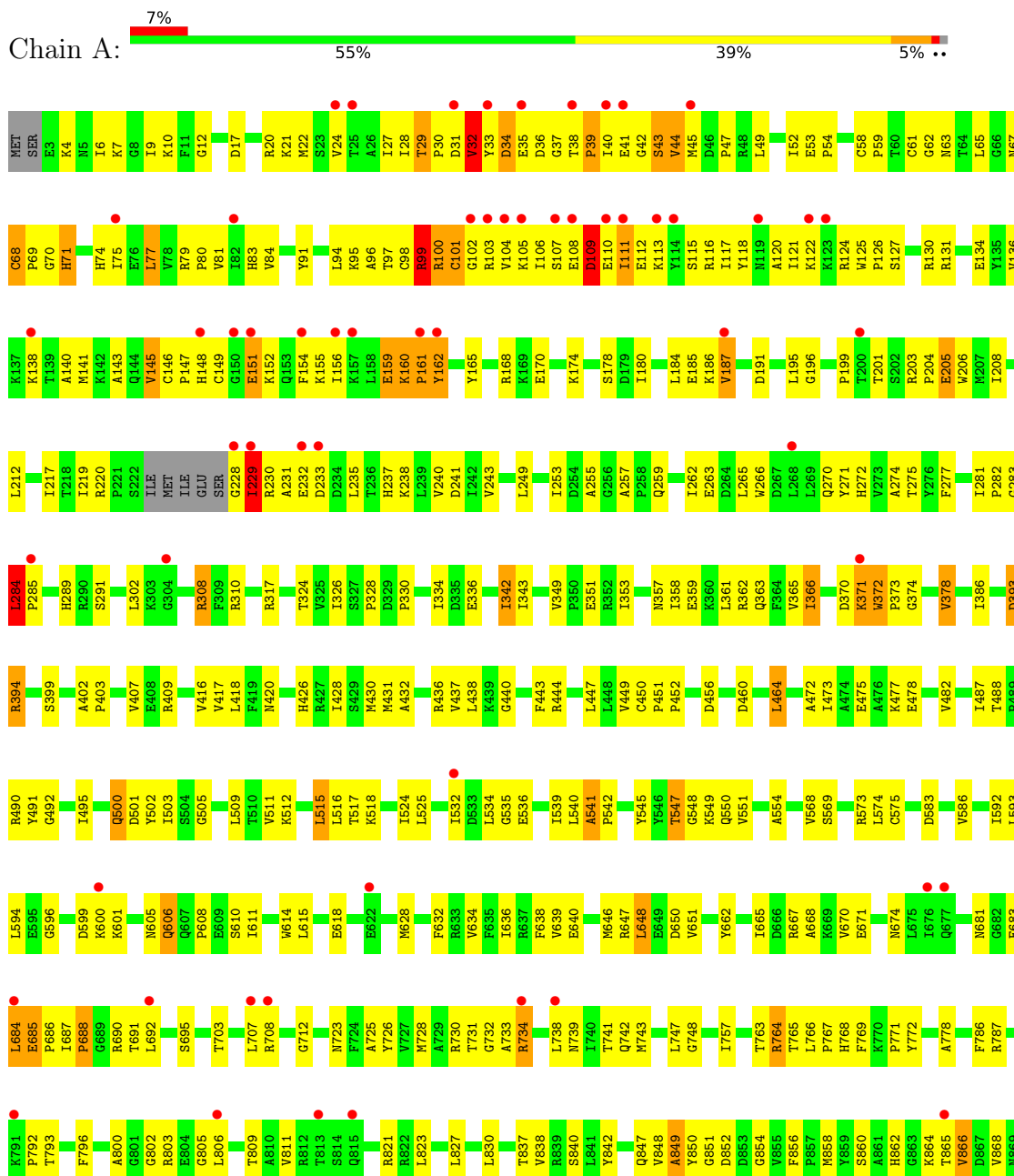


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total 7	Fe 3	S 4	0	0

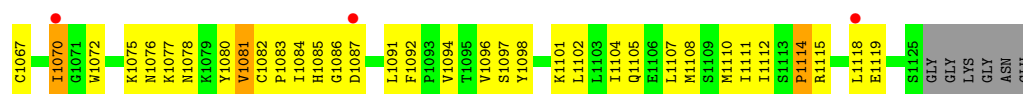
3 Residue-property plots

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



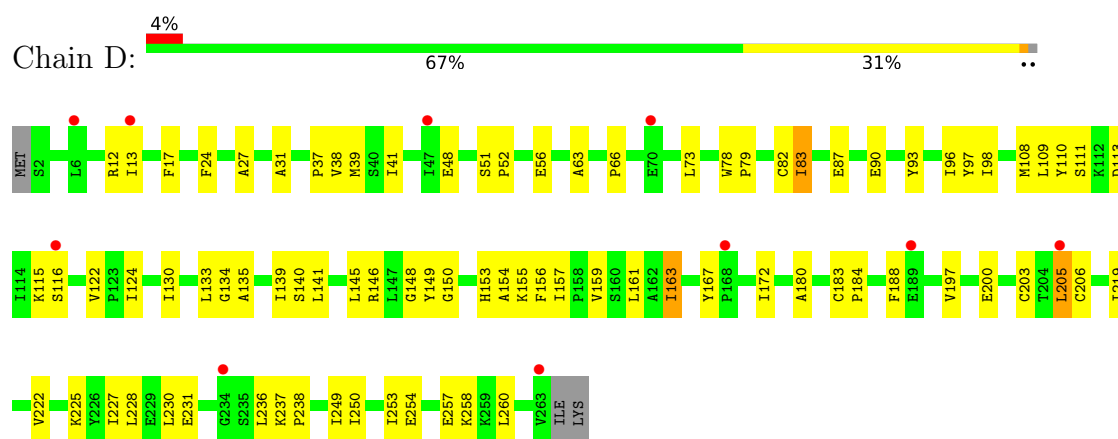




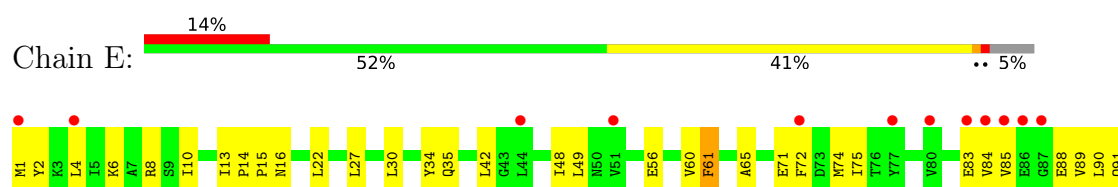
• Molecule 3: DNA-DIRECTED RNA POLYMERASE

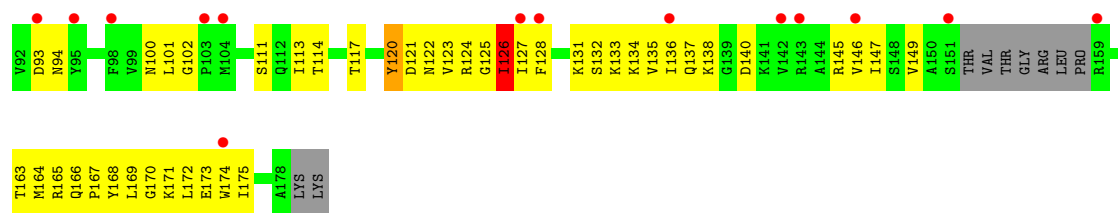


• Molecule 4: DNA-DIRECTED RNA POLYMERASE

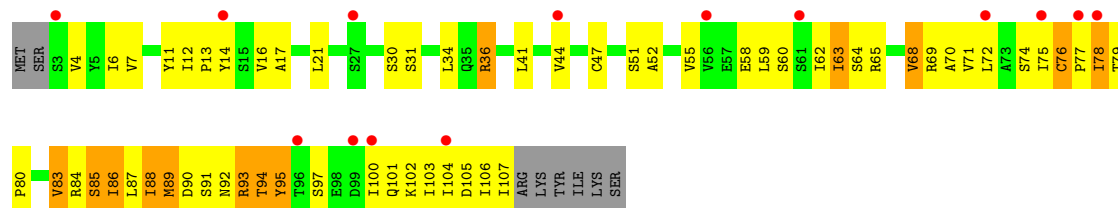


• Molecule 5: DNA-DIRECTED RNA POLYMERASE

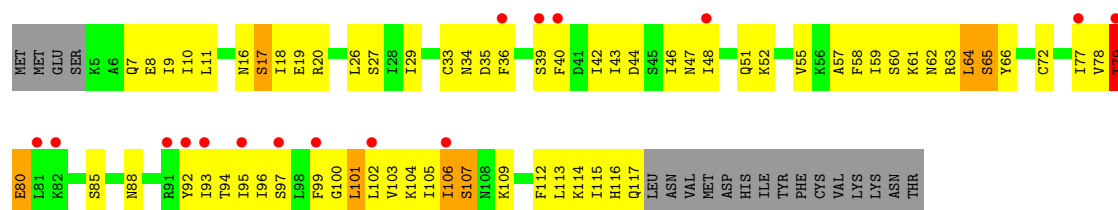




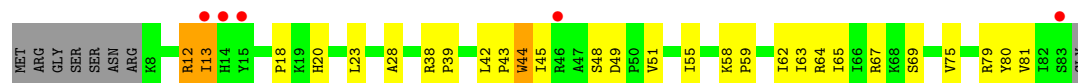
● Molecule 6: DNA-DIRECTED RNA POLYMERASE



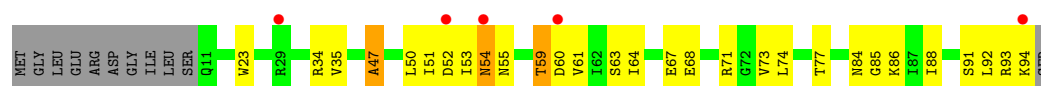
● Molecule 7: DNA-DIRECTED RNA POLYMERASE



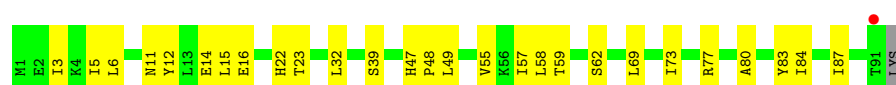
● Molecule 8: DNA-DIRECTED RNA POLYMERASE



● Molecule 9: DNA-DIRECTED RNA POLYMERASE



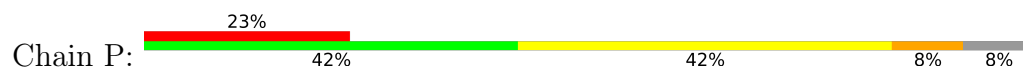
● Molecule 10: DNA-DIRECTED RNA POLYMERASE



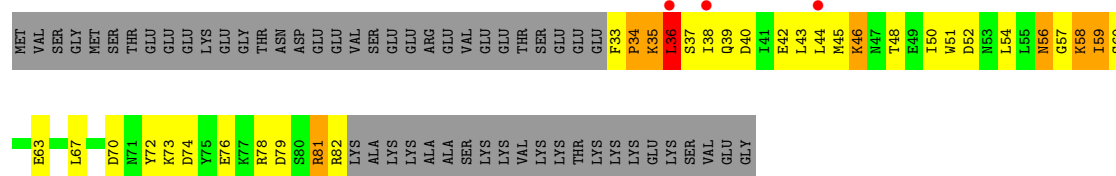
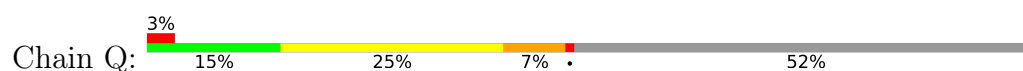
- Molecule 11: DNA-DIRECTED RNA POLYMERASE



- Molecule 12: DNA-DIRECTED RNA POLYMERASE



- Molecule 13: DNA-DIRECTED RNA POLYMERASE



4 Data and refinement statistics

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) 99.4 (40.10-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.242 , 0.300 0.236 , 0.294	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)	0.35 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.34	0/7108	0.72	1/9618 (0.0%)
2	B	0.32	0/8923	0.70	0/12071
3	C	0.32	0/2930	0.75	0/3944
4	D	0.28	0/2123	0.66	0/2870
5	E	0.27	0/1379	0.66	0/1861
6	F	0.32	0/836	0.70	0/1133
7	G	0.28	0/913	0.72	0/1224
8	H	0.29	0/638	0.70	0/864
9	K	0.33	0/682	0.72	1/921 (0.1%)
10	L	0.27	0/717	0.65	0/968
11	N	0.32	0/532	0.71	0/718
12	P	0.36	0/365	0.67	0/489
13	Q	0.28	0/434	0.63	1/580 (0.2%)
All	All	0.32	0/27580	0.70	3/37261 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	VAL	N-CA-C	6.34	116.45	110.30
9	K	85	GLY	N-CA-C	-6.20	107.70	115.08
13	Q	56	ASN	N-CA-C	5.06	116.88	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6957	7029	7013	429	0
2	B	8756	8908	8888	454	0
3	C	2906	3068	3063	208	0
4	D	2087	2128	2125	68	0
5	E	1359	1413	1411	80	0
6	F	827	839	839	88	0
7	G	901	915	912	88	0
8	H	624	660	658	26	0
9	K	673	717	716	23	0
10	L	707	742	739	20	0
11	N	521	537	535	42	0
12	P	357	387	387	26	0
13	Q	428	426	426	40	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	1481	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 27.

All (1481) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	1.44	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:211:ALA:HB1	3:C:212:ASN:C	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:864:LYS:HA	1:A:865:THR:CB	2.21	0.70
13:Q:78:ARG:HD3	13:Q:78:ARG:C	2.17	0.69
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
1:A:535:GLY:O	1:A:536:GLU:C	2.36	0.67
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
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
11:N:48:MET:HA	11:N:48:MET:HE2	1.76	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
3:C:213:ILE:HB	3:C:214:ASP:C	2.21	0.66
2:B:112:ALA:O	2:B:113:GLU:HB2	1.95	0.66
2:B:981:LYS:HZ1	4:D:205:LEU:HD13	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ASN:HB2	2:B:922:MET:SD	2.36	0.66
2:B:893:MET:HE2	10:L:48:PRO:HB2	1.77	0.66
5:E:117:THR:HG23	5:E:131:LYS:HZ1	1.61	0.65
3:C:101:THR:HG22	3:C:121:MET:HE1	1.78	0.65
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
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
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
2:B:233:LEU:HD11	2:B:311:ARG:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LYS:O	1:A:600:LYS:HG2	1.99	0.62
1:A:733:ALA:O	1:A:734:ARG:C	2.43	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
5:E:1:MET:HE1	5:E:85:VAL:HG22	1.81	0.61
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
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
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
2:B:592:VAL:CG2	2:B:596:ASP:CG	2.73	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: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
2:B:406:TRP:HB3	2:B:407:VAL:C	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD12	1:A:243:VAL:HG22	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
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
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:230:MET:HE2	2:B:230:MET:HA	1.84	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
2:B:30:HIS:HB3	2:B:125:MET:HE1	1.83	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
2:B:873:ARG:HB3	2:B:999:MET:HE1	1.84	0.59
3:C:81:PRO:HB3	3:C:306:LEU:HG	1.85	0.59
11:N:47:ARG:CZ	11:N:48:MET:HE3	2.33	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
3:C:101:THR:C	3:C:102:LEU:HD22	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:13:LEU:HD23	3:C:13:LEU:C	2.28	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: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:431:MET:HE1	1:A:482:VAL:HG13	1.85	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:108:ASN:O	2:B:109:ASN:HB2	2.02	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
5:E:125:GLY:C	5:E:126:ILE:HG23	2.29	0.57
13:Q:58:LYS:O	13:Q:59:ILE:HB	2.03	0.57
3:C:154:SER:HB3	3:C:170:ASP:HB2	1.85	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
2:B:1014:ILE:O	2:B:1015:LEU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:854:LEU:C	2:B:854:LEU:HD23	2.30	0.57
3:C:41:VAL:O	3:C:42:LEU:C	2.48	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
1:A:65:LEU:HD23	1:A:65:LEU:C	2.29	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:190:ALA:HB2	2:B:325:VAL:HG22	1.86	0.57
2:B:255:LEU:C	2:B:257:PRO:HD2	2.30	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:162:SER:O	3:C:163:MET:C	2.48	0.56
3:C:211:ALA:HB1	3:C:212:ASN:CA	2.34	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
1:A:80:PRO:HG3	1:A:178:SER:HA	1.88	0.56
5:E:121:ASP:C	5:E:125:GLY:HA2	2.30	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
2:B:778:MET:HE3	2:B:779:PRO:HD2	1.87	0.56
1:A:28:ILE:HD12	1:A:44:VAL:HA	1.88	0.56
1:A:456:ASP:OD1	1:A:460:ASP:CG	2.37	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
1:A:431:MET:HE2	1:A:482:VAL:HA	1.87	0.56
4:D:197:VAL:HG11	4:D:200:GLU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:646:MET:HE2	1:A:725:ALA:HB2	1.89	0.55
2:B:833:GLN:CB	2:B:834:ALA:CB	2.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:1:MET:HE1	5:E:85:VAL:CG2	2.38	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
2:B:284:LYS:O	2:B:285:ARG:C	2.51	0.54
3:C:348:GLU:O	3:C:349:VAL:HB	2.08	0.54
7:G:95:ILE:C	7:G:96:ILE:HG13	2.33	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: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
1:A:228:GLY:C	1:A:229:ILE:HG23	2.33	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
1:A:241:ASP:HB3	1:A:272:HIS:CD2	2.42	0.54
1:A:618:GLU:CD	1:A:874:ARG:HD3	2.33	0.54
2:B:734:GLY:HA3	2:B:735:TYR:CD2	2.42	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
13:Q:35:LYS:O	13:Q:36:LEU:C	2.50	0.54
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:LEU:H	2:B:919:PRO:HD2	1.73	0.53
2:B:1053:LEU:HD23	2:B:1053:LEU:C	2.33	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
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
2:B:162:ARG:NH1	2:B:415:GLN:C	2.66	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
3:C:145:GLU:C	3:C:237:ILE:HD11	2.33	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
1:A:651:VAL:HG12	1:A:651:VAL:O	2.07	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
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: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
7:G:63:ARG:C	7:G:64:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:734:GLY:CA	2:B:735:TYR:CB	2.81	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:431:MET:CE	1:A:482:VAL:HG13	2.40	0.52
1:A:684:LEU:O	1:A:685:GLU:C	2.53	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: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: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
2:B:928:MET:HE3	2:B:953:ILE:HG21	1.92	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:511:VAL:O	1:A:512:LYS:C	2.53	0.51
2:B:101:LEU:HD12	2:B:103:MET:HE3	1.92	0.51
2:B:454:GLY:HA3	2:B:580:ARG:HD3	1.93	0.51
3:C:66:PRO:C	3:C:385:MET:HE1	2.35	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:220:VAL:O	2:B:221:PRO:C	2.53	0.51
2:B:688:GLN:HG3	11:N:64:ARG:HG2	1.91	0.51
2:B:1081:VAL:C	2:B:1091:LEU:HD11	2.35	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:418:LEU:HD23	1:A:430:MET:HE2	1.92	0.51
1:A:509:LEU:O	1:A:548:GLY:HA3	2.11	0.51
1:A:517:THR:O	1:A:518:LYS:C	2.54	0.51
2:B:406:TRP:CA	2:B:407:VAL:CB	2.89	0.51
2:B:421:ASN:OD1	2:B:421:ASN:C	2.53	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: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
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:274:THR:HG22	3:C:276:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:541:ALA:O	1:A:542:PRO:C	2.54	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:775:LYS:HG3	2:B:777:VAL:HG23	1.93	0.51
3:C:143:LYS:O	3:C:234:ILE:HB	2.10	0.51
3:C:168:GLN:CD	3:C:204:ASN:OD1	2.53	0.51
4:D:141:LEU:HD12	4:D:141:LEU:C	2.36	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:420:THR:O	2:B:421:ASN:CG	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1086:GLY:O	2:B:1087:ASP:HB2	2.11	0.50
3:C:237:ILE:HG12	3:C:238:LYS:N	2.25	0.50
6:F:88:ILE:C	6:F:90:ASP:N	2.69	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
7:G:101:LEU:HD22	7:G:101:LEU:C	2.36	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
6:F:106:ILE:O	6:F:107:ILE:C	2.54	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
3:C:104:LEU:C	3:C:104:LEU:HD23	2.37	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
3:C:144:LEU:HD22	3:C:235:LYS:HZ1	1.75	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:196:THR:HG22	2:B:302:PRO:C	2.37	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
3:C:237:ILE:C	3:C:237:ILE:HD13	2.37	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:448:LEU:C	2:B:448:LEU:HD23	2.37	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
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
2:B:800:VAL:HB	12:P:36:MET:HE1	1.95	0.49
1:A:742:GLN:HG2	1:A:747:LEU:HA	1.94	0.49
2:B:893:MET:HE3	2:B:894:LEU:O	2.13	0.49
2:B:895:ILE:HB	2:B:900:MET:HE2	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
1:A:33:TYR:C	1:A:41:GLU:HB2	2.38	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
5:E:1:MET:HE2	5:E:83:GLU:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:72:ARG:HD2	2:B:72:ARG:C	2.38	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
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:604:SER:C	2:B:605:ILE:HD13	2.38	0.49
2:B:666:SER:N	2:B:667:PRO:HD2	2.28	0.49
2:B:743:MET:HE1	2:B:875:PRO:HB2	1.95	0.49
3:C:126:LEU:HB3	3:C:130:TYR:HB2	1.94	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: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:125:MET:HE2	2:B:153:GLY:HA2	1.95	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
5:E:140:ASP:CG	5:E:171:LYS:HE2	2.37	0.48
8:H:18:PRO:HB3	8:H:67:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:212:LEU:C	1:A:212:LEU:HD23	2.38	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
2:B:855:ILE:HD11	12:P:36:MET:HE3	1.94	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: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:614:TRP:O	1:A:615:LEU:C	2.57	0.48
1:A:687:ILE:CG1	1:A:688:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
6:F:84:ARG:O	6:F:85:SER:C	2.57	0.48
9:K:53:ILE:O	9:K:54:ASN:C	2.56	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:738:LEU:C	1:A:738:LEU:HD12	2.38	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
5:E:169:LEU:C	5:E:175:ILE:HD11	2.39	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:238:ASP:CG	2:B:259:LEU:HD11	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:778:MET:HE3	2:B:779:PRO:CD	2.44	0.47
3:C:139:GLU:O	3:C:142:ARG:HG2	2.15	0.47
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
7:G:10:ILE:C	7:G:11:LEU:HD12	2.39	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:209:LYS:O	2:B:210:ASP:CG	2.58	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
2:B:228:ILE:HG23	2:B:271:ALA:HB1	1.97	0.47
2:B:476:MET:HE1	2:B:645:ILE:HB	1.97	0.47
2:B:539:LEU:HD11	2:B:543:ILE:HD11	1.97	0.47
2:B:743:MET:HE3	2:B:748:VAL:CG2	2.45	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:1061:ILE:HD11	2:B:1101:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:GLY:O	1:A:103:ARG:C	2.58	0.46
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
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
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:592:VAL:HG22	2:B:596:ASP:CG	2.41	0.46
2:B:874:ILE:HG23	2:B:875:PRO:HD2	1.97	0.46
5:E:117:THR:HG23	5:E:131:LYS:NZ	2.29	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:67:ASN:C	1:A:69:PRO:HD3	2.40	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
3:C:235:LYS:HZ3	3:C:261:VAL:HA	1.81	0.46
4:D:236:LEU:HD12	4:D:236:LEU:N	2.31	0.46
6:F:59:LEU:C	6:F:69:ARG:NH1	2.73	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:95:LYS:HD3	1:A:141:MET:HE3	1.97	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: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
5:E:60:VAL:HG22	5:E:61:PHE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:683:TYR:O	2:B:684:ALA:HB2	2.14	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
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
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:485:GLU:O	2:B:486:LYS:C	2.58	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
2:B:808:LYS:O	2:B:809:GLY:C	2.59	0.46
1:A:61:CYS:HB2	1:A:68:CYS:SG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:GLU:CD	4:D:56:GLU:H	2.25	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
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
9:K:59:THR:CG2	9:K:63:SER:HB3	2.46	0.45
1:A:31:ASP:C	1:A:32:VAL:CG2	2.89	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: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
1:A:38:THR:H	1:A:39:PRO:HD2	1.81	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: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:96:ALA:HB1	1:A:105:LYS:HZ3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:525:LEU:C	2:B:525:LEU:HD13	2.41	0.45
2:B:1046:MET:HE2	2:B:1046:MET:HA	1.99	0.45
3:C:16:LYS:HE2	3:C:49:ASP:HA	1.99	0.45
3:C:122:MET:HE1	3:C:261:VAL:HG21	1.99	0.45
3:C:219:LEU:HA	3:C:222:LEU:HD23	1.99	0.45
4:D:130:ILE:O	11:N:2:MET:HE2	2.17	0.45
5:E:100:ASN:CG	6:F:36:ARG:HH11	2.25	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
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
1:A:823:LEU:C	1:A:823:LEU:HD12	2.42	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
2:B:893:MET:HE1	10:L:49:LEU:CD2	2.47	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:430:MET:HE1	2:B:1031:PHE:CZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:363:VAL:HG12	3:C:364:GLU:N	2.32	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
9:K:50:LEU:O	9:K:51:ILE:C	2.60	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
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
12:P:5:ARG:N	12:P:17:GLN:C	2.75	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:430:MET:HE1	2:B:1031:PHE:CE1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:LEU:O	2:B:171:ALA:C	2.60	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
5:E:1:MET:HE2	5:E:83:GLU:CG	2.47	0.44
7:G:55:VAL:HB	7:G:116:HIS:O	2.17	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
2:B:110:ILE:HD13	2:B:110:ILE:N	2.33	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
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
6:F:88:ILE:C	6:F:90:ASP:H	2.24	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: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
4:D:111:SER:C	4:D:113:ASP:H	2.24	0.44
1:A:40:ILE:HD13	1:A:47:PRO:HG2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:LYS:O	1:A:22:MET:C	2.61	0.44
1:A:281:ILE:CD1	1:A:284:LEU:HD12	2.48	0.44
1:A:363:GLN:C	1:A:366:ILE:HG22	2.43	0.44
2:B:125:MET:HE2	2:B:153:GLY:CA	2.48	0.44
2:B:928:MET:HE3	2:B:953:ILE:CG2	2.47	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
1:A:79:ARG:CB	1:A:266:TRP:CZ3	3.01	0.44
1:A:723:ASN:OD1	1:A:723:ASN:C	2.61	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
4:D:109:LEU:C	4:D:109:LEU:HD23	2.42	0.44
4:D:260:LEU:C	4:D:260:LEU:HD23	2.42	0.44
6:F:75:ILE:HG22	6:F:77:PRO:HG3	1.99	0.44
12:P:5:ARG:HB2	12:P:17:GLN:CD	2.43	0.44
1:A:219:ILE:HD11	2:B:1105:GLN:CB	2.48	0.44
1:A:366:ILE:HD13	1:A:366:ILE:C	2.43	0.44
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
2:B:300:PHE:O	2:B:301:LEU:C	2.61	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
5:E:100:ASN:CG	6:F:36:ARG:NH1	2.75	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:372:TRP:CD1	1:A:372:TRP:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:GLN:O	2:B:666:SER:C	2.61	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: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:95:LYS:HB2	1:A:141:MET:HE3	1.98	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:672:GLN:CD	2:B:884:ARG:HA	2.43	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: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
2:B:760:LEU:C	2:B:760:LEU:HD23	2.43	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:155:LYS:O	1:A:156:ILE:C	2.62	0.43
1:A:271:TYR:HE1	1:A:285:PRO:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG22	1:A:386:ILE:HB	2.01	0.43
2:B:125:MET:HE2	2:B:153:GLY:C	2.44	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: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
3:C:320:MET:HE2	3:C:329:ILE:HD13	2.00	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
7:G:96:ILE:HD13	7:G:99:PHE:CD1	2.53	0.43
1:A:22:MET:CE	2:B:1108:MET:HE3	2.49	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
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
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
2:B:995:LYS:CE	2:B:999:MET:HE3	2.49	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HD13	1:A:342:ILE:O	2.18	0.42
1:A:840:SER:C	1:A:842:TYR:H	2.27	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
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: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: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
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
1:A:802:GLY:O	1:A:803:ARG:C	2.62	0.42
2:B:778:MET:HE3	2:B:779:PRO:N	2.33	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
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
10:L:22:HIS:O	10:L:23:THR:C	2.61	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
1:A:431:MET:HE2	1:A:482:VAL:HG22	2.00	0.42
1:A:805:GLY:O	1:A:806:LEU:C	2.62	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
2:B:230:MET:HE1	2:B:315:ALA:HB1	2.01	0.42
2:B:345:ARG:HG3	2:B:576:GLY:C	2.44	0.42
2:B:752:MET:HE1	2:B:910:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:VAL:O	6:F:71:VAL:HG12	2.19	0.42
7:G:26:LEU:HD23	7:G:43:ILE:HD13	2.01	0.42
7:G:61:LYS:O	7:G:62:ASN:CB	2.66	0.42
13:Q:51:TRP:O	13:Q:52:ASP:C	2.63	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:34:TYR:O	5:E:35:GLN:C	2.61	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: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: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
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:718:ASN:C	2:B:719:ARG:HG3	2.44	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:837:THR:HG23	1:A:847:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:VAL:HG23	2:B:75:GLU:HG3	2.02	0.42
2:B:705:LEU:O	2:B:706:VAL:C	2.62	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
11:N:44:CYS:C	11:N:46:ARG:H	2.28	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
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
4:D:153:HIS:C	4:D:155:LYS:H	2.27	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
7:G:43:ILE:HG22	7:G:44:ASP:N	2.33	0.42
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: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
8:H:13:ILE:HG23	8:H:13:ILE:O	2.20	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:82:GLY:HA2	3:C:85:MET:HE2	2.02	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
8:H:12:ARG:O	8:H:13:ILE:C	2.62	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: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:228:GLY:C	1:A:230:ARG:H	2.28	0.41
1:A:308:ARG:HD3	1:A:308:ARG:HA	1.88	0.41
1:A:342:ILE:CG2	1:A:343:ILE:N	2.82	0.41
1:A:708:ARG:CD	1:A:748:GLY:HA3	2.50	0.41
2:B:209:LYS:C	2:B:210:ASP:CG	2.86	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:122:MET:HE2	3:C:124:ILE:HD11	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:D:134:GLY:O	4:D:135:ALA:C	2.63	0.41
5:E:1:MET:HG2	5:E:83:GLU:CD	2.46	0.41
12:P:29:CYS:C	12:P:31:TYR:N	2.78	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: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:245:LYS:O	3:C:246:GLY:C	2.63	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
11:N:18:TRP:O	11:N:19:GLN:C	2.64	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:103:MET:HE3	2:B:119:ILE:HD11	2.02	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
3:C:372:ASN:HA	3:C:375:ILE:HG22	2.01	0.41
4:D:258:LYS:HD2	4:D:258:LYS:C	2.46	0.41
9:K:51:ILE:HG21	9:K:71:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:85:MET:HE3	3:C:104:LEU:CG	2.51	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:96:ALA:CB	1:A:105:LYS:HZ3	2.34	0.41
1:A:326:ILE:HA	1:A:443:PHE:O	2.21	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
2:B:660:TYR:CD1	2:B:928:MET:HE2	2.56	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
5:E:133:LYS:O	5:E:133:LYS:HG3	2.20	0.41
6:F:62:ILE:O	6:F:62:ILE:HG22	2.20	0.41
6:F:75:ILE:C	6:F:76:CYS:SG	3.03	0.41
6:F:91:SER:HB3	6:F:92:ASN:C	2.45	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
13:Q:57:GLY:O	13:Q:58:LYS:C	2.64	0.41
1:A:145:VAL:HG13	1:A:146:CYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:610:SER:O	1:A:611:ILE:C	2.64	0.41
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
3:C:196:PHE:CD1	3:C:196:PHE:C	2.96	0.41
4:D:97:TYR:C	4:D:98:ILE:HD12	2.46	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:593:THR:O	2:B:594:ARG:C	2.65	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
3:C:281:GLU:CD	3:C:326:VAL:HG12	2.46	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:228:LEU:C	4:D:228:LEU:HD23	2.45	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
9:K:84:ASN:C	9:K:86:LYS:H	2.29	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:633:PRO:C	2:B:636:LEU:HD23	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:THR:HG22	3:C:351:VAL:N	2.36	0.40
4:D:96:ILE:HD12	4:D:96:ILE:C	2.47	0.40
4:D:159:VAL:HG22	4:D:161:LEU:H	1.86	0.40
9:K:52:ASP:CG	9:K:53:ILE:N	2.79	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
2:B:62:ARG:HB2	2:B:104:ILE:HB	2.03	0.40
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:914:ASN:C	2:B:916:HIS:H	2.29	0.40
2:B:1082:CYS:CB	2:B:1083:PRO:HD2	2.51	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
1:A:852:ASP:CG	8:H:75:VAL:HG21	2.47	0.40
2:B:562:VAL:O	2:B:563:THR:C	2.65	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
3:C:235:LYS:HZ3	3:C:261:VAL:HG13	1.85	0.40
6:F:6:ILE:HG22	6:F:7:VAL:N	2.36	0.40
6:F:89:MET:C	6:F:91:SER:H	2.30	0.40
7:G:34:ASN:C	7:G:36:PHE:H	2.29	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	868/880 (99%)	712 (82%)	124 (14%)	32 (4%)	2	18
2	B	1097/1131 (97%)	928 (85%)	133 (12%)	36 (3%)	3	21
3	C	372/395 (94%)	304 (82%)	49 (13%)	19 (5%)	1	13
4	D	260/265 (98%)	218 (84%)	37 (14%)	5 (2%)	6	33
5	E	167/180 (93%)	150 (90%)	16 (10%)	1 (1%)	21	56
6	F	103/113 (91%)	78 (76%)	17 (16%)	8 (8%)	1	5
7	G	111/132 (84%)	83 (75%)	20 (18%)	8 (7%)	1	6
8	H	74/84 (88%)	63 (85%)	8 (11%)	3 (4%)	2	17
9	K	82/95 (86%)	69 (84%)	9 (11%)	4 (5%)	1	13
10	L	89/92 (97%)	83 (93%)	4 (4%)	2 (2%)	5	29
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	2
All	All	3376/3585 (94%)	2802 (83%)	441 (13%)	133 (4%)	2	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	721 (95%)	37 (5%)	22	55
2	B	951/975 (98%)	903 (95%)	48 (5%)	22	55
3	C	324/341 (95%)	305 (94%)	19 (6%)	18	50
4	D	235/238 (99%)	234 (100%)	1 (0%)	84	86
5	E	150/158 (95%)	142 (95%)	8 (5%)	20	53
6	F	99/107 (92%)	89 (90%)	10 (10%)	7	30
7	G	106/125 (85%)	99 (93%)	7 (7%)	15	47
8	H	69/75 (92%)	68 (99%)	1 (1%)	59	77
9	K	74/83 (89%)	73 (99%)	1 (1%)	59	77
10	L	79/80 (99%)	79 (100%)	0	100	100
11	N	59/60 (98%)	58 (98%)	1 (2%)	53	75
12	P	40/43 (93%)	39 (98%)	1 (2%)	42	69
13	Q	48/96 (50%)	45 (94%)	3 (6%)	16	48
All	All	2992/3147 (95%)	2855 (95%)	137 (5%)	24	58

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	52	ILE
1	A	68	CYS
1	A	77	LEU
1	A	99	ARG
1	A	100	ARG
1	A	109	ASP
1	A	111	ILE
1	A	124	ARG
1	A	145	VAL
1	A	159	GLU
1	A	160	LYS

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Mol	Chain	Res	Type
1	A	162	TYR
1	A	187	VAL
1	A	205	GLU
1	A	229	ILE
1	A	232	GLU
1	A	233	ASP
1	A	284	LEU
1	A	289	HIS
1	A	342	ILE
1	A	366	ILE
1	A	378	VAL
1	A	420	ASN
1	A	426	HIS
1	A	464	LEU
1	A	478	GLU
1	A	500	GLN
1	A	515	LEU
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	809	THR
2	B	54	THR
2	B	66	ILE
2	B	72	ARG
2	B	93	LEU
2	B	101	LEU
2	B	110	ILE
2	B	166	THR
2	B	207	ARG
2	B	208	LEU
2	B	217	PHE
2	B	224	ILE
2	B	230	MET
2	B	233	LEU
2	B	318	LEU
2	B	326	ILE
2	B	330	LEU
2	B	345	ARG

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Mol	Chain	Res	Type
2	B	352	LEU
2	B	374	LYS
2	B	376	LYS
2	B	421	ASN
2	B	470	VAL
2	B	529	LEU
2	B	592	VAL
2	B	643	LEU
2	B	657	ILE
2	B	697	LEU
2	B	711	LEU
2	B	730	ILE
2	B	733	THR
2	B	735	TYR
2	B	783	VAL
2	B	872	LEU
2	B	887	GLN
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	1029	LEU
2	B	1061	ILE
2	B	1070	ILE
2	B	1077	LYS
2	B	1081	VAL
2	B	1102	LEU
3	C	70	ILE
3	C	159	ASP
3	C	180	THR
3	C	190	ARG
3	C	196	PHE
3	C	208	ILE
3	C	210	PHE
3	C	216	ILE
3	C	219	LEU
3	C	231	ILE
3	C	232	LYS

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Mol	Chain	Res	Type
3	C	237	ILE
3	C	244	LYS
3	C	291	GLU
3	C	306	LEU
3	C	307	ASP
3	C	315	LEU
3	C	319	VAL
3	C	386	VAL
4	D	163	ILE
5	E	16	ASN
5	E	27	LEU
5	E	61	PHE
5	E	90	LEU
5	E	93	ASP
5	E	120	TYR
5	E	122	ASN
5	E	126	ILE
6	F	36	ARG
6	F	41	LEU
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	52	LYS
7	G	64	LEU
7	G	79	THR
7	G	101	LEU
7	G	109	LYS
8	H	48	SER
9	K	59	THR
11	N	61	HIS
12	P	5	ARG
13	Q	36	LEU
13	Q	46	LYS
13	Q	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	272	HIS
1	A	357	ASN
1	A	363	GLN
1	A	420	ASN
2	B	613	GLN
2	B	640	HIS
2	B	664	ASN
2	B	686	ASN
2	B	723	ASN
2	B	798	ASN
2	B	885	HIS
2	B	926	GLN
2	B	957	GLN
2	B	997	HIS
2	B	1078	ASN
3	C	339	ASN
7	G	25	ASN
7	G	88	ASN
10	L	82	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	872/880 (99%)	0.40	61 (6%)	22	14	50, 78, 123, 165	0
2	B	1103/1131 (97%)	0.40	53 (4%)	35	22	49, 77, 118, 173	0
3	C	376/395 (95%)	0.53	31 (8%)	17	11	52, 86, 126, 185	0
4	D	262/265 (98%)	0.38	10 (3%)	44	27	67, 87, 118, 140	0
5	E	171/180 (95%)	1.10	26 (15%)	5	4	63, 123, 158, 178	0
6	F	105/113 (92%)	1.24	14 (13%)	7	6	94, 137, 169, 215	0
7	G	113/132 (85%)	1.10	16 (14%)	6	5	69, 103, 127, 157	0
8	H	76/84 (90%)	0.46	5 (6%)	24	15	62, 79, 104, 121	0
9	K	84/95 (88%)	0.23	5 (5%)	27	17	58, 71, 111, 137	0
10	L	91/92 (98%)	0.18	1 (1%)	78	61	62, 84, 107, 159	0
11	N	65/66 (98%)	0.40	6 (9%)	14	9	62, 81, 102, 112	0
12	P	44/48 (91%)	1.21	11 (25%)	2	2	66, 88, 119, 152	0
13	Q	50/104 (48%)	0.70	3 (6%)	27	17	89, 115, 145, 158	0
All	All	3412/3585 (95%)	0.50	242 (7%)	22	14	49, 83, 135, 215	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	340	SER	6.2
5	E	72	PHE	4.9
7	G	92	TYR	4.9
1	A	122	LYS	4.9
2	B	476	MET	4.9
3	C	181	VAL	4.7
3	C	230	LYS	4.7
1	A	40	ILE	4.6
4	D	205	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
5	E	143	ARG	4.6
1	A	151	GLU	4.5
1	A	105	LYS	4.3
1	A	82	ILE	4.3
11	N	65	PRO	4.2
2	B	254	GLU	4.2
2	B	261	GLN	4.2
1	A	103	ARG	4.2
4	D	47	ILE	4.1
1	A	684	LEU	4.1
2	B	1118	LEU	4.1
5	E	104	MET	4.1
11	N	63	THR	4.0
1	A	138	LYS	3.9
6	F	104	ILE	3.9
12	P	18	LEU	3.8
11	N	1	MET	3.8
1	A	119	ASN	3.8
12	P	10	TRP	3.8
6	F	72	LEU	3.7
1	A	865	THR	3.6
2	B	876	SER	3.6
7	G	48	ILE	3.6
7	G	93	ILE	3.6
7	G	91	ARG	3.6
8	H	83	SER	3.5
1	A	879	LYS	3.5
1	A	285	PRO	3.5
6	F	14	TYR	3.4
2	B	7	ASN	3.4
2	B	26	LEU	3.4
1	A	148	HIS	3.4
2	B	380	ARG	3.4
1	A	111	ILE	3.4
5	E	98	PHE	3.3
6	F	100	ILE	3.3
11	N	45	CYS	3.3
1	A	161	PRO	3.3
7	G	40	PHE	3.3
1	A	114	TYR	3.2
2	B	399	HIS	3.2
7	G	95	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	734	ARG	3.2
1	A	233	ASP	3.2
2	B	217	PHE	3.2
2	B	592	VAL	3.2
5	E	86	GLU	3.1
2	B	271	ALA	3.1
7	G	82	LYS	3.1
1	A	108	GLU	3.1
2	B	769	PRO	3.1
1	A	229	ILE	3.1
1	A	24	VAL	3.1
1	A	157	LYS	3.1
6	F	78	ILE	3.1
13	Q	36	LEU	3.1
6	F	27	SER	3.1
7	G	102	LEU	3.0
2	B	435	SER	3.0
3	C	216	ILE	3.0
11	N	10	CYS	3.0
2	B	175	VAL	3.0
7	G	99	PHE	3.0
2	B	730	ILE	3.0
6	F	3	SER	2.9
5	E	146	VAL	2.9
5	E	136	ILE	2.9
5	E	85	VAL	2.9
5	E	1	MET	2.9
4	D	6	LEU	2.9
1	A	813	THR	2.9
1	A	107	SER	2.9
2	B	379	GLY	2.9
2	B	1070	ILE	2.9
2	B	267	ASN	2.9
1	A	150	GLY	2.9
1	A	707	LEU	2.9
12	P	23	GLY	2.9
1	A	123	LYS	2.9
8	H	13	ILE	2.9
9	K	29	ARG	2.8
1	A	371	LYS	2.8
1	A	815	GLN	2.8
3	C	341	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	339	ASN	2.8
2	B	260	GLU	2.8
1	A	41	GLU	2.8
3	C	234	ILE	2.8
1	A	33	TYR	2.8
2	B	199	TYR	2.8
6	F	77	PRO	2.8
3	C	231	ILE	2.8
1	A	38	THR	2.7
3	C	101	THR	2.7
8	H	15	TYR	2.7
3	C	42	LEU	2.7
1	A	102	GLY	2.7
1	A	600	LYS	2.7
13	Q	44	LEU	2.7
3	C	173	MET	2.7
1	A	532	ILE	2.7
1	A	104	VAL	2.7
7	G	81	LEU	2.7
2	B	275	ILE	2.6
5	E	103	PRO	2.6
2	B	733	THR	2.6
3	C	188	ILE	2.6
3	C	25	PRO	2.6
3	C	163	MET	2.6
5	E	151	SER	2.6
6	F	61	SER	2.6
1	A	738	LEU	2.6
5	E	142	VAL	2.6
7	G	97	SER	2.6
8	H	14	HIS	2.6
2	B	218	PRO	2.6
4	D	263	VAL	2.6
12	P	32	LYS	2.6
2	B	487	ILE	2.5
13	Q	38	ILE	2.5
5	E	87	GLY	2.5
2	B	382	LEU	2.5
6	F	99	ASP	2.5
1	A	232	GLU	2.5
4	D	116	SER	2.5
3	C	218	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	224	ILE	2.5
5	E	127	ILE	2.5
3	C	86	THR	2.5
7	G	36	PHE	2.5
2	B	781	PRO	2.5
1	A	708	ARG	2.5
5	E	44	LEU	2.5
9	K	94	LYS	2.5
3	C	110	ILE	2.5
2	B	256	PHE	2.5
1	A	162	TYR	2.5
12	P	43	LYS	2.5
6	F	75	ILE	2.5
2	B	108	ASN	2.5
6	F	56	VAL	2.5
5	E	128	PHE	2.4
1	A	25	THR	2.4
2	B	838	THR	2.4
5	E	93	ASP	2.4
2	B	53	PRO	2.4
2	B	517	TYR	2.4
5	E	77	TYR	2.4
5	E	84	VAL	2.4
2	B	229	LEU	2.4
4	D	234	GLY	2.4
1	A	75	ILE	2.4
2	B	438	ARG	2.4
7	G	79	THR	2.4
7	G	77	ILE	2.4
7	G	106	ILE	2.4
2	B	551	GLU	2.4
1	A	187	VAL	2.4
1	A	228	GLY	2.4
1	A	304	GLY	2.4
9	K	54	ASN	2.4
1	A	35	GLU	2.4
4	D	168	PRO	2.4
1	A	791	LYS	2.3
2	B	171	ALA	2.3
9	K	60	ASP	2.3
1	A	268	LEU	2.3
2	B	144	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	206	GLU	2.3
3	C	235	LYS	2.3
1	A	878	TRP	2.3
3	C	145	GLU	2.3
12	P	28	TYR	2.3
1	A	113	LYS	2.3
1	A	110	GLU	2.3
5	E	51	VAL	2.3
3	C	161	ALA	2.3
3	C	229	THR	2.3
3	C	209	SER	2.3
2	B	343	ASN	2.3
12	P	20	VAL	2.3
7	G	39	SER	2.2
1	A	156	ILE	2.2
5	E	174	TRP	2.2
4	D	70	GLU	2.2
1	A	31	ASP	2.2
3	C	193	LEU	2.2
10	L	91	THR	2.2
2	B	540	ALA	2.2
3	C	236	GLY	2.2
1	A	154	PHE	2.2
3	C	394	LEU	2.2
2	B	886	GLY	2.2
3	C	6	ASP	2.2
1	A	200	THR	2.1
2	B	237	THR	2.1
3	C	232	LYS	2.1
1	A	622	GLU	2.1
2	B	211	GLY	2.1
12	P	5	ARG	2.1
12	P	45	VAL	2.1
2	B	1060	THR	2.1
1	A	806	LEU	2.1
2	B	330	LEU	2.1
3	C	219	LEU	2.1
12	P	17	GLN	2.1
2	B	246	SER	2.1
5	E	83	GLU	2.1
6	F	44	VAL	2.1
1	A	45	MET	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	159	ARG	2.1
4	D	189	GLU	2.1
2	B	806	GLU	2.1
1	A	692	LEU	2.1
11	N	5	ILE	2.1
9	K	52	ASP	2.1
3	C	205	THR	2.1
12	P	9	CYS	2.1
3	C	100	VAL	2.0
5	E	80	VAL	2.0
8	H	46	ARG	2.0
2	B	219	ALA	2.0
2	B	593	THR	2.0
6	F	96	THR	2.0
2	B	13	ARG	2.0
5	E	4	LEU	2.0
1	A	676	ILE	2.0
3	C	158	ILE	2.0
5	E	95	TYR	2.0
2	B	1087	ASP	2.0
1	A	677	GLN	2.0
2	B	516	GLU	2.0
4	D	13	ILE	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 oligosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	A	1884	1/1	0.69	0.28	81,81,81,81	0
14	ZN	A	1882	1/1	0.90	0.25	81,81,81,81	0
14	ZN	B	2127	1/1	0.91	0.19	81,81,81,81	0
14	ZN	B	2128	1/1	0.93	0.25	81,81,81,81	0
14	ZN	A	1881	1/1	0.93	0.13	81,81,81,81	0
14	ZN	A	1883	1/1	0.94	0.15	81,81,81,81	0
14	ZN	P	1049	1/1	0.95	0.06	118,118,118,118	0
14	ZN	C	1395	1/1	0.95	0.07	81,81,81,81	0
16	SF4	D	1264	7/8	0.95	0.13	81,81,81,81	0
14	ZN	A	1880	1/1	0.96	0.05	81,81,81,81	0
14	ZN	B	2126	1/1	0.96	0.05	81,81,81,81	0
14	ZN	N	1066	1/1	0.97	0.06	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.