



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:22 PM UTC

PDB ID : 4KN4 / pdb_00004kn4
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Benzoxazinorifamycin-2b
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.96 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

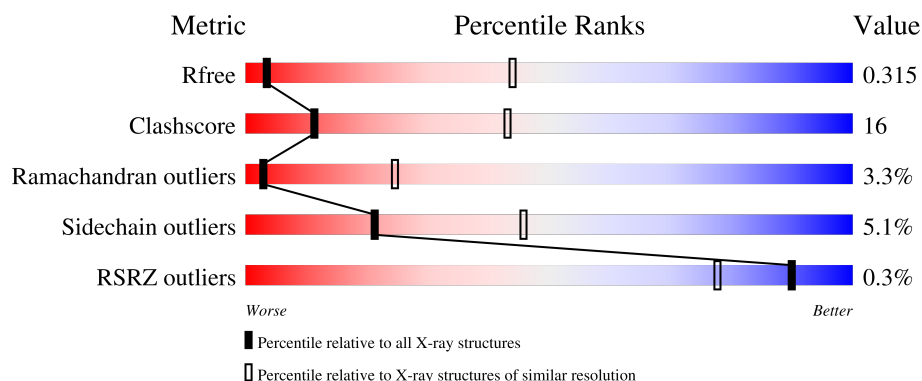
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	329	71% 23% ••
1	B	329	47% 18% • 33%
1	F	329	53% 16% • 30%
1	G	329	% 51% 14% • 34%
2	C	1342	65% 30% ••

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Mol	Chain	Length	Quality of chain
2	H	1342	67%28%
3	D	1407	48%31% 18%
3	I	1407	50%29% 18%
4	E	91	73%22%
4	J	91	59%21% 16%
5	X	613	%59%23% 16%
5	Y	613	55%18% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56333 atoms, of which 122 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

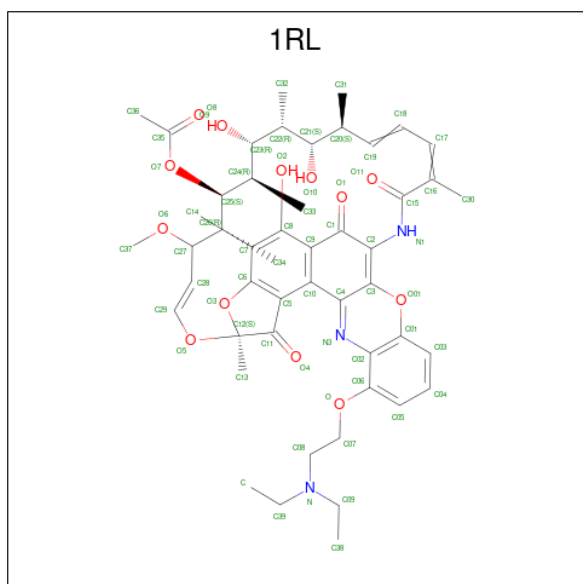
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is Benzoxazinorifamycin-2b (CCD ID: 1RL) (formula: $C_{49}H_{61}N_3O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			126	49	61	3	13		
6	H	1	Total	C	H	N	O	0	0
			126	49	61	3	13		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

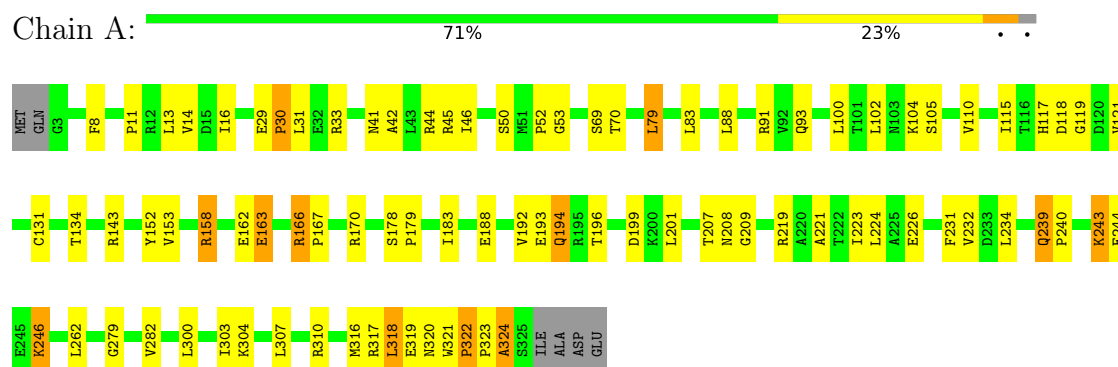
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		
8	I	1	Total	Mg	0	0
			1	1		

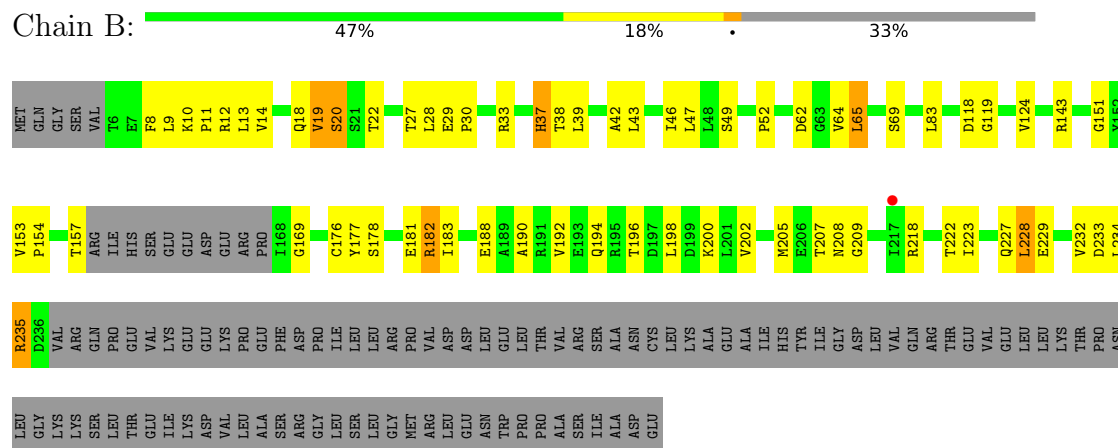
3 Residue-property plots

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.

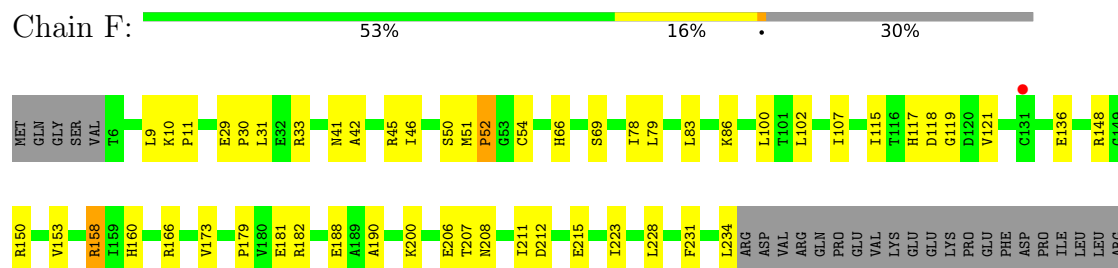
• Molecule 1: DNA-directed RNA polymerase subunit alpha



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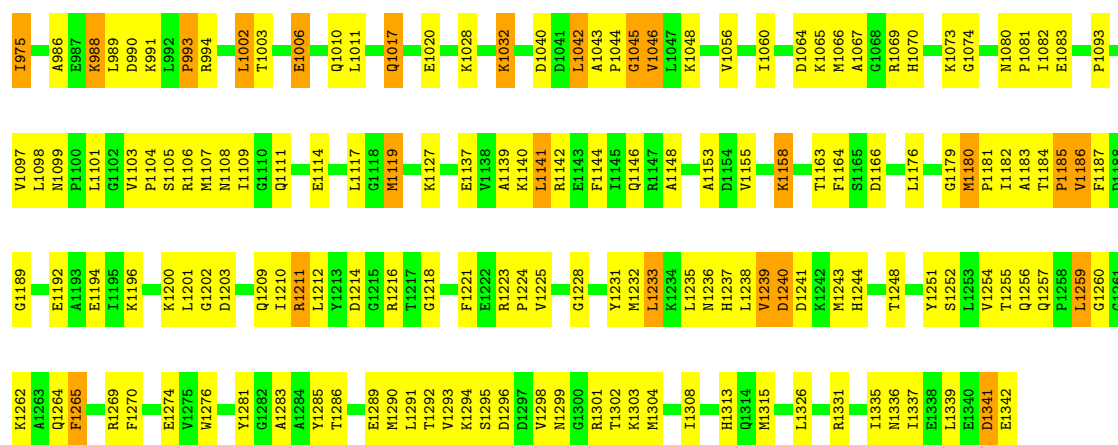
[illegible]

- Molecule 1: DNA-directed RNA polymerase subunit alpha

[illegible]

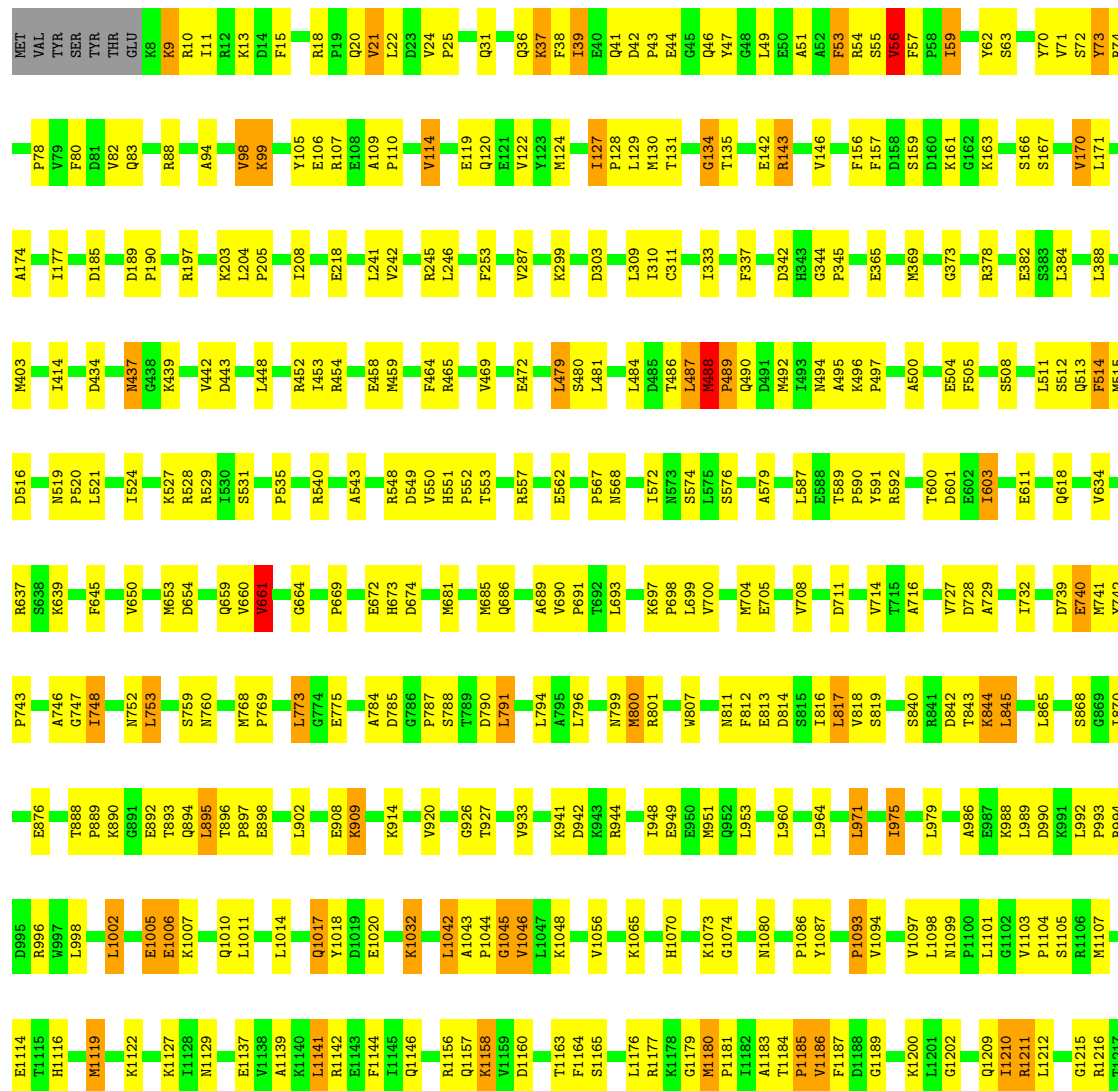
- Molecule 2: DNA-directed RNA polymerase subunit beta

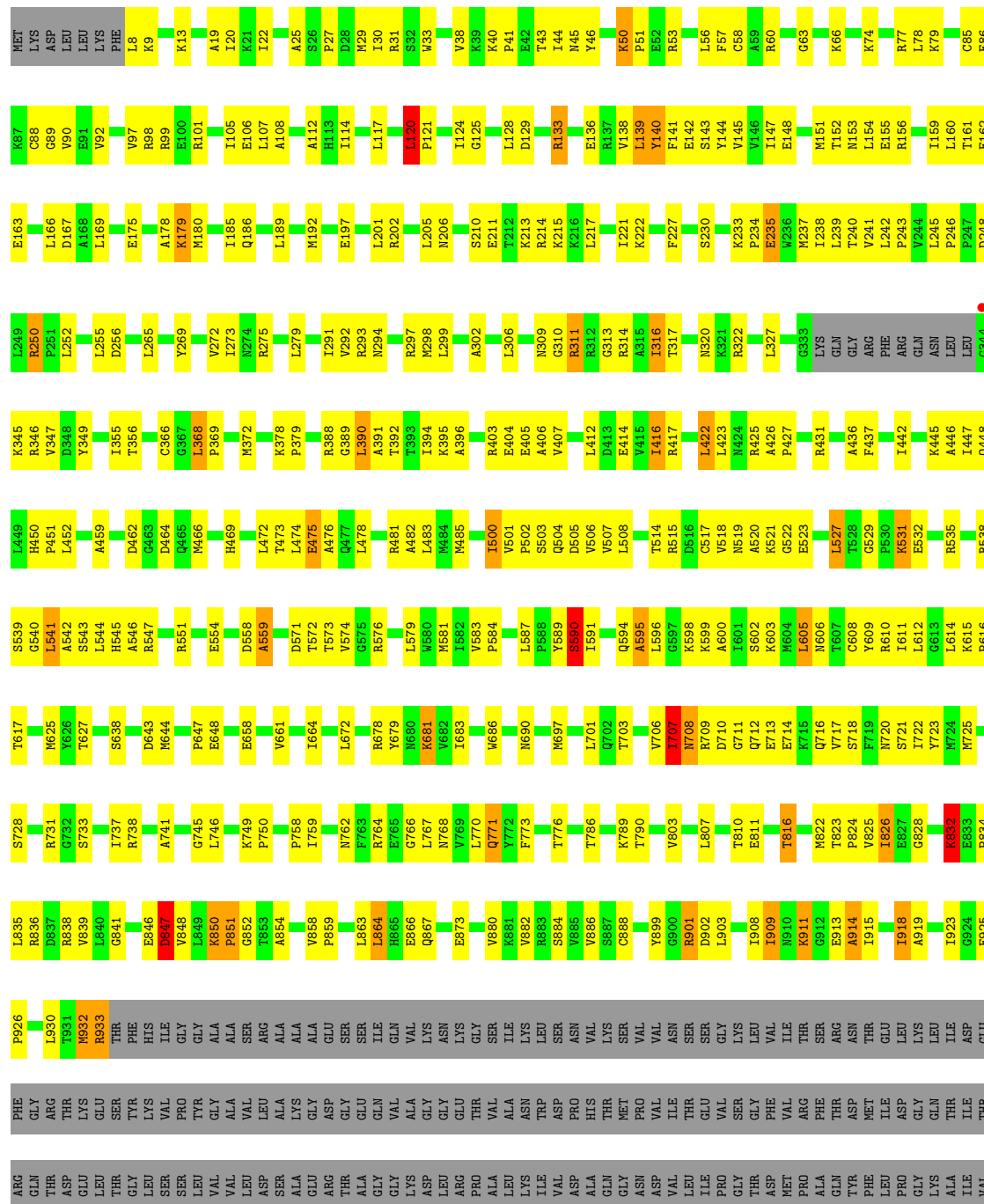
[illegible]

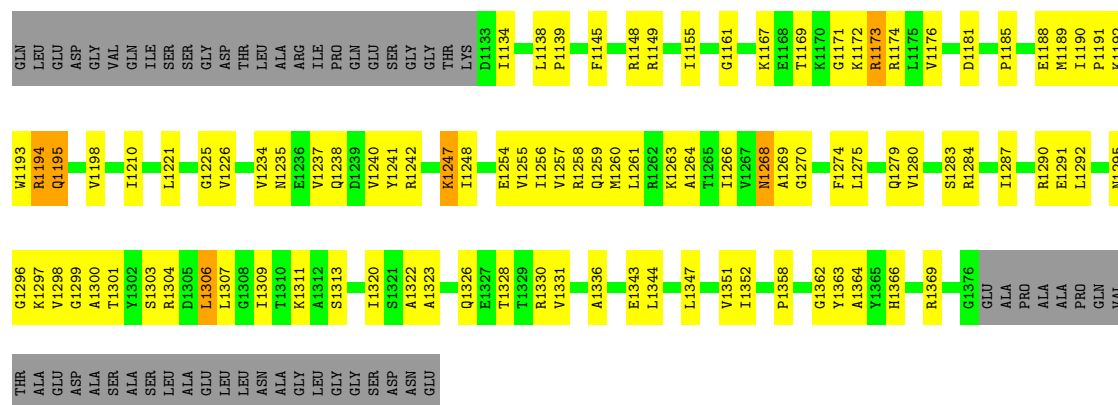


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain H: 67% 28% . .

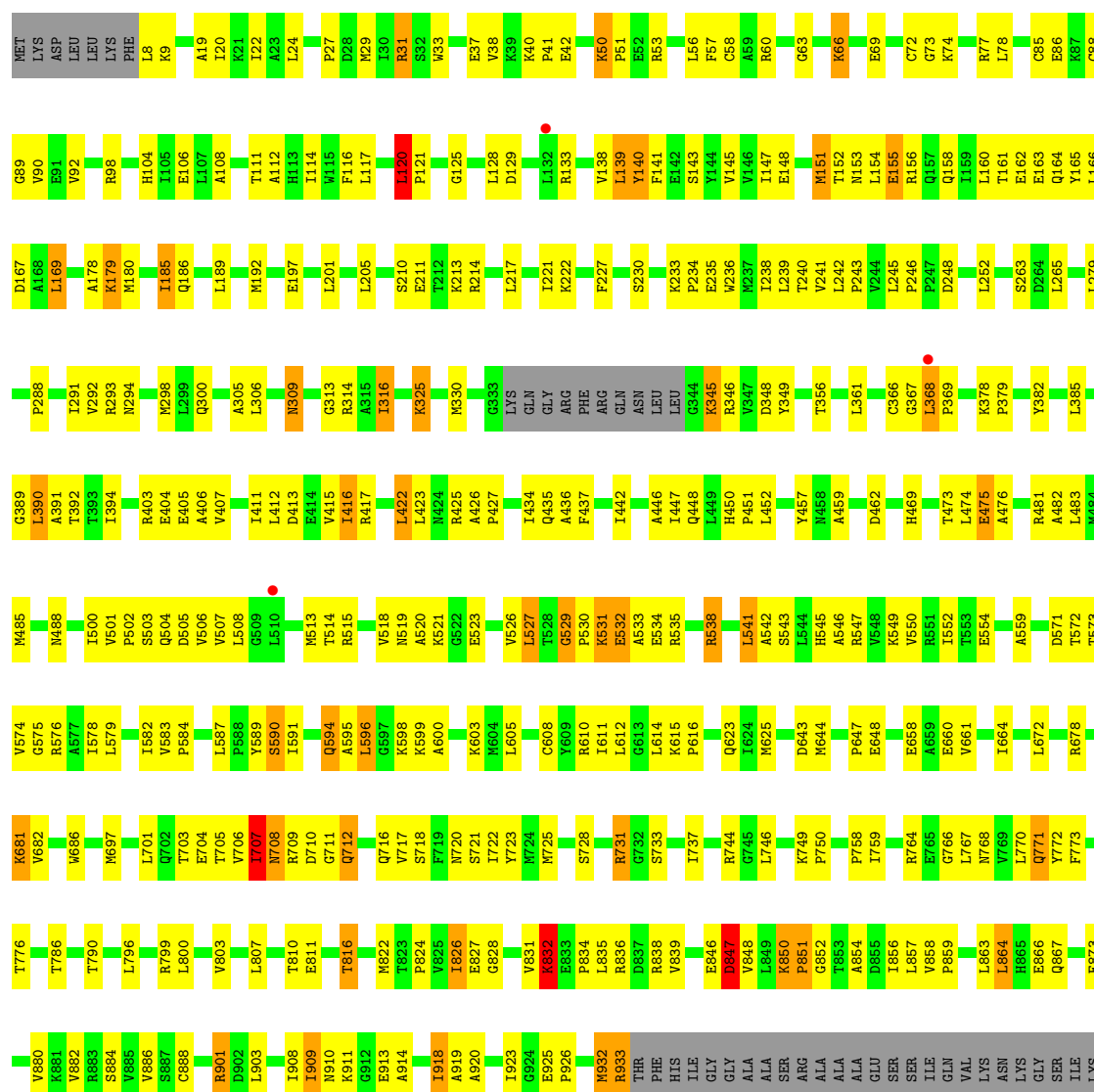


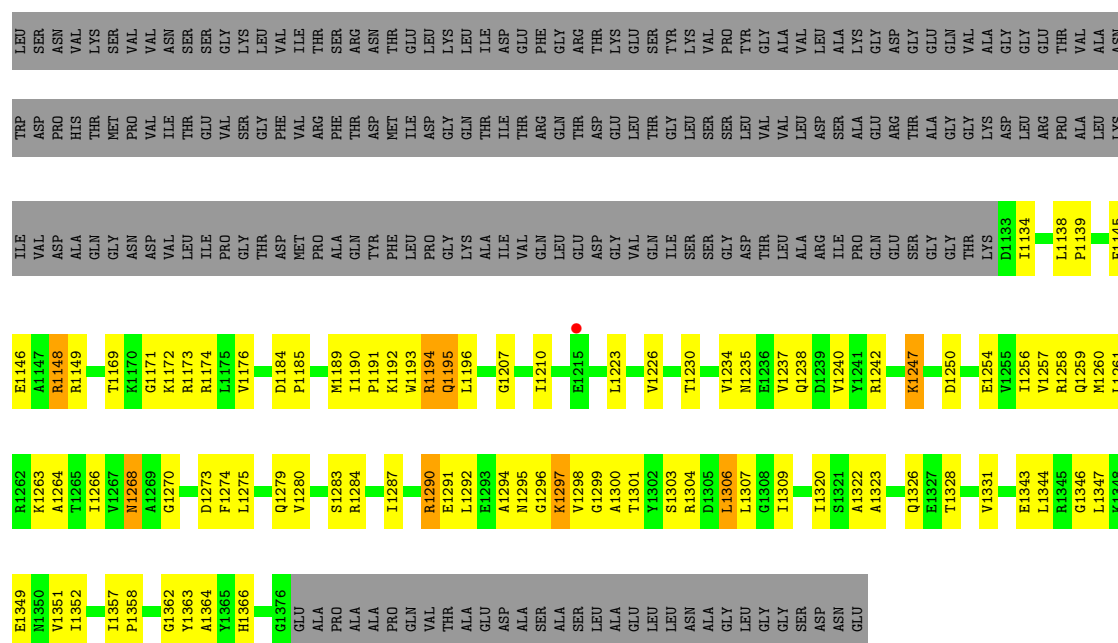




● Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain I: 50% 29% 18%





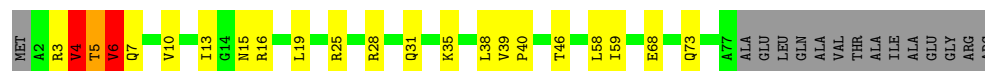
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 73% 22% . . .



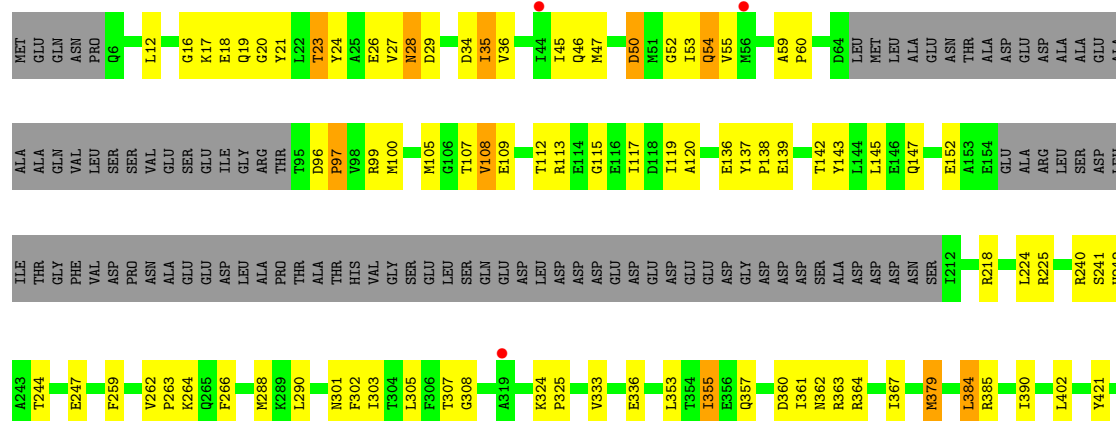
- Molecule 4: DNA-directed RNA polymerase subunit omega

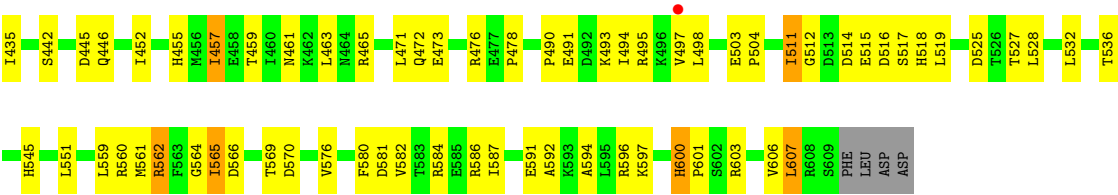
Chain J: 59% 21% . . 16%



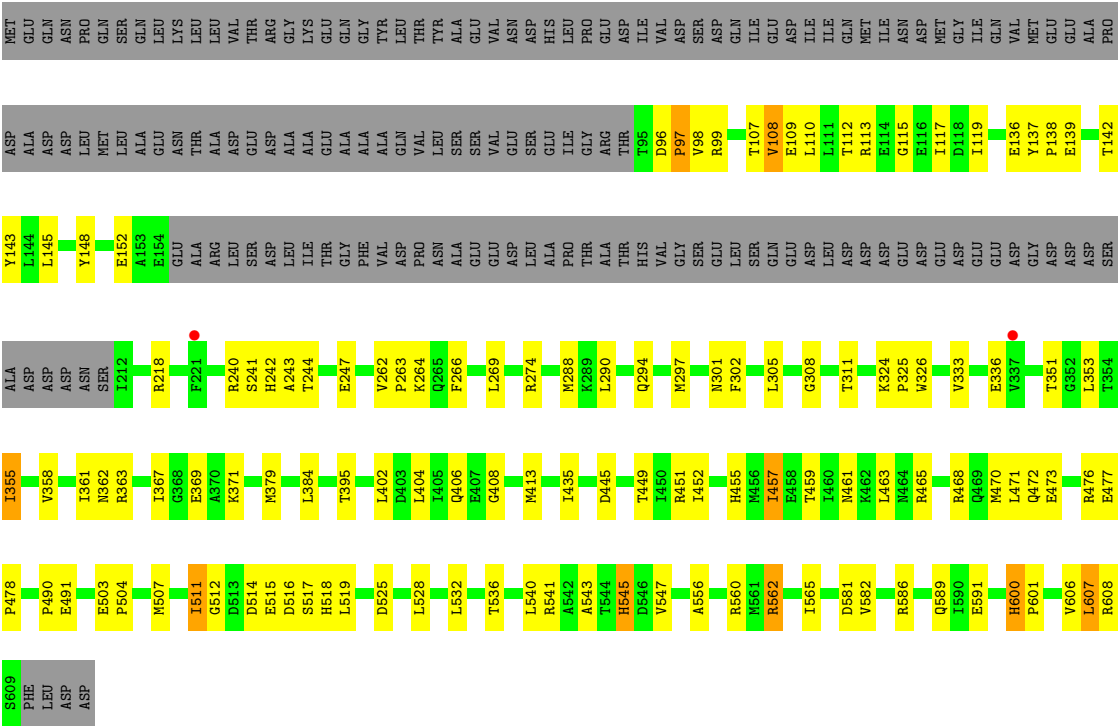
- Molecule 5: RNA polymerase sigma factor RpoD

Chain X: % 59% 23% . 16%





● Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.68Å 203.97Å 307.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 3.96 29.77 – 3.96	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.77-3.96) 89.6 (29.77-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.251 , 0.315 0.252 , 0.315	Depositor DCC
R_{free} test set	4761 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	151.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	56333	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: 1RL, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/2548	0.72	1/3454 (0.0%)
1	B	0.25	0/1725	0.69	0/2337
1	F	0.26	0/1797	0.74	3/2436 (0.1%)
1	G	0.25	0/1690	0.68	0/2290
2	C	0.25	0/10690	0.72	7/14423 (0.0%)
2	H	0.25	0/10690	0.72	5/14423 (0.0%)
3	D	0.26	0/9198	0.74	7/12413 (0.1%)
3	I	0.26	0/9198	0.74	7/12413 (0.1%)
4	E	0.25	0/710	0.69	0/956
4	J	0.25	0/607	0.68	0/817
5	X	0.25	0/4253	0.70	0/5719
5	Y	0.25	0/3783	0.68	0/5083
All	All	0.25	0/56889	0.72	30/76764 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	120	LEU	CA-C-N	-7.20	112.00	120.13
3	I	120	LEU	C-N-CA	-7.20	112.00	120.13
3	D	120	LEU	CA-C-N	-7.01	112.21	120.13
3	D	120	LEU	C-N-CA	-7.01	112.21	120.13
2	C	42	ASP	CA-C-N	6.78	128.31	119.84
2	C	42	ASP	C-N-CA	6.78	128.31	119.84
2	H	1184	THR	CA-C-N	5.97	127.31	119.84
2	H	1184	THR	C-N-CA	5.97	127.31	119.84
3	I	529	GLY	CA-C-N	5.91	126.06	119.32
3	I	529	GLY	C-N-CA	5.91	126.06	119.32
3	D	854	ALA	CB-CA-C	-5.88	109.81	116.63
3	I	854	ALA	CB-CA-C	-5.84	109.86	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	986	ALA	CB-CA-C	-5.77	109.94	116.63
2	C	1184	THR	CA-C-N	5.75	127.02	119.84
2	C	1184	THR	C-N-CA	5.75	127.02	119.84
1	F	212	ASP	CA-C-N	5.59	125.43	119.28
1	F	212	ASP	C-N-CA	5.59	125.43	119.28
3	D	368	LEU	CA-C-N	5.56	125.57	119.90
3	D	368	LEU	C-N-CA	5.56	125.57	119.90
2	C	986	ALA	CB-CA-C	-5.54	110.21	116.63
3	D	529	GLY	CA-C-N	5.51	125.60	119.32
3	D	529	GLY	C-N-CA	5.51	125.60	119.32
3	I	368	LEU	CA-C-N	5.32	125.33	119.90
3	I	368	LEU	C-N-CA	5.32	125.33	119.90
1	F	78	ILE	N-CA-C	5.28	116.00	110.62
2	C	566	GLY	CA-C-N	5.24	124.94	119.64
2	C	566	GLY	C-N-CA	5.24	124.94	119.64
1	A	152	TYR	CB-CA-C	-5.12	110.26	117.23
2	H	242	VAL	CA-C-N	5.04	125.07	119.32
2	H	242	VAL	C-N-CA	5.04	125.07	119.32

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	2514	0	2566	68	0
1	B	1706	0	1738	62	0
1	F	1775	0	1800	40	0
1	G	1671	0	1706	46	0
2	C	10523	0	10546	385	0
2	H	10523	0	10546	357	0
3	D	9060	0	9256	404	0
3	I	9060	0	9255	364	0
4	E	708	0	719	21	0
4	J	605	0	612	18	0
5	X	4198	0	4250	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	3732	0	3809	81	0
6	C	65	61	61	5	0
6	H	65	61	61	10	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56211	122	56925	1828	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 16.

All (1828) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.32	1.10
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.34	1.09
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.30	1.06
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.34	1.04
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.35	1.03
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.40	1.01
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.45	0.98
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.46	0.98
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.46	0.97
4:J:5:THR:HA	4:J:6:VAL:HB	1.46	0.96
2:H:54:ARG:H	2:H:55:SER:HB2	1.28	0.95
4:E:5:THR:HA	4:E:6:VAL:HB	1.46	0.95
2:H:487:LEU:HB3	2:H:488:MET:HA	1.48	0.94
2:H:488:MET:HB2	2:H:490:GLN:H	1.29	0.94
6:H:1401:1RL:H322	6:H:1401:1RL:H313	1.48	0.93
2:C:163:LYS:H	2:C:163:LYS:HD3	1.32	0.92
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.48	0.92
4:E:5:THR:HA	4:E:6:VAL:CB	2.00	0.90
6:C:1401:1RL:H322	6:C:1401:1RL:H313	1.53	0.90
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.55	0.88
4:J:5:THR:HA	4:J:6:VAL:CB	2.02	0.87
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.03	0.87
2:H:488:MET:HB2	2:H:490:GLN:N	1.89	0.87
2:C:54:ARG:H	2:C:55:SER:HB2	1.38	0.87
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.55	0.86
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.56	0.86
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.56	0.85
2:H:487:LEU:CB	2:H:488:MET:HA	2.06	0.84
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.08	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.05	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.60	0.82
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.62	0.82
4:J:5:THR:CA	4:J:6:VAL:HB	2.09	0.82
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.08	0.81
2:H:908:GLU:HG2	2:H:909:LYS:H	1.43	0.81
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.63	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.61	0.80
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.62	0.79
2:H:800:MET:HA	2:H:800:MET:HE3	1.63	0.79
3:D:643:ASP:O	3:D:720:ASN:ND2	2.16	0.79
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.63	0.78
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.64	0.78
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.14	0.78
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.63	0.78
2:H:487:LEU:HB3	2:H:488:MET:CA	2.13	0.77
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.77
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.66	0.77
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.65	0.76
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.67	0.76
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.68	0.76
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.50	0.75
4:E:5:THR:CA	4:E:6:VAL:HB	2.15	0.75
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.69	0.75
1:G:45:ARG:O	3:I:538:ARG:NH2	2.20	0.75
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.75
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.68	0.75
2:C:131:THR:HG21	2:C:135:THR:HG22	1.67	0.74
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.68	0.74
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.69	0.74
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.68	0.74
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.18	0.74
2:H:99:LYS:HD3	2:H:99:LYS:N	2.02	0.73
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.68	0.73
2:C:800:MET:HA	2:C:800:MET:HE3	1.69	0.73
5:X:35:ILE:HG13	5:X:36:VAL:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:ARG:N	2:H:55:SER:HB2	2.01	0.73
2:H:142:GLU:HG2	2:H:515:MET:SD	2.27	0.73
3:I:850:LYS:O	3:I:852:GLY:N	2.21	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.54	0.73
2:C:131:THR:CG2	2:C:135:THR:HG22	2.19	0.72
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.71	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.19	0.72
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.25	0.72
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.19	0.72
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.70	0.72
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.71	0.72
1:B:29:GLU:HA	1:B:200:LYS:CB	2.18	0.72
3:D:822:MET:SD	3:D:838:ARG:NH1	2.63	0.72
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.72	0.72
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.23	0.71
3:D:151:MET:SD	3:D:151:MET:N	2.63	0.71
1:G:65:LEU:HD23	1:G:65:LEU:H	1.55	0.71
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.70	0.71
3:D:850:LYS:O	3:D:852:GLY:N	2.22	0.71
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.72	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.72	0.71
2:H:516:ASP:HB2	6:H:1401:1RL:H201	1.73	0.71
2:C:55:SER:CB	2:C:56:VAL:HG22	2.17	0.71
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.72	0.71
2:H:131:THR:CG2	2:H:135:THR:HG22	2.21	0.70
3:D:1362:GLY:O	3:D:1364:ALA:N	2.24	0.70
2:C:134:GLY:O	2:C:527:LYS:NZ	2.24	0.70
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.74	0.70
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.55	0.70
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.27	0.70
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.74	0.70
2:H:55:SER:CB	2:H:56:VAL:HG22	2.22	0.70
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.57	0.70
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.74	0.69
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.74	0.69
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.22	0.69
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.56	0.69
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.58	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.75	0.69
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:GLN:O	2:C:22:LEU:N	2.25	0.69
2:C:37:LYS:HA	2:C:37:LYS:HE3	1.75	0.69
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.69
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.73	0.69
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.76	0.69
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.57	0.68
3:D:1191:PRO:O	3:D:1193:TRP:N	2.26	0.68
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.57	0.68
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.75	0.68
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.75	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.58	0.68
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.68
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.76	0.68
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.75	0.68
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.68
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.76	0.68
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.75	0.68
3:D:405:GLU:O	3:D:407:VAL:N	2.27	0.68
2:H:664:GLY:O	2:H:686:GLN:NE2	2.27	0.68
3:I:720:ASN:O	3:I:722:ILE:N	2.27	0.68
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.76	0.67
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.76	0.67
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.77	0.67
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.76	0.67
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.29	0.67
3:I:1191:PRO:O	3:I:1193:TRP:N	2.27	0.67
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.29	0.67
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.25	0.67
2:C:54:ARG:CG	2:C:55:SER:HB2	2.25	0.67
2:H:21:VAL:HG13	2:H:22:LEU:H	1.59	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.77	0.67
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.25	0.66
2:H:54:ARG:H	2:H:55:SER:CB	2.05	0.66
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.75	0.66
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.27	0.66
5:X:240:ARG:HD3	5:X:244:THR:HB	1.75	0.66
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.76	0.66
3:D:245:LEU:O	3:D:250:ARG:NH1	2.29	0.66
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.77	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:511:ILE:HG23	5:X:512:GLY:H	1.58	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
2:C:529:ARG:CZ	6:C:1401:1RL:H171	2.25	0.66
3:I:139:LEU:HD13	3:I:140:TYR:N	2.11	0.66
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.25	0.66
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.25	0.66
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.61	0.66
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.77	0.66
3:D:610:ARG:HG2	3:D:864:LEU:HD22	1.78	0.66
3:D:711:GLY:O	3:D:712:GLN:HG2	1.95	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.29	0.66
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.11	0.66
3:D:139:LEU:HD13	3:D:140:TYR:N	2.11	0.65
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.77	0.65
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.77	0.65
2:C:54:ARG:N	2:C:55:SER:HB2	2.09	0.65
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.31	0.65
3:D:932:MET:O	3:D:933:ARG:HG3	1.96	0.65
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.78	0.65
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.78	0.65
2:C:402:ARG:NH2	2:C:419:ILE:O	2.30	0.65
3:D:546:ALA:N	3:D:547:ARG:HA	2.11	0.65
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.77	0.65
3:I:643:ASP:O	3:I:720:ASN:ND2	2.21	0.65
2:C:845:LEU:HD13	2:C:845:LEU:H	1.60	0.65
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.25	0.65
2:H:1239:VAL:O	2:H:1241:ASP:N	2.30	0.65
2:C:119:GLU:CD	2:C:489:PRO:HG2	2.22	0.65
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.77	0.65
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.78	0.65
1:B:12:ARG:H	1:B:30:PRO:HG2	1.60	0.65
1:B:49:SER:HA	1:B:151:GLY:HA2	1.78	0.65
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.97	0.65
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.77	0.65
3:I:546:ALA:N	3:I:547:ARG:HA	2.11	0.65
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.78	0.65
1:G:227:GLN:C	1:G:228:LEU:HD23	2.21	0.65
2:H:127:ILE:H	2:H:127:ILE:HD13	1.62	0.65
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.62	0.65
2:H:131:THR:HG21	2:H:135:THR:HG22	1.76	0.65
2:H:488:MET:HE3	2:H:489:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.79	0.65
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.78	0.65
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.30	0.65
3:D:546:ALA:H	3:D:547:ARG:HA	1.61	0.64
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.77	0.64
5:X:476:ARG:H	5:X:476:ARG:HD2	1.62	0.64
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.78	0.64
3:I:546:ALA:H	3:I:547:ARG:HA	1.62	0.64
2:H:845:LEU:HD13	2:H:845:LEU:H	1.62	0.64
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.33	0.64
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.27	0.64
3:I:151:MET:SD	3:I:151:MET:N	2.70	0.64
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.78	0.64
3:I:450:HIS:NE2	3:I:625:MET:SD	2.71	0.64
3:I:822:MET:SD	3:I:838:ARG:NH1	2.71	0.64
3:D:720:ASN:O	3:D:722:ILE:N	2.31	0.64
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.80	0.64
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.81	0.63
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.80	0.63
2:H:1252:SER:OG	2:H:1255:THR:O	2.15	0.63
3:I:711:GLY:O	3:I:712:GLN:HG2	1.99	0.63
2:C:660:VAL:HG22	2:C:661:VAL:H	1.62	0.63
3:D:389:GLY:O	3:D:391:ALA:N	2.32	0.63
3:I:1362:GLY:O	3:I:1364:ALA:N	2.31	0.63
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.80	0.63
3:I:709:ARG:O	3:I:711:GLY:N	2.32	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.98	0.63
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.63
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.81	0.63
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.80	0.62
2:C:488:MET:N	2:C:489:PRO:HD3	2.15	0.62
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.81	0.62
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.62
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.25	0.62
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.23	0.62
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.14	0.62
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.81	0.62
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.80	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.32	0.62
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.34	0.62
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.32	0.62
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.81	0.62
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.62
2:C:54:ARG:H	2:C:55:SER:CB	2.12	0.62
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.62
2:H:459:MET:SD	2:H:511:LEU:HD22	2.40	0.62
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.81	0.62
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.35	0.62
5:X:517:SER:O	5:X:518:HIS:ND1	2.32	0.62
2:H:504:GLU:O	2:H:508:SER:HB3	2.00	0.62
2:H:529:ARG:NE	6:H:1401:1RL:H171	2.15	0.62
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.80	0.62
5:X:457:ILE:O	5:X:461:ASN:ND2	2.33	0.62
3:I:768:ASN:O	3:I:771:GLN:NE2	2.33	0.61
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.35	0.61
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.61
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.82	0.61
4:E:5:THR:HA	4:E:6:VAL:CG1	2.29	0.61
3:I:389:GLY:O	3:I:391:ALA:N	2.33	0.61
2:C:533:LEU:HG	6:C:1401:1RL:H142	1.83	0.61
2:H:505:PHE:O	2:H:512:SER:OG	2.16	0.61
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.65	0.61
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.30	0.61
1:G:29:GLU:HA	1:G:200:LYS:CB	2.30	0.61
2:H:590:PRO:O	2:H:659:GLN:NE2	2.33	0.61
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.83	0.61
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.83	0.61
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.82	0.61
2:H:99:LYS:HD3	2:H:99:LYS:H	1.65	0.61
3:D:316:ILE:HG23	3:D:317:THR:H	1.66	0.61
5:X:139:GLU:HA	5:X:142:THR:HG22	1.82	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.15	0.61
2:C:768:MET:O	2:C:785:ASP:N	2.33	0.61
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.81	0.61
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.81	0.61
3:I:145:VAL:HG22	3:I:180:MET:SD	2.40	0.61
2:C:189:ASP:OD1	2:C:193:ASN:N	2.29	0.61
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.61
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.16	0.61
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.83	0.60
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.26	0.60
2:C:127:ILE:H	2:C:127:ILE:HD13	1.67	0.60
2:C:1200:LYS:O	2:C:1202:GLY:N	2.33	0.60
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.84	0.60
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.82	0.60
3:D:120:LEU:CB	3:D:121:PRO:CD	2.78	0.60
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.37	0.60
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.65	0.60
2:H:163:LYS:H	2:H:163:LYS:HD3	1.66	0.60
3:I:589:TYR:O	3:I:591:ILE:N	2.35	0.60
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.83	0.60
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.84	0.60
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.31	0.60
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.35	0.60
3:D:79:LYS:HE3	5:X:569:THR:N	2.17	0.60
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.35	0.60
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.84	0.60
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.82	0.60
5:X:379:MET:HE2	5:X:379:MET:HA	1.84	0.60
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.32	0.60
2:H:660:VAL:HG22	2:H:661:VAL:H	1.65	0.60
2:H:768:MET:O	2:H:785:ASP:N	2.35	0.60
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.84	0.59
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.32	0.59
6:H:1401:1RL:O10	6:H:1401:1RL:O9	2.17	0.59
3:I:405:GLU:O	3:I:407:VAL:N	2.35	0.59
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.32	0.59
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.84	0.59
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.38	0.59
3:D:546:ALA:H	3:D:547:ARG:CA	2.14	0.59
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.36	0.59
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.84	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.33	0.59
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.59
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.85	0.59
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.35	0.59
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.38	0.59
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.35	0.59
2:C:309:LEU:HD23	2:C:309:LEU:H	1.68	0.59
3:D:56:LEU:O	3:D:250:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:240:ARG:O	5:X:242:HIS:N	2.35	0.59
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.67	0.59
3:I:88:CYS:O	3:I:90:VAL:N	2.36	0.59
2:C:752:ASN:O	2:C:753:LEU:HG	2.03	0.59
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.67	0.59
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.85	0.59
2:C:143:ARG:NH1	2:C:512:SER:O	2.36	0.58
2:H:20:GLN:O	2:H:22:LEU:N	2.36	0.58
2:H:309:LEU:HD23	2:H:309:LEU:H	1.68	0.58
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.38	0.58
3:I:514:THR:HG23	3:I:576:ARG:HE	1.68	0.58
3:I:828:GLY:HA2	3:I:832:LYS:N	2.18	0.58
3:I:1173:ARG:HB3	3:I:1174:ARG:O	2.02	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.33	0.58
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.38	0.58
3:D:316:ILE:HG13	3:D:317:THR:N	2.18	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.85	0.58
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.68	0.58
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.03	0.58
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.38	0.58
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.85	0.58
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.28	0.58
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.36	0.58
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.34	0.58
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.33	0.58
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.21	0.58
2:C:660:VAL:O	2:C:661:VAL:HG22	2.03	0.58
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.85	0.58
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.16	0.58
3:D:932:MET:SD	3:D:932:MET:N	2.74	0.58
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.86	0.58
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.85	0.58
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.58
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.34	0.58
2:C:142:GLU:HG2	2:C:515:MET:SD	2.43	0.58
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.03	0.58
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.04	0.58
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.86	0.58
5:X:584:ARG:O	5:X:587:ILE:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.37	0.58
3:I:827:GLU:O	3:I:831:VAL:HG12	2.03	0.58
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.39	0.58
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.39	0.58
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.36	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.69	0.58
2:C:106:GLU:N	2:C:107:ARG:HA	2.18	0.57
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.84	0.57
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.86	0.57
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.39	0.57
2:C:510:GLN:O	2:C:511:LEU:HB2	2.04	0.57
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.18	0.57
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.86	0.57
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.34	0.57
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.04	0.57
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.57
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.69	0.57
2:C:526:HIS:HA	2:C:529:ARG:NH1	2.19	0.57
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.85	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.34	0.57
2:H:106:GLU:N	2:H:107:ARG:HA	2.19	0.57
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.70	0.57
3:D:316:ILE:HG23	3:D:317:THR:N	2.19	0.57
2:H:54:ARG:CG	2:H:55:SER:HB2	2.34	0.57
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.38	0.57
3:I:828:GLY:HA2	3:I:832:LYS:H	1.69	0.57
2:C:1252:SER:OG	2:C:1255:THR:O	2.21	0.57
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.20	0.57
2:H:38:PHE:O	2:H:39:ILE:HB	2.05	0.57
1:A:207:THR:OG1	1:A:208:ASN:N	2.38	0.57
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.86	0.57
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.40	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.35	0.57
2:H:531:SER:OG	6:H:1401:1RL:O2	2.20	0.57
3:I:546:ALA:H	3:I:547:ARG:CA	2.17	0.57
3:I:583:VAL:HG13	3:I:584:PRO:HD2	1.87	0.57
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.86	0.57
1:B:227:GLN:O	1:B:228:LEU:HG	2.04	0.57
2:C:740:GLU:HB2	2:C:741:MET:SD	2.44	0.57
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.35	0.56
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.34	0.56
3:D:573:THR:HG22	3:D:576:ARG:CD	2.34	0.56
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.69	0.56
3:I:197:GLU:O	3:I:201:LEU:HD23	2.05	0.56
1:B:65:LEU:HD23	1:B:65:LEU:H	1.69	0.56
3:D:546:ALA:HB3	3:D:547:ARG:O	2.05	0.56
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.04	0.56
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.19	0.56
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.38	0.56
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.35	0.56
2:C:741:MET:SD	2:C:741:MET:N	2.78	0.56
2:C:1255:THR:O	2:C:1257:GLN:N	2.36	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.28	0.56
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.87	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.21	0.56
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.87	0.56
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.05	0.56
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.33	0.56
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.37	0.56
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.20	0.56
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.85	0.56
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.21	0.56
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.36	0.56
3:I:545:HIS:HB2	3:I:546:ALA:HA	1.86	0.56
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.86	0.56
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.70	0.56
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.88	0.56
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.88	0.56
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.41	0.56
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.06	0.56
2:H:170:VAL:HG23	2:H:171:LEU:H	1.70	0.56
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.05	0.56
3:I:1297:LYS:HA	3:I:1297:LYS:CE	2.36	0.56
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.88	0.56
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.88	0.56
3:I:120:LEU:CB	3:I:121:PRO:CD	2.83	0.56
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.88	0.56
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.39	0.56
1:A:42:ALA:O	1:A:46:ILE:HG12	2.06	0.56
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.06	0.56
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.87	0.55
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.24	0.55
3:D:29:MET:HA	3:D:29:MET:HE3	1.87	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.87	0.55
5:X:445:ASP:OD1	5:X:445:ASP:N	2.39	0.55
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.31	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.39	0.55
1:G:19:VAL:O	1:G:20:SER:OG	2.17	0.55
2:H:1304:MET:HE1	2:H:1308:ILE:HD11	1.88	0.55
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.88	0.55
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.72	0.55
3:D:128:LEU:HA	3:D:192:MET:HE1	1.88	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.89	0.55
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.89	0.55
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.21	0.55
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.88	0.55
3:D:697:MET:SD	3:D:741:ALA:HB3	2.47	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.42	0.55
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.31	0.55
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.88	0.55
2:H:540:ARG:NH2	2:H:568:ASN:OD1	2.40	0.55
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.89	0.55
2:H:747:GLY:O	2:H:748:ILE:HG13	2.06	0.55
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.06	0.55
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.88	0.55
5:X:363:ARG:O	5:X:367:ILE:HG12	2.07	0.55
3:I:918:ILE:HD13	3:I:919:ALA:N	2.22	0.55
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.07	0.55
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.08	0.54
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.72	0.54
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.89	0.54
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.37	0.54
3:D:142:GLU:HA	3:D:180:MET:HE2	1.90	0.54
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.89	0.54
1:F:9:LEU:O	1:G:227:GLN:NE2	2.40	0.54
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.88	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.89	0.54
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:894:GLN:O	2:C:895:LEU:HB2	2.07	0.54
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.40	0.54
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.37	0.54
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.89	0.54
3:D:546:ALA:H	3:D:547:ARG:C	2.15	0.54
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.89	0.54
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.38	0.54
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.38	0.54
3:I:77:ARG:HG3	3:I:78:LEU:H	1.72	0.54
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.41	0.54
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.21	0.54
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.90	0.54
1:A:91:ARG:NH2	1:A:209:GLY:O	2.40	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.90	0.54
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.89	0.54
3:I:473:THR:HB	3:I:476:ALA:HB2	1.90	0.54
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.73	0.54
2:C:681:MET:O	2:C:685:MET:HG2	2.07	0.54
3:D:858:VAL:HB	3:D:859:PRO:CD	2.29	0.54
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.90	0.54
2:C:496:LYS:N	2:C:497:PRO:HD2	2.21	0.54
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.40	0.54
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.54
3:I:29:MET:HA	3:I:29:MET:HE3	1.90	0.54
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.89	0.54
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.08	0.54
3:D:316:ILE:HG13	3:D:317:THR:H	1.72	0.54
5:X:503:GLU:N	5:X:504:PRO:HA	2.22	0.54
2:H:488:MET:HB2	2:H:489:PRO:CA	2.38	0.54
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.90	0.54
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.90	0.54
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.89	0.54
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.90	0.54
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.88	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.89	0.54
2:H:143:ARG:NH1	2:H:512:SER:O	2.41	0.54
2:C:562:GLU:HG2	2:C:574:SER:CB	2.38	0.53
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.89	0.53
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.37	0.53
2:H:21:VAL:HG13	2:H:22:LEU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.88	0.53
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.22	0.53
3:D:88:CYS:O	3:D:90:VAL:N	2.42	0.53
2:H:514:PHE:O	6:H:1401:1RL:H321	2.09	0.53
3:I:152:THR:O	3:I:154:LEU:N	2.40	0.53
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.90	0.53
2:C:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.90	0.53
3:D:85:CYS:HB3	3:D:88:CYS:O	2.08	0.53
3:D:422:LEU:HA	3:D:436:ALA:HA	1.89	0.53
3:I:227:PHE:O	3:I:230:SER:OG	2.18	0.53
3:I:824:PRO:O	3:I:826:ILE:HG13	2.08	0.53
1:B:64:VAL:HG13	1:B:69:SER:OG	2.08	0.53
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.90	0.53
3:D:545:HIS:HB2	3:D:546:ALA:HA	1.91	0.53
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.42	0.53
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.07	0.53
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.89	0.53
3:I:546:ALA:HB3	3:I:547:ARG:O	2.09	0.53
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.42	0.53
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.20	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.42	0.53
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.89	0.53
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.91	0.53
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.08	0.53
2:C:55:SER:HB3	2:C:56:VAL:CB	2.38	0.53
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.90	0.53
5:X:580:PHE:O	5:X:582:VAL:N	2.42	0.53
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.90	0.53
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.41	0.53
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.91	0.53
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.23	0.53
3:D:608:CYS:O	3:D:612:LEU:HB2	2.09	0.53
3:D:1173:ARG:HB3	3:D:1174:ARG:O	2.08	0.53
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.24	0.53
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.91	0.53
3:D:20:ILE:HD11	3:D:1320:ILE:HD11	1.90	0.53
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ILE:HG23	3:I:156:ARG:C	2.33	0.53
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.90	0.53
1:B:151:GLY:O	1:B:177:TYR:HB2	2.09	0.53
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.41	0.53
5:X:35:ILE:HG23	5:X:36:VAL:N	2.24	0.53
5:X:355:ILE:O	5:X:355:ILE:HD13	2.08	0.53
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.90	0.53
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.39	0.53
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.08	0.52
3:D:546:ALA:N	3:D:547:ARG:CA	2.70	0.52
3:D:768:ASN:O	3:D:771:GLN:NE2	2.42	0.52
5:X:515:GLU:N	5:X:516:ASP:HA	2.24	0.52
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.90	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.09	0.52
2:C:975:ILE:O	2:C:975:ILE:HD13	2.08	0.52
2:H:840:SER:OG	2:H:1048:LYS:O	2.27	0.52
2:H:1141:LEU:H	2:H:1141:LEU:HD13	1.74	0.52
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.90	0.52
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.45	0.52
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.24	0.52
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.25	0.52
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.52
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.44	0.52
2:C:660:VAL:HG22	2:C:661:VAL:N	2.25	0.52
2:C:690:VAL:HG11	2:C:830:THR:HG21	1.91	0.52
3:D:77:ARG:HG3	3:D:78:LEU:H	1.74	0.52
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.44	0.52
2:H:9:LYS:HD3	2:H:9:LYS:N	2.24	0.52
3:I:508:LEU:O	3:I:508:LEU:HD23	2.09	0.52
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.90	0.52
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.91	0.52
2:C:728:ASP:OD2	2:C:729:ALA:N	2.42	0.52
2:C:1109:ILE:HD13	3:D:644:MET:HE1	1.92	0.52
2:C:1251:TYR:O	5:X:525:ASP:N	2.42	0.52
2:C:1304:MET:HE1	2:C:1308:ILE:HD11	1.91	0.52
3:D:227:PHE:O	3:D:230:SER:OG	2.19	0.52
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.91	0.52
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.90	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.52
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.91	0.52
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:807:LEU:HD12	3:I:807:LEU:O	2.10	0.52
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.74	0.52
1:B:65:LEU:HD23	1:B:65:LEU:N	2.25	0.52
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.45	0.52
3:D:1290:ARG:NH1	3:D:1296:GLY:O	2.43	0.52
5:X:600:HIS:H	5:X:601:PRO:CD	2.22	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.90	0.52
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.43	0.52
1:B:42:ALA:O	1:B:46:ILE:HG12	2.10	0.52
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.91	0.52
2:C:540:ARG:NH2	2:C:568:ASN:OD1	2.43	0.52
2:C:690:VAL:HG13	2:C:691:PRO:HD2	1.90	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.42	0.52
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.74	0.52
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.92	0.52
5:X:112:THR:HG22	5:X:113:ARG:H	1.74	0.52
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.90	0.52
2:C:72:SER:O	2:C:98:VAL:HG23	2.10	0.52
2:C:590:PRO:O	2:C:659:GLN:NE2	2.41	0.52
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.40	0.52
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.91	0.52
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.92	0.52
2:H:896:THR:HG23	2:H:897:PRO:HD2	1.91	0.52
2:C:528:ARG:NH2	2:C:576:SER:O	2.43	0.52
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.91	0.52
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.92	0.52
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.24	0.52
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.92	0.52
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.92	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.43	0.52
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.52
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	1.92	0.52
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.43	0.52
2:C:539:THR:O	2:C:540:ARG:HG3	2.10	0.52
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.45	0.52
5:X:600:HIS:H	5:X:601:PRO:HD2	1.74	0.51
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.92	0.51
2:H:131:THR:HG22	2:H:135:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.40	0.51
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.91	0.51
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.92	0.51
2:C:660:VAL:C	2:C:661:VAL:HG13	2.34	0.51
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.10	0.51
1:G:49:SER:HA	1:G:151:GLY:HA2	1.92	0.51
2:H:1268:GLN:O	3:I:346:ARG:HA	2.10	0.51
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.40	0.51
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.41	0.51
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.41	0.51
3:I:515:ARG:NH2	3:I:718:SER:O	2.44	0.51
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.51
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.51
2:C:840:SER:OG	2:C:1048:LYS:O	2.27	0.51
3:D:514:THR:HG21	3:D:595:ALA:O	2.10	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.92	0.51
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.93	0.51
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.43	0.51
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.10	0.51
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.44	0.51
1:G:227:GLN:C	1:G:229:GLU:H	2.19	0.51
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.34	0.51
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.92	0.51
2:H:519:ASN:ND2	2:H:689:ALA:O	2.44	0.51
2:C:694:ARG:NH2	2:C:768:MET:SD	2.84	0.51
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.25	0.51
3:D:828:GLY:HA2	3:D:832:LYS:H	1.74	0.51
4:E:5:THR:HA	4:E:6:VAL:HG12	1.92	0.51
2:H:403:MET:HG3	2:H:414:ILE:HB	1.93	0.51
1:B:19:VAL:O	1:B:20:SER:HB3	2.10	0.51
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.93	0.51
2:C:127:ILE:HD13	2:C:127:ILE:N	2.26	0.51
1:A:79:LEU:O	1:A:83:LEU:HD13	2.11	0.51
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.40	0.51
3:D:451:PRO:HG2	3:D:625:MET:SD	2.50	0.51
1:G:118:ASP:OD1	1:G:119:GLY:N	2.43	0.51
2:H:528:ARG:NH2	2:H:576:SER:O	2.44	0.51
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.51
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.40	0.51
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.41	0.51
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.41	0.51
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.91	0.51
5:X:301:ASN:O	5:X:305:LEU:HD13	2.11	0.51
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.46	0.50
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.41	0.50
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.46	0.50
2:H:134:GLY:O	2:H:527:LYS:NZ	2.44	0.50
2:H:660:VAL:HG22	2:H:661:VAL:N	2.27	0.50
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.40	0.50
3:D:125:GLY:O	3:D:129:ASP:N	2.43	0.50
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.92	0.50
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.75	0.50
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.50
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.41	0.50
3:I:390:LEU:HD21	3:I:407:VAL:HG11	1.94	0.50
3:I:1290:ARG:NH1	3:I:1296:GLY:O	2.43	0.50
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.50
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.12	0.50
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.77	0.50
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.50
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.50
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.93	0.50
5:X:525:ASP:OD1	5:X:527:THR:HG22	2.11	0.50
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.45	0.50
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.92	0.50
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.92	0.50
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.93	0.50
2:H:514:PHE:HB2	6:H:1401:1RL:O8	2.12	0.50
2:H:521:LEU:CD2	2:H:686:GLN:HB3	2.42	0.50
2:H:685:MET:HE1	2:H:1073:LYS:HE2	1.93	0.50
2:H:753:LEU:HD12	2:H:753:LEU:O	2.11	0.50
2:H:844:LYS:HB2	2:H:844:LYS:NZ	2.26	0.50
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.76	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.42	0.50
3:I:832:LYS:HA	3:I:832:LYS:HZ1	1.76	0.50
4:J:3:ARG:O	4:J:4:VAL:HG13	2.11	0.50
2:C:1107:MET:SD	2:C:1107:MET:N	2.85	0.50
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.94	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.93	0.50
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:660:VAL:C	2:H:661:VAL:HG13	2.37	0.50
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.46	0.50
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.50
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.94	0.50
3:D:298:MET:HE3	5:X:402:LEU:HB3	1.94	0.50
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.51	0.50
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.12	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.12	0.50
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.92	0.50
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.94	0.50
3:I:356:THR:O	3:I:448:GLN:HA	2.11	0.50
3:I:546:ALA:H	3:I:547:ARG:C	2.20	0.50
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.92	0.50
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.93	0.50
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.46	0.50
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.45	0.50
2:H:740:GLU:HB2	2:H:741:MET:SD	2.51	0.50
3:I:773:PHE:O	3:I:776:THR:HG22	2.12	0.50
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.11	0.50
2:C:21:VAL:HG13	2:C:22:LEU:N	2.27	0.50
2:C:800:MET:HA	2:C:800:MET:CE	2.41	0.50
2:C:876:GLU:N	2:C:876:GLU:OE2	2.45	0.50
3:D:590:SER:O	3:D:594:GLN:N	2.44	0.50
3:D:810:THR:OG1	3:D:811:GLU:N	2.44	0.50
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.26	0.50
4:E:45:LYS:O	4:E:49:ILE:HG12	2.12	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
2:H:975:ILE:HD13	2:H:975:ILE:O	2.11	0.50
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.27	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.94	0.50
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.42	0.50
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.42	0.50
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.12	0.50
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.42	0.50
2:H:1107:MET:N	2:H:1107:MET:SD	2.85	0.50
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.27	0.50
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.44	0.49
3:D:356:THR:O	3:D:448:GLN:HA	2.12	0.49
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.45	0.49
2:H:487:LEU:HB3	2:H:488:MET:CG	2.40	0.49
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.94	0.49
3:D:213:LYS:O	3:D:217:LEU:HG	2.11	0.49
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.73	0.49
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.41	0.49
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.77	0.49
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	1.94	0.49
1:A:192:VAL:O	1:A:194:GLN:N	2.44	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.27	0.49
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.94	0.49
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.95	0.49
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.27	0.49
1:F:11:PRO:CG	1:G:228:LEU:H	2.26	0.49
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.47	0.49
2:H:1042:LEU:HD13	2:H:1042:LEU:N	2.25	0.49
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.47	0.49
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.76	0.49
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.28	0.49
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.94	0.49
1:A:310:ARG:HA	1:A:310:ARG:HE	1.76	0.49
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.42	0.49
1:G:227:GLN:O	1:G:229:GLU:N	2.45	0.49
3:I:125:GLY:O	3:I:129:ASP:N	2.45	0.49
3:I:482:ALA:C	3:I:483:LEU:HD12	2.38	0.49
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.43	0.49
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.94	0.49
2:H:697:LYS:HG3	2:H:698:PRO:HD2	1.94	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.12	0.49
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.94	0.49
3:D:85:CYS:SG	3:D:86:GLU:N	2.85	0.49
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.43	0.49
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.94	0.49
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.76	0.49
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.27	0.49
2:H:1251:TYR:O	5:Y:525:ASP:N	2.45	0.49
3:I:316:ILE:HD13	3:I:316:ILE:N	2.28	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.49
1:A:134:THR:HG21	2:C:727:VAL:HG23	1.95	0.49
1:A:317:ARG:C	1:A:318:LEU:HD13	2.38	0.49
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.49
2:C:897:PRO:HB3	5:X:564:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.12	0.49
5:Y:240:ARG:O	5:Y:242:HIS:N	2.46	0.49
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.44	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.46	0.49
1:B:118:ASP:OD1	1:B:119:GLY:N	2.45	0.49
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.49
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.95	0.49
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.43	0.49
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.43	0.49
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.93	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.13	0.48
3:D:545:HIS:HB2	3:D:546:ALA:CA	2.42	0.48
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.95	0.48
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.43	0.48
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.93	0.48
2:C:130:MET:HE3	2:C:136:PHE:CZ	2.49	0.48
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.28	0.48
2:H:747:GLY:C	2:H:748:ILE:HG13	2.38	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.28	0.48
2:C:403:MET:HG3	2:C:414:ILE:HB	1.95	0.48
2:C:572:ILE:HD13	6:C:1401:1RL:O1	2.12	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.48
3:D:807:LEU:HD12	3:D:807:LEU:O	2.12	0.48
2:H:71:VAL:O	2:H:72:SER:OG	2.26	0.48
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.95	0.48
3:I:919:ALA:O	3:I:923:ILE:HG12	2.14	0.48
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.28	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.48
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.45	0.48
5:X:561:MET:SD	5:X:576:VAL:HG22	2.53	0.48
2:H:548:ARG:NH2	2:H:567:PRO:O	2.46	0.48
2:H:876:GLU:N	2:H:876:GLU:OE2	2.46	0.48
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.95	0.48
3:I:239:LEU:HD12	3:I:239:LEU:O	2.13	0.48
5:Y:96:ASP:CG	5:Y:97:PRO:HD2	2.37	0.48
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.95	0.48
2:C:57:PHE:CE1	2:C:475:VAL:HG11	2.48	0.48
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.48
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.28	0.48
3:D:139:LEU:C	3:D:139:LEU:HD22	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.95	0.48
3:D:482:ALA:C	3:D:483:LEU:HD12	2.39	0.48
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.79	0.48
2:H:127:ILE:HD13	2:H:127:ILE:N	2.27	0.48
2:H:514:PHE:HB2	6:H:1401:1RL:C35	2.44	0.48
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.95	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.29	0.48
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
3:D:147:ILE:HG13	3:D:148:GLU:N	2.28	0.48
1:F:118:ASP:OD1	1:F:119:GLY:N	2.46	0.48
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.95	0.48
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.14	0.48
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.95	0.48
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.48
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.38	0.48
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.43	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.14	0.48
3:D:500:ILE:H	3:D:500:ILE:HD13	1.79	0.48
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.95	0.48
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.49	0.48
3:I:1173:ARG:HG2	3:I:1189:MET:HE1	1.95	0.48
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.96	0.48
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.14	0.48
2:C:490:GLN:O	5:X:472:GLN:HG3	2.13	0.48
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.94	0.48
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.94	0.48
3:D:473:THR:HB	3:D:476:ALA:HB2	1.96	0.48
3:D:786:THR:O	3:D:790:THR:HG23	2.12	0.48
2:H:484:LEU:H	2:H:484:LEU:HD22	1.78	0.48
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.95	0.48
3:I:85:CYS:HB3	3:I:88:CYS:O	2.14	0.48
3:I:128:LEU:HD12	3:I:192:MET:CE	2.44	0.48
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.49	0.48
2:C:804:PHE:O	3:D:638:SER:OG	2.28	0.48
2:C:989:LEU:HG	2:C:990:ASP:H	1.79	0.48
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.13	0.48
3:D:8:LEU:HD23	3:D:8:LEU:N	2.29	0.48
3:D:412:LEU:O	3:D:416:ILE:HD12	2.14	0.48
3:D:647:PRO:HG3	3:D:697:MET:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LEU:CD2	1:G:220:ALA:HB2	2.44	0.48
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.44	0.48
3:I:213:LYS:O	3:I:217:LEU:HG	2.13	0.48
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.96	0.48
5:Y:297:MET:HE2	5:Y:326:TRP:CZ3	2.49	0.48
1:A:102:LEU:HD12	1:A:115:ILE:HG12	1.95	0.48
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.37	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:753:LEU:O	2:C:753:LEU:HD12	2.13	0.48
1:F:45:ARG:NE	1:G:38:THR:OG1	2.45	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:741:MET:SD	2:H:741:MET:N	2.86	0.48
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.96	0.48
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.95	0.48
3:I:834:PRO:C	3:I:835:LEU:HD12	2.39	0.48
3:I:858:VAL:HB	3:I:859:PRO:CD	2.29	0.48
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.14	0.48
2:C:690:VAL:HG11	2:C:830:THR:CG2	2.44	0.47
2:C:799:ASN:O	2:C:800:MET:HE3	2.13	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.47	0.47
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.47
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.44	0.47
2:H:521:LEU:HD23	2:H:686:GLN:HB3	1.96	0.47
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.96	0.47
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.28	0.47
3:I:1247:LYS:HD3	3:I:1247:LYS:N	2.26	0.47
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.96	0.47
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.96	0.47
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.96	0.47
3:I:8:LEU:HD23	3:I:8:LEU:N	2.29	0.47
3:I:24:LEU:HD11	3:I:116:PHE:CZ	2.50	0.47
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.13	0.47
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.14	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
2:C:119:GLU:OE1	2:C:490:GLN:HB3	2.15	0.47
2:C:149:LEU:HD12	2:C:452:ARG:O	2.14	0.47
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.29	0.47
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.96	0.47
3:D:834:PRO:C	3:D:835:LEU:HD12	2.39	0.47
2:H:159:SER:OG	2:H:442:VAL:HG11	2.15	0.47
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.97	0.47
3:I:385:LEU:HD21	3:I:411:ILE:HG13	1.97	0.47
3:I:786:THR:O	3:I:790:THR:HG23	2.14	0.47
3:I:810:THR:OG1	3:I:811:GLU:N	2.45	0.47
2:C:748:ILE:C	2:C:748:ILE:HD12	2.40	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.47	0.47
3:D:611:ILE:HG13	3:D:612:LEU:CD2	2.45	0.47
3:D:901:ARG:HB3	3:D:908:ILE:HA	1.95	0.47
3:D:914:ALA:O	3:D:918:ILE:HG22	2.14	0.47
5:X:113:ARG:O	5:X:117:ILE:HD13	2.14	0.47
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.44	0.47
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.96	0.47
2:H:971:LEU:HD12	2:H:1018:TYR:HD1	1.78	0.47
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.49	0.47
2:C:748:ILE:HD12	2:C:748:ILE:O	2.14	0.47
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.45	0.47
3:D:828:GLY:HA2	3:D:832:LYS:N	2.29	0.47
5:X:262:VAL:HG12	5:X:264:LYS:H	1.78	0.47
5:X:503:GLU:HB3	5:X:504:PRO:O	2.13	0.47
5:X:532:LEU:O	5:X:536:THR:HG23	2.15	0.47
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.47	0.47
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.97	0.47
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.96	0.47
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.45	0.47
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.96	0.47
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.80	0.47
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.80	0.47
2:C:41:GLN:CD	2:C:42:ASP:H	2.23	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
2:C:747:GLY:C	2:C:748:ILE:HG13	2.39	0.47
5:X:264:LYS:HD2	5:X:264:LYS:N	2.29	0.47
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.47	0.47
2:H:773:LEU:C	2:H:773:LEU:HD22	2.39	0.47
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.95	0.47
3:I:1171:GLY:N	3:I:1172:LYS:O	2.47	0.47
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.15	0.47
1:A:303:ILE:O	1:A:307:LEU:HD13	2.14	0.47
1:B:19:VAL:O	1:B:19:VAL:HG12	2.15	0.47
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.50	0.47
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.96	0.47
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.79	0.47
3:D:139:LEU:HD22	3:D:139:LEU:O	2.15	0.47
3:D:166:LEU:HD12	3:D:167:ASP:N	2.30	0.47
3:D:294:ASN:ND2	3:D:298:MET:SD	2.87	0.47
3:D:355:ILE:HG12	3:D:464:ASP:O	2.14	0.47
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.95	0.47
4:E:5:THR:HB	4:E:7:GLN:HB2	1.97	0.47
5:X:45:ILE:C	5:X:45:ILE:HD12	2.40	0.47
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.97	0.47
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.96	0.47
5:X:551:LEU:HD22	5:X:597:LYS:HD2	1.97	0.47
1:G:42:ALA:O	1:G:46:ILE:HG12	2.15	0.47
2:H:73:TYR:O	2:H:74:ARG:HB2	2.14	0.47
2:H:127:ILE:O	2:H:127:ILE:HG12	2.14	0.47
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.30	0.47
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.95	0.47
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.96	0.47
3:I:139:LEU:C	3:I:139:LEU:HD22	2.39	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.44	0.47
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.30	0.47
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.96	0.47
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.47
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.49	0.47
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.95	0.47
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.97	0.47
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.45	0.47
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.50	0.47
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.14	0.47
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.13	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.96	0.47
3:D:141:PHE:O	3:D:297:ARG:HD3	2.15	0.47
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.80	0.47
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.45	0.47
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.95	0.47
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.26	0.47
2:C:71:VAL:O	2:C:72:SER:OG	2.30	0.47
2:C:519:ASN:ND2	2:C:689:ALA:O	2.47	0.47
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.45	0.47
3:D:145:VAL:HG22	3:D:180:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.97	0.47
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.45	0.47
2:H:989:LEU:HG	2:H:990:ASP:H	1.80	0.47
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.45	0.47
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.80	0.47
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.29	0.47
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.50	0.46
2:C:542:ARG:O	2:C:544:GLY:N	2.41	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.14	0.46
3:D:543:SER:O	3:D:574:VAL:HB	2.14	0.46
3:D:573:THR:HG22	3:D:576:ARG:CG	2.44	0.46
1:F:11:PRO:HG2	1:G:228:LEU:H	1.80	0.46
2:H:494:ASN:OD1	2:H:495:ALA:N	2.47	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.50	0.46
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.96	0.46
3:I:678:ARG:O	3:I:681:LYS:HG3	2.15	0.46
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.50	0.46
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.97	0.46
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.49	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.97	0.46
2:H:119:GLU:HG2	2:H:120:GLN:N	2.29	0.46
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.31	0.46
5:Y:355:ILE:O	5:Y:358:VAL:HG22	2.14	0.46
1:A:134:THR:HG21	2:C:727:VAL:O	2.16	0.46
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.46	0.46
1:A:318:LEU:HD13	1:A:318:LEU:N	2.30	0.46
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.50	0.46
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.40	0.46
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.49	0.46
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.46
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.51	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.46
3:D:147:ILE:HG23	3:D:156:ARG:C	2.41	0.46
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.98	0.46
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.30	0.46
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.98	0.46
2:C:510:GLN:C	2:C:512:SER:H	2.24	0.46
2:C:773:LEU:C	2:C:773:LEU:HD22	2.40	0.46
2:C:1239:VAL:HG12	2:C:1240:ASP:N	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.50	0.46
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.30	0.46
3:I:161:THR:HG22	3:I:162:GLU:N	2.30	0.46
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.40	0.46
1:A:69:SER:OG	1:A:70:THR:N	2.48	0.46
2:C:106:GLU:HG2	2:C:109:ALA:H	1.80	0.46
2:C:163:LYS:H	2:C:163:LYS:CD	2.12	0.46
2:C:1006:GLU:O	2:C:1006:GLU:HG2	2.16	0.46
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.46
3:D:706:VAL:C	3:D:707:ILE:HG13	2.41	0.46
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.31	0.46
2:H:1233:LEU:HD12	2:H:1233:LEU:O	2.15	0.46
3:I:403:ARG:O	3:I:405:GLU:N	2.49	0.46
5:Y:297:MET:HE2	5:Y:326:TRP:CE3	2.51	0.46
2:C:850:ILE:HG23	2:C:885:GLY:O	2.16	0.46
3:D:22:ILE:HG12	3:D:1336:ALA:HA	1.98	0.46
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.81	0.46
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.79	0.46
2:H:748:ILE:C	2:H:748:ILE:HD12	2.40	0.46
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.50	0.46
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.98	0.46
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.97	0.46
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.98	0.46
3:D:235:GLU:OE1	3:D:235:GLU:N	2.48	0.46
2:H:453:ILE:O	2:H:453:ILE:HG23	2.16	0.46
3:I:147:ILE:HG13	3:I:148:GLU:N	2.29	0.46
3:I:366:CYS:SG	3:I:437:PHE:HB2	2.56	0.46
3:I:582:ILE:HG23	3:I:623:GLN:HB3	1.98	0.46
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.51	0.46
1:B:14:VAL:HG13	1:B:28:LEU:CD2	2.46	0.46
1:B:227:GLN:C	1:B:229:GLU:H	2.24	0.46
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.97	0.46
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.51	0.46
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.98	0.46
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.98	0.46
3:D:535:ARG:HB3	3:D:541:LEU:HD11	1.98	0.46
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.46
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.50	0.46
2:H:72:SER:O	2:H:98:VAL:HG23	2.16	0.46
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.45	0.46
2:H:748:ILE:HD12	2:H:748:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.97	0.46
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.98	0.46
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.16	0.46
2:C:202:ARG:NE	2:C:369:MET:HG2	2.31	0.46
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.31	0.46
3:D:161:THR:HG22	3:D:162:GLU:N	2.31	0.46
3:D:1241:TYR:CD1	3:D:1248:ILE:HG21	2.51	0.46
5:X:115:GLY:O	5:X:119:ILE:HG12	2.16	0.46
1:F:79:LEU:O	1:F:83:LEU:HD13	2.16	0.46
2:H:55:SER:CB	2:H:56:VAL:HG13	2.43	0.46
3:I:608:CYS:O	3:I:612:LEU:HB2	2.16	0.46
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.15	0.46
4:J:5:THR:HA	4:J:6:VAL:HG12	1.98	0.46
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.98	0.45
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.98	0.45
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.31	0.45
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.51	0.45
3:D:909:ILE:HD12	3:D:909:ILE:O	2.17	0.45
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.99	0.45
2:H:189:ASP:HB2	2:H:190:PRO:CD	2.47	0.45
2:H:1006:GLU:HG2	2:H:1006:GLU:O	2.16	0.45
5:Y:471:LEU:HD12	5:Y:472:GLN:N	2.31	0.45
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.42	0.45
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.17	0.45
2:H:1005:GLU:O	2:H:1007:LYS:N	2.49	0.45
6:H:1401:1RL:O2	6:H:1401:1RL:O1	2.35	0.45
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.46	0.45
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.31	0.45
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.98	0.45
1:B:22:THR:HG22	1:B:208:ASN:O	2.16	0.45
2:C:963:GLU:O	2:C:966:ILE:HG22	2.16	0.45
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.49	0.45
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.98	0.45
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.98	0.45
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.51	0.45
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.99	0.45
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.52	0.45
2:C:901:LEU:O	2:C:905:ILE:HG13	2.17	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.16	0.45
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.45	0.45
3:D:515:ARG:NH2	3:D:718:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.82	0.45
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.98	0.45
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.32	0.45
1:F:86:LYS:HE2	1:F:173:VAL:HG23	1.98	0.45
2:H:488:MET:H	2:H:489:PRO:HA	1.81	0.45
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.81	0.45
3:I:265:LEU:HD11	3:I:330:MET:SD	2.57	0.45
3:I:647:PRO:HG3	3:I:697:MET:HA	1.98	0.45
3:I:1306:LEU:HD13	3:I:1307:LEU:N	2.31	0.45
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.98	0.45
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.16	0.45
1:B:176:CYS:C	1:B:178:SER:H	2.25	0.45
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.45
3:D:162:GLU:HG2	3:D:163:GLU:N	2.31	0.45
3:D:316:ILE:O	3:D:317:THR:OG1	2.19	0.45
3:D:423:LEU:HB3	3:D:466:MET:HE2	1.99	0.45
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.47	0.45
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.99	0.45
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.99	0.45
1:F:41:ASN:HD21	2:H:1218:GLY:CA	2.29	0.45
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.99	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:CG2	2.47	0.45
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.99	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:HE3	1.82	0.45
3:I:58:CYS:SG	3:I:60:ARG:N	2.89	0.45
3:I:382:TYR:HB3	3:I:394:ILE:CD1	2.46	0.45
3:I:513:MET:O	3:I:575:GLY:HA3	2.16	0.45
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.46	0.45
3:I:733:SER:O	3:I:737:ILE:HG12	2.17	0.45
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.82	0.45
1:A:178:SER:HA	1:A:179:PRO:HD3	1.77	0.45
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.45
3:D:918:ILE:HD13	3:D:919:ALA:N	2.32	0.45
5:X:459:THR:O	5:X:463:LEU:HD13	2.15	0.45
2:H:500:ALA:O	2:H:504:GLU:HB2	2.17	0.45
2:H:994:ARG:HD3	2:H:994:ARG:N	2.32	0.45
3:I:138:VAL:O	3:I:143:SER:HB3	2.17	0.45
3:I:179:LYS:HD3	3:I:179:LYS:N	2.32	0.45
3:I:422:LEU:HA	3:I:436:ALA:HA	1.99	0.45
2:C:44:GLU:HG3	2:C:45:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.49	0.45
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.46	0.45
3:D:395:LYS:NZ	5:X:607:LEU:O	2.36	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.99	0.45
2:H:106:GLU:HG2	2:H:109:ALA:H	1.82	0.45
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.52	0.45
3:I:579:LEU:O	3:I:579:LEU:HD13	2.16	0.45
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.97	0.45
2:C:893:THR:O	2:C:894:GLN:HB2	2.17	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
3:I:390:LEU:N	3:I:390:LEU:HD12	2.31	0.45
3:I:886:VAL:HG23	3:I:1254:GLU:HB3	1.99	0.45
3:I:1247:LYS:H	3:I:1247:LYS:CD	2.26	0.45
3:I:1256:ILE:O	3:I:1260:MET:HB2	2.17	0.45
2:C:80:PHE:O	2:C:84:GLU:HB3	2.16	0.45
2:C:99:LYS:C	2:C:100:LEU:HD12	2.42	0.45
2:C:533:LEU:N	2:C:533:LEU:HD23	2.32	0.45
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.99	0.45
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.17	0.45
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.45
5:X:379:MET:HA	5:X:379:MET:CE	2.47	0.45
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.46	0.45
2:H:941:LYS:HD2	2:H:941:LYS:O	2.16	0.45
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.98	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.52	0.45
2:C:1290:MET:SD	2:C:1294:LYS:HD3	2.57	0.45
3:D:841:GLY:CA	3:D:901:ARG:HD3	2.46	0.45
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.99	0.45
5:X:519:LEU:O	5:X:519:LEU:HD13	2.17	0.45
2:H:135:THR:OG1	2:H:143:ARG:O	2.30	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.52	0.45
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.17	0.45
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.52	0.44
2:C:551:HIS:CD2	2:C:552:PRO:HD2	2.52	0.44
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.99	0.44
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.52	0.44
2:H:54:ARG:N	2:H:55:SER:C	2.75	0.44
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.50	0.44
1:A:321:TRP:HA	1:A:322:PRO:HA	1.71	0.44
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.00	0.44
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.97	0.44
3:D:678:ARG:HD2	3:D:678:ARG:C	2.42	0.44
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.16	0.44
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.98	0.44
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.99	0.44
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.98	0.44
2:H:843:THR:HB	2:H:845:LEU:CD2	2.47	0.44
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.98	0.44
2:C:542:ARG:HG2	2:C:543:ALA:N	2.32	0.44
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.58	0.44
5:X:288:MET:HA	5:X:302:PHE:CZ	2.52	0.44
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.44
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.18	0.44
3:I:1190:ILE:HD12	3:I:1190:ILE:N	2.32	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.99	0.44
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.47	0.44
3:D:1306:LEU:HD13	3:D:1307:LEU:N	2.33	0.44
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.52	0.44
2:H:488:MET:HB2	2:H:489:PRO:C	2.41	0.44
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.44
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.82	0.44
3:D:515:ARG:HH22	3:D:717:VAL:C	2.25	0.44
3:D:610:ARG:CG	3:D:864:LEU:HD22	2.45	0.44
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.44
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.42	0.44
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.49	0.44
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	1.99	0.44
3:I:252:LEU:H	3:I:252:LEU:HD23	1.81	0.44
3:I:886:VAL:HG13	3:I:1230:THR:HG21	2.00	0.44
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.43	0.44
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.47	0.44
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.99	0.44
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.53	0.44
2:H:699:LEU:HD11	2:H:1179:GLY:CA	2.44	0.44
3:I:288:PRO:HB2	3:I:291:ILE:HG12	2.00	0.44
1:A:221:ALA:HB1	1:B:228:LEU:HD13	2.00	0.44
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.98	0.44
2:C:51:ALA:C	2:C:53:PHE:H	2.25	0.44
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.18	0.44
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1158:LYS:HD2	2:C:1158:LYS:O	2.18	0.44
2:C:1243:MET:HE3	3:D:372:MET:HB2	1.98	0.44
3:D:205:LEU:HB3	3:D:217:LEU:HD22	1.99	0.44
3:D:233:LYS:HG3	3:D:234:PRO:HD2	2.00	0.44
3:D:766:GLY:C	3:D:767:LEU:HD22	2.43	0.44
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.53	0.44
5:X:528:LEU:C	5:X:528:LEU:HD12	2.43	0.44
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.44
2:H:653:MET:HG2	2:H:654:ASP:N	2.33	0.44
2:H:1277:ALA:HB3	3:I:434:ILE:HD13	2.00	0.44
3:I:508:LEU:HD23	3:I:508:LEU:C	2.43	0.44
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.48	0.44
1:A:29:GLU:O	1:A:31:LEU:N	2.50	0.44
2:C:42:ASP:O	2:C:44:GLU:HG2	2.17	0.44
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.53	0.44
3:D:841:GLY:HA3	3:D:901:ARG:HD3	1.99	0.44
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.18	0.44
2:H:122:VAL:HG13	2:H:124:MET:HG3	2.00	0.44
2:H:488:MET:HB2	2:H:489:PRO:HA	1.99	0.44
2:H:551:HIS:CD2	2:H:552:PRO:HD2	2.52	0.44
2:H:1298:VAL:HG13	2:H:1321:GLU:HG3	1.99	0.44
3:I:242:LEU:HD12	3:I:243:PRO:HD2	2.00	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.17	0.44
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.32	0.44
3:I:610:ARG:CG	3:I:864:LEU:HD22	2.48	0.44
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.33	0.44
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.51	0.44
5:Y:139:GLU:HG3	5:Y:351:THR:HA	2.00	0.44
2:C:752:ASN:C	2:C:753:LEU:HG	2.43	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.48	0.44
2:C:841:ARG:HA	2:C:1046:VAL:HG13	2.00	0.44
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.99	0.44
3:D:143:SER:HB2	5:X:100:MET:HE2	2.00	0.44
3:D:144:TYR:HB3	3:D:159:ILE:CG2	2.48	0.44
3:D:306:LEU:C	3:D:306:LEU:HD23	2.43	0.44
3:D:709:ARG:HD2	3:D:714:GLU:HB2	2.00	0.44
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.47	0.44
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.17	0.44
4:E:82:ALA:O	4:E:86:ILE:HG13	2.17	0.44
1:F:234:LEU:HD12	1:F:234:LEU:N	2.33	0.44
2:H:218:GLU:HG2	2:H:299:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:549:ASP:OD1	2:H:550:VAL:N	2.50	0.44
2:H:843:THR:HB	2:H:845:LEU:HD22	1.99	0.44
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.48	0.44
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.33	0.44
3:I:1258:ARG:HG3	3:I:1259:GLN:N	2.33	0.44
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.98	0.43
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.90	0.43
3:I:162:GLU:HG2	3:I:163:GLU:N	2.33	0.43
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.47	0.43
3:I:545:HIS:CB	3:I:546:ALA:HA	2.41	0.43
3:I:681:LYS:HB2	3:I:681:LYS:HZ3	1.83	0.43
3:I:1270:GLY:HA2	3:I:1298:VAL:C	2.43	0.43
4:J:4:VAL:O	4:J:5:THR:OG1	2.32	0.43
5:Y:395:THR:HA	5:Y:404:LEU:CD2	2.48	0.43
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.43
6:C:1401:1RL:O9	6:C:1401:1RL:O10	2.18	0.43
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.43
3:D:390:LEU:N	3:D:390:LEU:HD12	2.33	0.43
3:D:579:LEU:O	3:D:579:LEU:HD13	2.17	0.43
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.43
3:D:1190:ILE:HD12	3:D:1190:ILE:N	2.32	0.43
5:X:47:MET:O	5:X:55:VAL:HG11	2.18	0.43
5:X:532:LEU:C	5:X:532:LEU:HD13	2.43	0.43
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.33	0.43
2:H:1017:GLN:O	2:H:1020:GLU:HB3	2.18	0.43
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.48	0.43
3:I:288:PRO:HG2	5:Y:413:MET:HE2	1.99	0.43
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.18	0.43
3:I:534:GLU:O	3:I:538:ARG:HB2	2.18	0.43
3:I:582:ILE:HG23	3:I:623:GLN:CB	2.48	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
2:C:994:ARG:HD3	2:C:994:ARG:N	2.33	0.43
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.53	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43
3:D:202:ARG:O	3:D:206:ASN:ND2	2.51	0.43
3:D:648:GLU:OE2	3:D:648:GLU:N	2.51	0.43
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.32	0.43
2:H:465:ARG:O	2:H:469:VAL:HG23	2.18	0.43
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	2.00	0.43
2:H:1258:PRO:HG2	3:I:346:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:856:ILE:HG13	3:I:857:LEU:O	2.19	0.43
3:I:901:ARG:CB	3:I:908:ILE:HA	2.49	0.43
2:C:685:MET:HE2	2:C:1067:ALA:CB	2.48	0.43
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.49	0.43
2:C:993:PRO:HB2	2:C:994:ARG:H	1.60	0.43
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.80	0.43
3:D:63:GLY:O	3:D:98:ARG:NH2	2.50	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.51	0.43
2:H:37:LYS:HA	2:H:37:LYS:HE3	2.00	0.43
2:H:705:GLU:HB2	2:H:794:LEU:HB3	2.01	0.43
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.99	0.43
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.18	0.43
1:A:234:LEU:N	1:A:234:LEU:HD12	2.34	0.43
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.50	0.43
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.99	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.34	0.43
3:I:306:LEU:C	3:I:306:LEU:HD23	2.43	0.43
3:I:590:SER:O	3:I:594:GLN:N	2.51	0.43
3:I:909:ILE:HD12	3:I:909:ILE:O	2.18	0.43
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.18	0.43
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.43
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.00	0.43
2:C:106:GLU:H	2:C:107:ARG:HA	1.83	0.43
2:C:122:VAL:HG22	2:C:123:TYR:N	2.33	0.43
2:C:1140:LYS:C	2:C:1142:ARG:H	2.27	0.43
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.43
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.19	0.43
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.47	0.43
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.54	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:H:529:ARG:CD	6:H:1401:1RL:H171	2.48	0.43
2:H:892:GLU:O	2:H:893:THR:OG1	2.22	0.43
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.53	0.43
3:I:572:THR:HB	3:I:576:ARG:HD2	2.01	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.83	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
2:C:189:ASP:HB2	2:C:190:PRO:CD	2.49	0.43
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.19	0.43
3:D:240:THR:HG23	3:D:241:VAL:HG23	2.01	0.43
3:D:252:LEU:HD23	3:D:252:LEU:H	1.82	0.43
3:D:519:ASN:OD1	3:D:520:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:545:HIS:O	3:D:573:THR:OG1	2.35	0.43
3:I:305:ALA:O	3:I:309:ASN:ND2	2.51	0.43
3:I:766:GLY:C	3:I:767:LEU:HD22	2.44	0.43
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.84	0.43
2:C:135:THR:OG1	2:C:143:ARG:O	2.35	0.43
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.33	0.43
3:D:27:PRO:O	3:D:31:ARG:HD3	2.19	0.43
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.49	0.43
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.99	0.43
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.99	0.43
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.19	0.43
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.43
3:I:799:ARG:NH1	3:I:1146:GLU:OE1	2.51	0.43
2:C:49:LEU:HD23	2:C:49:LEU:C	2.44	0.43
2:C:73:TYR:O	2:C:74:ARG:HB2	2.18	0.43
2:C:82:VAL:HG13	2:C:83:GLN:N	2.34	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.00	0.43
3:D:690:ASN:ND2	3:D:745:GLY:HA3	2.34	0.43
3:D:824:PRO:O	3:D:826:ILE:HG13	2.19	0.43
3:D:919:ALA:O	3:D:923:ILE:HG12	2.18	0.43
5:X:264:LYS:H	5:X:264:LYS:HD2	1.83	0.43
2:H:73:TYR:N	2:H:73:TYR:CD2	2.85	0.43
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.43
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.52	0.43
2:H:800:MET:HA	2:H:800:MET:CE	2.40	0.43
2:H:868:SER:OG	2:H:942:ASP:OD1	2.36	0.43
2:H:888:THR:O	2:H:914:LYS:N	2.51	0.43
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.54	0.43
3:I:367:GLY:HA3	3:I:448:GLN:HB2	2.00	0.43
3:I:848:VAL:HG11	3:I:880:VAL:HA	2.00	0.43
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.43	0.43
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.99	0.43
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.48	0.43
2:C:736:VAL:HG11	2:C:740:GLU:CA	2.48	0.43
3:D:58:CYS:SG	3:D:60:ARG:N	2.92	0.43
3:D:124:ILE:CG1	3:D:189:LEU:HD11	2.49	0.43
3:D:403:ARG:O	3:D:405:GLU:N	2.52	0.43
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.48	0.43
3:D:1226:VAL:HG11	3:I:1292:LEU:HA	2.01	0.43
2:H:693:LEU:HD13	2:H:693:LEU:C	2.44	0.43
2:H:818:VAL:HG22	2:H:819:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.83	0.43
3:I:648:GLU:OE2	3:I:648:GLU:N	2.52	0.43
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.19	0.43
4:J:10:VAL:HG21	4:J:16:ARG:HG2	2.01	0.43
5:Y:108:VAL:HB	5:Y:110:LEU:HG	2.01	0.43
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.84	0.43
5:Y:600:HIS:N	5:Y:601:PRO:CD	2.82	0.43
1:A:300:LEU:O	1:A:300:LEU:HD13	2.19	0.42
2:C:52:ALA:O	2:C:53:PHE:HB2	2.19	0.42
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	2.01	0.42
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.84	0.42
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.48	0.42
3:D:107:LEU:HD23	3:D:299:LEU:HD21	2.00	0.42
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.54	0.42
3:D:579:LEU:HD23	3:D:627:THR:HG21	2.00	0.42
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.81	0.42
2:H:205:PRO:O	2:H:208:ILE:HG22	2.19	0.42
3:I:361:LEU:HD23	3:I:366:CYS:HA	2.00	0.42
3:I:519:ASN:OD1	3:I:520:ALA:N	2.52	0.42
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.49	0.42
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.34	0.42
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.33	0.42
2:C:10:ARG:NH1	2:C:775:GLU:OE2	2.52	0.42
2:C:494:ASN:OD1	2:C:495:ALA:N	2.52	0.42
2:C:759:SER:OG	2:C:760:ASN:N	2.52	0.42
2:C:971:LEU:C	2:C:971:LEU:HD13	2.43	0.42
2:H:185:ASP:OD1	2:H:185:ASP:N	2.51	0.42
2:H:845:LEU:HD13	2:H:845:LEU:N	2.30	0.42
2:H:998:LEU:O	2:H:998:LEU:HD13	2.19	0.42
2:H:1294:LYS:HE2	3:I:348:ASP:O	2.19	0.42
3:I:139:LEU:HD22	3:I:139:LEU:O	2.19	0.42
3:I:686:TRP:HB3	3:I:758:PRO:HG2	2.00	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.19	0.42
2:C:622:ASN:OD1	2:C:623:LEU:N	2.52	0.42
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.42
5:X:303:ILE:O	5:X:307:THR:OG1	2.22	0.42
2:H:59:ILE:HD13	2:H:479:LEU:HD12	2.01	0.42
2:H:600:THR:HG22	2:H:601:ASP:H	1.84	0.42
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.19	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.48	0.42
2:C:557:ARG:NH2	2:C:606:LEU:O	2.52	0.42
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.42
3:D:124:ILE:HA	3:D:237:MET:HE2	2.01	0.42
3:D:124:ILE:HD11	3:D:189:LEU:HD11	2.01	0.42
3:D:154:LEU:HD21	3:D:160:LEU:HD21	2.01	0.42
3:D:1171:GLY:HA3	3:D:1172:LYS:C	2.44	0.42
5:X:565:ILE:HG12	5:X:566:ASP:N	2.34	0.42
5:X:582:VAL:HG11	5:X:586:ARG:HG2	2.01	0.42
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.54	0.42
2:H:691:PRO:HA	2:H:788:SER:OG	2.19	0.42
3:I:128:LEU:HD12	3:I:192:MET:HE1	2.01	0.42
3:I:368:LEU:HD12	3:I:369:PRO:HD2	2.01	0.42
3:I:482:ALA:O	3:I:488:ASN:ND2	2.52	0.42
3:I:611:ILE:HG13	3:I:612:LEU:HD23	2.01	0.42
3:I:770:LEU:C	3:I:770:LEU:HD13	2.44	0.42
5:Y:143:TYR:CD1	5:Y:269:LEU:HD21	2.54	0.42
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.32	0.42
3:D:369:PRO:HG3	3:D:446:ALA:O	2.19	0.42
5:X:442:SER:OG	5:X:446:GLN:NE2	2.52	0.42
5:X:461:ASN:HB3	5:X:465:ARG:CZ	2.49	0.42
1:F:51:MET:HB2	1:F:179:PRO:HD2	2.01	0.42
2:H:10:ARG:NH1	2:H:775:GLU:OE2	2.51	0.42
2:H:948:ILE:HG13	2:H:949:GLU:N	2.34	0.42
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	2.01	0.42
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	2.01	0.42
2:C:177:ILE:N	2:C:177:ILE:HD12	2.34	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.54	0.42
3:D:242:LEU:HD12	3:D:243:PRO:HD2	2.01	0.42
3:D:313:GLY:O	3:D:314:ARG:HB2	2.20	0.42
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.53	0.42
3:D:886:VAL:HG23	3:D:1254:GLU:HB3	2.00	0.42
5:X:143:TYR:O	5:X:147:GLN:HG2	2.19	0.42
2:H:106:GLU:CB	2:H:107:ARG:CA	2.97	0.42
3:I:413:ASP:HA	3:I:416:ILE:HD12	2.01	0.42
3:I:481:ARG:HA	3:I:485:MET:HE2	2.02	0.42
3:I:526:VAL:HG12	3:I:549:LYS:HB2	2.00	0.42
3:I:901:ARG:HB3	3:I:908:ILE:HA	2.02	0.42
1:A:45:ARG:NE	1:B:38:THR:OG1	2.49	0.42
1:B:83:LEU:CD1	3:D:527:LEU:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:ILE:O	2:C:127:ILE:HG12	2.19	0.42
2:C:166:SER:C	2:C:168:GLY:H	2.26	0.42
2:C:603:ILE:HD12	2:C:603:ILE:O	2.19	0.42
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	2.02	0.42
3:D:596:LEU:N	3:D:596:LEU:HD23	2.34	0.42
3:D:605:LEU:O	3:D:605:LEU:HD13	2.20	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.49	0.42
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.50	0.42
5:X:108:VAL:HG23	5:X:109:GLU:N	2.30	0.42
1:F:42:ALA:O	1:F:46:ILE:HG12	2.20	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.85	0.42
2:H:177:ILE:N	2:H:177:ILE:HD12	2.35	0.42
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.55	0.42
2:H:1259:LEU:C	2:H:1259:LEU:HD12	2.44	0.42
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.92	0.42
3:I:596:LEU:N	3:I:596:LEU:HD23	2.34	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
3:I:706:VAL:C	3:I:707:ILE:HG13	2.43	0.42
3:I:932:MET:O	3:I:933:ARG:HG3	2.19	0.42
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	2.01	0.42
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.79	0.42
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.19	0.42
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	2.01	0.42
1:A:44:ARG:HG3	1:A:183:ILE:HG22	2.02	0.42
3:D:1270:GLY:CA	3:D:1299:GLY:HA2	2.49	0.42
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.35	0.42
2:H:894:GLN:O	2:H:895:LEU:HB2	2.20	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.19	0.42
3:I:72:CYS:SG	3:I:73:GLY:N	2.93	0.42
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.84	0.42
3:I:1297:LYS:HA	3:I:1297:LYS:HE2	2.00	0.42
4:J:19:LEU:HD13	4:J:19:LEU:C	2.45	0.42
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.42
1:A:323:PRO:CA	1:A:324:ALA:HB2	2.50	0.42
2:C:73:TYR:CG	2:C:74:ARG:N	2.86	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:948:ILE:HG13	2:C:949:GLU:N	2.34	0.42
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
3:D:292:VAL:HG13	3:D:293:ARG:N	2.34	0.42
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:517:CYS:N	3:D:544:LEU:O	2.47	0.42
5:X:12:LEU:HD21	5:X:27:VAL:HG21	1.98	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
1:G:86:LYS:NZ	3:I:526:VAL:O	2.52	0.42
1:G:207:THR:OG1	1:G:208:ASN:N	2.52	0.42
2:H:634:VAL:HG22	2:H:645:PHE:HE2	1.85	0.42
2:H:892:GLU:C	2:H:894:GLN:H	2.28	0.42
3:I:189:LEU:HB3	3:I:234:PRO:HB2	2.02	0.42
3:I:369:PRO:HG3	3:I:446:ALA:O	2.20	0.42
3:I:771:GLN:HE21	3:I:772:TYR:N	2.18	0.42
1:A:42:ALA:HA	1:B:38:THR:HG23	2.02	0.42
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.01	0.42
2:C:639:LYS:HE2	2:C:639:LYS:HA	2.02	0.42
2:C:818:VAL:HG22	2:C:819:SER:N	2.35	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
3:D:320:ASN:HB3	3:D:322:ARG:HG2	2.01	0.42
3:D:392:THR:HG22	5:X:603:ARG:HG2	2.00	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.49	0.42
4:E:26:ARG:HE	4:E:30:MET:HE3	1.85	0.42
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.35	0.42
2:H:59:ILE:HD11	2:H:63:SER:HB3	2.02	0.42
2:H:163:LYS:HG2	2:H:163:LYS:O	2.20	0.42
2:H:166:SER:O	2:H:167:SER:OG	2.32	0.42
2:H:484:LEU:HB3	2:H:486:THR:HG22	2.01	0.42
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.48	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.50	0.42
3:I:644:MET:O	3:I:764:ARG:NH1	2.53	0.42
5:Y:528:LEU:C	5:Y:528:LEU:HD12	2.44	0.42
1:B:9:LEU:H	1:B:9:LEU:HD23	1.85	0.41
1:B:190:ALA:HB2	1:B:200:LYS:HB3	2.01	0.41
2:C:91:THR:HG22	2:C:138:ILE:HA	2.02	0.41
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.55	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.53	0.41
2:H:384:LEU:O	2:H:388:LEU:HG	2.20	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.35	0.41
2:H:639:LYS:HA	2:H:639:LYS:HE2	2.00	0.41
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.50	0.41
2:H:759:SER:OG	2:H:760:ASN:N	2.53	0.41
2:H:893:THR:O	2:H:894:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:971:LEU:HD12	2:H:1018:TYR:CD1	2.54	0.41
3:I:240:THR:HG23	3:I:241:VAL:HG23	2.01	0.41
3:I:252:LEU:HG	3:I:252:LEU:O	2.20	0.41
3:I:1173:ARG:NH1	3:I:1176:VAL:HG21	2.34	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.52	0.41
2:C:152:SER:HA	2:C:153:PRO:HD3	1.89	0.41
2:C:166:SER:O	2:C:168:GLY:N	2.45	0.41
2:C:873:ILE:HD11	2:C:931:VAL:HG22	2.02	0.41
2:C:896:THR:HG23	2:C:897:PRO:HD2	2.02	0.41
3:D:395:LYS:HG3	5:X:536:THR:HG21	2.02	0.41
3:D:846:GLU:O	3:D:847:ASP:C	2.63	0.41
4:E:3:ARG:O	4:E:4:VAL:HG13	2.20	0.41
5:X:511:ILE:HG23	5:X:512:GLY:N	2.32	0.41
1:F:54:CYS:SG	1:F:148:ARG:NH1	2.93	0.41
2:H:727:VAL:HG22	2:H:773:LEU:HB3	2.00	0.41
2:H:752:ASN:C	2:H:753:LEU:HG	2.45	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
3:I:233:LYS:HG3	3:I:234:PRO:HD2	2.01	0.41
3:I:508:LEU:HD12	3:I:725:MET:HG2	2.03	0.41
3:I:550:VAL:HG23	3:I:552:ILE:HD11	2.02	0.41
3:I:846:GLU:O	3:I:847:ASP:C	2.63	0.41
3:I:863:LEU:HB2	3:I:866:GLU:HB2	2.03	0.41
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.20	0.41
2:C:516:ASP:O	2:C:522:SER:OG	2.29	0.41
2:C:519:ASN:CB	2:C:520:PRO:HD2	2.47	0.41
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.41
3:D:394:ILE:HG21	5:X:536:THR:HA	2.03	0.41
3:D:412:LEU:O	3:D:416:ILE:HG23	2.19	0.41
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.35	0.41
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.34	0.41
3:I:63:GLY:O	3:I:98:ARG:NH2	2.52	0.41
3:I:451:PRO:HG2	3:I:625:MET:SD	2.60	0.41
2:C:93:SER:HB2	2:C:126:GLU:CD	2.45	0.41
2:C:201:ARG:HD2	2:C:370:MET:SD	2.60	0.41
2:C:538:LEU:HD12	2:C:538:LEU:N	2.35	0.41
3:D:310:GLY:O	3:D:314:ARG:HG2	2.19	0.41
3:D:514:THR:HG23	3:D:576:ARG:HE	1.86	0.41
3:D:911:LYS:HG3	4:E:15:ASN:ND2	2.36	0.41
3:D:1171:GLY:CA	3:D:1172:LYS:C	2.92	0.41
3:D:1173:ARG:HG2	3:D:1189:MET:HE1	2.01	0.41
5:X:96:ASP:CG	5:X:97:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:LEU:HD23	2:H:49:LEU:C	2.45	0.41
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.20	0.41
3:I:503:SER:O	3:I:507:VAL:HG23	2.20	0.41
3:I:573:THR:HG22	3:I:576:ARG:CD	2.50	0.41
3:I:704:GLU:O	3:I:705:THR:OG1	2.26	0.41
3:I:1226:VAL:O	3:I:1230:THR:HG23	2.20	0.41
1:B:182:ARG:NH1	3:D:581:MET:SD	2.93	0.41
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.41
2:C:533:LEU:HD23	2:C:533:LEU:H	1.85	0.41
2:C:546:GLU:O	2:C:547:VAL:HB	2.20	0.41
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.02	0.41
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.41
3:D:474:LEU:HD13	3:D:478:LEU:HD13	2.01	0.41
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.41
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.50	0.41
3:D:909:ILE:H	3:D:909:ILE:HG13	1.62	0.41
2:H:54:ARG:CA	2:H:55:SER:HB2	2.51	0.41
2:H:870:ILE:HG22	2:H:944:ARG:NH1	2.35	0.41
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.35	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.50	0.41
3:I:221:ILE:HG13	3:I:222:LYS:N	2.36	0.41
3:I:527:LEU:HD13	3:I:531:LYS:HB3	2.02	0.41
3:I:583:VAL:HG13	3:I:587:LEU:HD22	2.01	0.41
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.03	0.41
1:A:104:LYS:HD3	1:A:105:SER:N	2.35	0.41
1:A:104:LYS:HD2	1:A:110:VAL:HG22	2.02	0.41
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.55	0.41
2:C:106:GLU:CB	2:C:107:ARG:HA	2.46	0.41
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.50	0.41
2:H:1332:SER:O	3:I:243:PRO:HG2	2.21	0.41
3:I:139:LEU:HD21	3:I:185:ILE:HD13	2.02	0.41
3:I:886:VAL:HG22	3:I:1257:VAL:CG1	2.51	0.41
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.20	0.41
3:I:1138:LEU:N	3:I:1139:PRO:CD	2.84	0.41
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.34	0.41
1:A:300:LEU:HD13	1:A:300:LEU:C	2.46	0.41
2:C:487:LEU:HD12	2:C:487:LEU:H	1.86	0.41
2:C:898:GLU:OE1	2:C:898:GLU:N	2.51	0.41
2:C:908:GLU:CG	2:C:909:LYS:H	2.33	0.41
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.21	0.41
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:269:TYR:HA	3:D:272:VAL:HG12	2.02	0.41
3:D:545:HIS:HB2	3:D:546:ALA:HB2	2.03	0.41
3:D:770:LEU:C	3:D:770:LEU:HD13	2.45	0.41
3:D:932:MET:C	3:D:933:ARG:HG3	2.45	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB3	2.02	0.41
3:D:1256:ILE:HA	3:D:1259:GLN:HE21	1.85	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.36	0.41
2:H:603:ILE:HD12	2:H:603:ILE:O	2.20	0.41
2:H:790:ASP:C	2:H:791:LEU:HG	2.46	0.41
2:H:1156:ARG:O	2:H:1157:GLN:HB2	2.21	0.41
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.35	0.41
5:Y:145:LEU:C	5:Y:145:LEU:HD13	2.45	0.41
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.32	0.41
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.50	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:106:GLU:H	2:H:107:ARG:HA	1.86	0.41
2:H:496:LYS:N	2:H:497:PRO:CD	2.84	0.41
3:I:313:GLY:O	3:I:314:ARG:HB2	2.21	0.41
3:I:660:GLU:O	3:I:664:ILE:HG12	2.20	0.41
3:I:1210:ILE:O	3:I:1210:ILE:HG13	2.21	0.41
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.36	0.41
5:Y:532:LEU:C	5:Y:532:LEU:HD13	2.46	0.41
1:A:282:VAL:CG2	1:A:316:MET:HE2	2.51	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.89	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
2:C:667:LEU:O	2:C:1069:ARG:NH2	2.54	0.41
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	2.03	0.41
2:C:988:LYS:O	2:C:991:LYS:HE3	2.20	0.41
2:C:1066:MET:HG2	2:C:1232:MET:HE2	2.03	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
3:D:221:ILE:HG13	3:D:222:LYS:N	2.35	0.41
3:D:481:ARG:HA	3:D:485:MET:HE2	2.03	0.41
3:D:697:MET:HE1	3:D:738:ARG:HA	2.03	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.61	0.41
3:D:803:VAL:HB	3:D:1313:SER:HB3	2.03	0.41
3:D:1210:ILE:O	3:D:1210:ILE:HG13	2.21	0.41
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.21	0.41
4:E:30:MET:O	4:E:35:LYS:HG2	2.20	0.41
5:X:52:GLY:O	5:X:53:ILE:HB	2.19	0.41
5:X:54:GLN:CA	5:X:54:GLN:HE21	2.34	0.41
5:X:244:THR:O	5:X:247:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:494:ILE:O	5:X:498:LEU:HD23	2.21	0.41
1:F:10:LYS:HE3	1:G:226:GLU:HB3	2.03	0.41
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.36	0.41
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.55	0.41
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.61	0.41
2:H:82:VAL:HG13	2:H:83:GLN:N	2.35	0.41
2:H:378:ARG:NE	2:H:382:GLU:OE2	2.54	0.41
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.56	0.41
2:H:637:ARG:NE	3:I:770:LEU:HD23	2.36	0.41
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.55	0.41
2:H:951:MET:HE3	2:H:951:MET:HA	2.03	0.41
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.36	0.41
3:I:316:ILE:HD13	3:I:316:ILE:H	1.86	0.41
3:I:501:VAL:HA	3:I:502:PRO:HD3	1.97	0.41
3:I:822:MET:HG2	3:I:839:VAL:HG22	2.02	0.41
3:I:884:SER:OG	3:I:1254:GLU:OE1	2.31	0.41
3:I:1171:GLY:HA3	3:I:1172:LYS:C	2.44	0.41
3:I:1171:GLY:CA	3:I:1172:LYS:C	2.94	0.41
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.21	0.41
5:Y:333:VAL:HG22	5:Y:336:GLU:HB2	2.03	0.41
1:B:14:VAL:HG13	1:B:28:LEU:HD23	2.03	0.41
3:D:147:ILE:HA	3:D:178:ALA:CB	2.51	0.41
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.41
1:G:181:GLU:HB2	1:G:206:GLU:O	2.21	0.41
2:H:146:VAL:HG13	2:H:513:GLN:HG3	2.03	0.41
2:H:524:ILE:HD12	2:H:708:VAL:HG13	2.03	0.41
2:H:681:MET:O	2:H:685:MET:HG2	2.21	0.41
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.86	0.41
3:I:155:GLU:CD	3:I:158:GLN:HB2	2.46	0.41
3:I:1169:THR:HA	3:I:1173:ARG:HB3	2.02	0.41
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.54	0.40
1:A:143:ARG:HD2	1:A:143:ARG:N	2.36	0.40
1:A:246:LYS:HD3	1:A:246:LYS:N	2.35	0.40
1:B:232:VAL:HG12	1:B:233:ASP:O	2.21	0.40
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.51	0.40
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.40
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.54	0.40
3:D:238:ILE:O	3:D:238:ILE:HG13	2.20	0.40
3:D:503:SER:O	3:D:507:VAL:HG23	2.21	0.40
3:D:573:THR:HG23	3:D:576:ARG:H	1.85	0.40
3:D:733:SER:O	3:D:737:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:361:ILE:HG13	5:X:362:ASN:N	2.36	0.40
1:F:102:LEU:HG	1:F:115:ILE:HG12	2.03	0.40
1:G:185:TYR:HA	1:G:202:VAL:O	2.21	0.40
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.86	0.40
3:I:532:GLU:O	3:I:535:ARG:HB2	2.21	0.40
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.40
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	2.02	0.40
5:Y:361:ILE:HG13	5:Y:362:ASN:N	2.36	0.40
5:Y:540:LEU:HD13	5:Y:607:LEU:HD22	2.04	0.40
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.57	0.40
1:B:234:LEU:O	1:B:235:ARG:HB2	2.21	0.40
2:C:98:VAL:HG11	2:C:124:MET:SD	2.60	0.40
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.40
2:C:106:GLU:CB	2:C:107:ARG:CA	2.98	0.40
2:C:342:ASP:O	2:C:437:ASN:ND2	2.54	0.40
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	2.02	0.40
3:D:179:LYS:H	3:D:179:LYS:HD3	1.87	0.40
3:D:265:LEU:HD21	3:D:327:LEU:HD23	2.02	0.40
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.40
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.36	0.40
5:X:224:LEU:HB2	5:X:259:PHE:CZ	2.56	0.40
5:X:455:HIS:O	5:X:459:THR:HG23	2.21	0.40
1:G:219:ARG:O	1:G:222:THR:HG22	2.21	0.40
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.21	0.40
2:H:442:VAL:HG12	2:H:443:ASP:N	2.37	0.40
2:H:876:GLU:HG3	2:H:927:THR:HG22	2.03	0.40
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.56	0.40
3:I:292:VAL:HG13	3:I:293:ARG:N	2.35	0.40
3:I:598:LYS:HG3	3:I:599:LYS:N	2.36	0.40
4:J:5:THR:HB	4:J:7:GLN:HB2	2.03	0.40
2:C:56:VAL:HB	2:C:57:PHE:H	1.60	0.40
2:C:600:THR:HG22	2:C:601:ASP:H	1.87	0.40
2:C:611:GLU:CD	2:C:616:ILE:HD11	2.47	0.40
2:C:1017:GLN:O	2:C:1020:GLU:HB3	2.20	0.40
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	2.02	0.40
3:D:558:ASP:OD1	3:D:559:ALA:N	2.54	0.40
3:D:610:ARG:N	3:D:610:ARG:HD2	2.36	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.21	0.40
5:X:493:LYS:O	5:X:497:VAL:HG23	2.21	0.40
5:X:559:LEU:HD12	5:X:594:ALA:HB1	2.03	0.40
1:F:51:MET:HA	1:F:52:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:HIS:O	1:F:117:HIS:ND1	2.50	0.40
2:H:31:GLN:O	2:H:130:MET:HE1	2.21	0.40
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.22	0.40
3:I:85:CYS:SG	3:I:86:GLU:N	2.93	0.40
3:I:165:TYR:CE1	3:I:169:LEU:HD23	2.56	0.40
3:I:238:ILE:O	3:I:238:ILE:HG13	2.20	0.40
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.40
3:I:807:LEU:HD12	3:I:807:LEU:C	2.46	0.40
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.47	0.40
5:Y:288:MET:HA	5:Y:302:PHE:CZ	2.57	0.40
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.57	0.40
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.21	0.40
3:D:213:LYS:O	3:D:215:LYS:N	2.54	0.40
3:D:233:LYS:CG	3:D:234:PRO:HD2	2.51	0.40
3:D:1221:LEU:C	3:D:1221:LEU:HD13	2.47	0.40
4:E:19:LEU:HD13	4:E:19:LEU:C	2.47	0.40
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.57	0.40
2:H:898:GLU:CB	5:Y:540:LEU:HD21	2.52	0.40
2:H:975:ILE:HD13	2:H:975:ILE:C	2.46	0.40
3:I:29:MET:HE2	3:I:33:TRP:NE1	2.36	0.40
3:I:483:LEU:HD12	3:I:483:LEU:N	2.36	0.40
1:B:183:ILE:HD11	1:B:205:MET:HG3	2.04	0.40
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.54	0.40
2:C:117:ILE:HD13	2:C:487:LEU:HB3	2.04	0.40
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	2.03	0.40
3:D:43:THR:OG1	3:D:44:ILE:N	2.55	0.40
3:D:166:LEU:HD12	3:D:166:LEU:C	2.47	0.40
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.21	0.40
3:D:1258:ARG:HG3	3:D:1259:GLN:N	2.37	0.40
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.21	0.40
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.86	0.40
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.52	0.40
2:H:51:ALA:C	2:H:53:PHE:H	2.30	0.40
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.03	0.40
2:H:1296:ASP:OD2	2:H:1320:PRO:HB2	2.21	0.40
3:I:40:LYS:HA	3:I:41:PRO:HD3	1.80	0.40
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.35	0.40
3:I:263:SER:HB2	5:Y:507:MET:HE2	2.03	0.40
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.57	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	321/329 (98%)	263 (82%)	42 (13%)	16 (5%)	1	18
1	B	217/329 (66%)	187 (86%)	25 (12%)	5 (2%)	5	31
1	F	227/329 (69%)	195 (86%)	27 (12%)	5 (2%)	5	31
1	G	213/329 (65%)	188 (88%)	22 (10%)	3 (1%)	9	39
2	C	1333/1342 (99%)	1087 (82%)	204 (15%)	42 (3%)	3	25
2	H	1333/1342 (99%)	1091 (82%)	197 (15%)	45 (3%)	3	24
3	D	1154/1407 (82%)	933 (81%)	180 (16%)	41 (4%)	2	23
3	I	1154/1407 (82%)	934 (81%)	180 (16%)	40 (4%)	3	23
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	1	17
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	1	14
5	X	511/613 (83%)	453 (89%)	44 (9%)	14 (3%)	4	28
5	Y	454/613 (74%)	414 (91%)	30 (7%)	10 (2%)	5	31
All	All	7079/8222 (86%)	5886 (83%)	962 (14%)	231 (3%)	3	24

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	319	GLU
1	B	20	SER
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	53	PHE
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO

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Mol	Chain	Res	Type
2	C	686	GLN
2	C	748	ILE
2	C	753	LEU
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1363	TYR
4	E	6	VAL
5	X	241	SER
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL
2	H	39	ILE
2	H	53	PHE
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	542	ALA
3	I	710	ASP
3	I	847	ASP
3	I	851	PRO
4	J	4	VAL
4	J	6	VAL
4	J	35	LYS

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Mol	Chain	Res	Type
5	Y	241	SER
1	A	193	GLU
1	A	201	LEU
1	A	232	VAL
1	B	19	VAL
1	B	52	PRO
2	C	437	ASN
2	C	812	PHE
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	214	ARG
3	D	417	ARG
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	728	SER
3	D	851	PRO
3	D	901	ARG
3	D	914	ALA
3	D	1192	LYS
4	E	35	LYS
5	X	20	GLY
5	X	23	THR
5	X	108	VAL
5	X	490	PRO
5	X	514	ASP
5	X	581	ASP
1	G	188	GLU
1	G	228	LEU
2	H	170	VAL
2	H	437	ASN
2	H	669	PRO
2	H	753	LEU
2	H	812	PHE
2	H	1006	GLU
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
3	I	89	GLY
3	I	214	ARG

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Mol	Chain	Res	Type
3	I	345	LYS
3	I	417	ARG
3	I	595	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	901	ARG
3	I	914	ALA
3	I	1192	LYS
3	I	1195	GLN
3	I	1268	ASN
3	I	1363	TYR
5	Y	308	GLY
5	Y	490	PRO
1	A	93	GLN
1	A	196	THR
1	B	188	GLU
2	C	143	ARG
2	C	1240	ASP
3	D	53	ARG
3	D	210	SER
3	D	316	ILE
3	D	559	ALA
3	D	590	SER
3	D	672	LEU
3	D	703	THR
3	D	707	ILE
3	D	913	GLU
3	D	1195	GLN
4	E	4	VAL
5	X	308	GLY
5	X	491	GLU
1	F	33	ARG
1	F	188	GLU
2	H	44	GLU
2	H	487	LEU
2	H	543	ALA
2	H	1046	VAL
2	H	1137	GLU
2	H	1240	ASP
2	H	1256	GLN
3	I	53	ARG

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Mol	Chain	Res	Type
3	I	153	ASN
3	I	210	SER
3	I	559	ALA
3	I	590	SER
3	I	728	SER
3	I	913	GLU
5	Y	108	VAL
5	Y	491	GLU
5	Y	514	ASP
1	A	166	ARG
1	A	188	GLU
1	B	235	ARG
2	C	44	GLU
2	C	487	LEU
2	C	1006	GLU
2	C	1080	ASN
2	C	1137	GLU
2	C	1139	ALA
3	D	153	ASN
3	D	832	LYS
3	D	888	CYS
4	E	5	THR
5	X	600	HIS
1	F	153	VAL
1	F	166	ARG
2	H	143	ARG
2	H	488	MET
2	H	535	PRO
2	H	895	LEU
2	H	1045	GLY
2	H	1080	ASN
2	H	1139	ALA
3	I	672	LEU
3	I	703	THR
3	I	832	LYS
3	I	888	CYS
3	I	1194	ARG
5	Y	107	THR
5	Y	581	ASP
1	A	14	VAL
1	A	322	PRO
1	A	324	ALA

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Mol	Chain	Res	Type
2	C	699	LEU
2	C	746	ALA
2	C	1203	ASP
2	C	1315	MET
3	D	816	THR
5	X	50	ASP
5	X	107	THR
2	H	1093	PRO
2	H	1315	MET
3	I	1290	ARG
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	A	194	GLN
2	C	69	GLN
2	C	895	LEU
2	C	1045	GLY
2	C	1046	VAL
2	C	1093	PRO
2	C	1201	LEU
3	D	255	LEU
3	D	902	ASP
3	D	1173	ARG
3	D	1194	ARG
4	E	59	ILE
2	H	56	VAL
2	H	739	ASP
2	H	746	ALA
2	H	1238	LEU
3	I	596	LEU
3	I	712	GLN
3	I	731	ARG
3	I	816	THR
5	X	97	PRO
4	J	59	ILE
1	A	153	VAL
2	C	56	VAL
2	C	373	GLY
5	X	35	ILE
2	C	59	ILE
2	H	59	ILE
2	H	373	GLY

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Mol	Chain	Res	Type
3	I	850	LYS
5	Y	97	PRO
1	A	30	PRO
3	D	850	LYS
3	D	1185	PRO
2	H	78	PRO
2	H	134	GLY
2	H	43	PRO
2	H	489	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	281/286 (98%)	272 (97%)	9 (3%)	34	56
1	B	189/286 (66%)	183 (97%)	6 (3%)	34	56
1	F	197/286 (69%)	194 (98%)	3 (2%)	57	70
1	G	185/286 (65%)	184 (100%)	1 (0%)	81	82
2	C	1150/1157 (99%)	1084 (94%)	66 (6%)	18	44
2	H	1150/1157 (99%)	1084 (94%)	66 (6%)	18	44
3	D	971/1168 (83%)	909 (94%)	62 (6%)	16	41
3	I	971/1168 (83%)	908 (94%)	63 (6%)	15	41
4	E	74/75 (99%)	71 (96%)	3 (4%)	27	50
4	J	65/75 (87%)	61 (94%)	4 (6%)	16	42
5	X	460/540 (85%)	444 (96%)	16 (4%)	32	54
5	Y	407/540 (75%)	392 (96%)	15 (4%)	30	53
All	All	6100/7024 (87%)	5786 (95%)	314 (5%)	21	46

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	117	HIS
1	A	158	ARG
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	65	LEU
1	B	182	ARG
1	B	196	THR
1	B	228	LEU
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	80	PHE
2	C	88	ARG
2	C	98	VAL
2	C	127	ILE
2	C	161	LYS
2	C	163	LYS
2	C	203	LYS
2	C	479	LEU
2	C	487	LEU
2	C	603	ILE
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	704	MET
2	C	711	ASP
2	C	740	GLU
2	C	773	LEU
2	C	791	LEU
2	C	800	MET

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Mol	Chain	Res	Type
2	C	807	TRP
2	C	817	LEU
2	C	843	THR
2	C	844	LYS
2	C	845	LEU
2	C	890	LYS
2	C	909	LYS
2	C	920	VAL
2	C	944	ARG
2	C	953	LEU
2	C	964	LEU
2	C	975	ILE
2	C	988	LYS
2	C	1002	LEU
2	C	1010	GLN
2	C	1011	LEU
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1060	ILE
2	C	1106	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1210	ILE
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1262	LYS
2	C	1264	GLN
2	C	1265	PHE
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
3	D	9	LYS
3	D	13	LYS
3	D	50	LYS
3	D	66	LYS

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Mol	Chain	Res	Type
3	D	74	LYS
3	D	92	VAL
3	D	114	ILE
3	D	117	LEU
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	155	GLU
3	D	169	LEU
3	D	175	GLU
3	D	179	LYS
3	D	185	ILE
3	D	211	GLU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	416	ILE
3	D	422	LEU
3	D	442	ILE
3	D	475	GLU
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	521	LYS
3	D	523	GLU
3	D	527	LEU
3	D	531	LYS
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	590	SER
3	D	605	LEU
3	D	681	LYS
3	D	707	ILE
3	D	713	GLU
3	D	771	GLN
3	D	816	THR
3	D	826	ILE
3	D	832	LYS
3	D	847	ASP

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Mol	Chain	Res	Type
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	882	VAL
3	D	909	ILE
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1297	LYS
3	D	1306	LEU
3	D	1366	HIS
4	E	4	VAL
4	E	6	VAL
4	E	73	GLN
5	X	21	TYR
5	X	28	ASN
5	X	54	GLN
5	X	99	ARG
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	452	ILE
5	X	457	ILE
5	X	473	GLU
5	X	511	ILE
5	X	545	HIS
5	X	562	ARG
5	X	565	ILE
5	X	607	LEU
1	F	158	ARG
1	F	160	HIS
1	F	181	GLU
1	G	37	HIS
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG

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Mol	Chain	Res	Type
2	H	37	LYS
2	H	41	GLN
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	98	VAL
2	H	99	LYS
2	H	127	ILE
2	H	161	LYS
2	H	203	LYS
2	H	311	CYS
2	H	479	LEU
2	H	481	LEU
2	H	488	MET
2	H	514	PHE
2	H	603	ILE
2	H	661	VAL
2	H	690	VAL
2	H	704	MET
2	H	711	ASP
2	H	740	GLU
2	H	773	LEU
2	H	791	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	865	LEU
2	H	890	LYS
2	H	909	LYS
2	H	920	VAL
2	H	953	LEU
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	988	LYS
2	H	1002	LEU
2	H	1005	GLU

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Mol	Chain	Res	Type
2	H	1010	GLN
2	H	1011	LEU
2	H	1017	GLN
2	H	1032	LYS
2	H	1042	LEU
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1210	ILE
2	H	1211	ARG
2	H	1233	LEU
2	H	1248	THR
2	H	1262	LYS
2	H	1264	GLN
2	H	1276	TRP
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
3	I	9	LYS
3	I	31	ARG
3	I	50	LYS
3	I	66	LYS
3	I	74	LYS
3	I	92	VAL
3	I	114	ILE
3	I	117	LEU
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	155	GLU
3	I	169	LEU
3	I	179	LYS
3	I	185	ILE
3	I	211	GLU
3	I	235	GLU
3	I	248	ASP
3	I	309	ASN

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Mol	Chain	Res	Type
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	422	LEU
3	I	442	ILE
3	I	474	LEU
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	521	LYS
3	I	523	GLU
3	I	527	LEU
3	I	531	LYS
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	605	LEU
3	I	681	LYS
3	I	707	ILE
3	I	771	GLN
3	I	816	THR
3	I	826	ILE
3	I	832	LYS
3	I	847	ASP
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	882	VAL
3	I	909	ILE
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1196	LEU
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1366	HIS

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Mol	Chain	Res	Type
4	J	4	VAL
4	J	6	VAL
4	J	13	ILE
4	J	73	GLN
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	473	GLU
5	Y	511	ILE
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	75	GLN
1	A	84	ASN
1	A	239	GLN
1	A	268	ASN
1	B	84	ASN
1	B	147	GLN
2	C	133	ASN
2	C	139	ASN
2	C	437	ASN
2	C	450	ASN
2	C	513	GLN
2	C	573	ASN
2	C	673	HIS
2	C	684	ASN
2	C	808	ASN
2	C	932	GLN
2	C	952	GLN
2	C	955	GLN

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Mol	Chain	Res	Type
2	C	1010	GLN
2	C	1017	GLN
2	C	1072	ASN
2	C	1134	GLN
2	C	1264	GLN
3	D	164	GLN
3	D	209	ASN
3	D	680	ASN
3	D	690	ASN
3	D	739	GLN
3	D	777	HIS
3	D	1197	ASN
3	D	1218	HIS
3	D	1268	ASN
4	E	31	GLN
5	X	40	GLN
5	X	54	GLN
5	X	317	ASN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	455	HIS
1	F	103	ASN
1	G	23	HIS
1	G	66	HIS
2	H	46	GLN
2	H	450	ASN
2	H	510	GLN
2	H	513	GLN
2	H	573	ASN
2	H	582	ASN
2	H	649	GLN
2	H	684	ASN
2	H	834	GLN
2	H	1010	GLN
2	H	1072	ASN
2	H	1108	ASN
2	H	1116	HIS
2	H	1134	GLN
2	H	1220	GLN
2	H	1264	GLN
3	I	164	GLN

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Mol	Chain	Res	Type
3	I	209	ASN
3	I	274	ASN
3	I	309	ASN
3	I	320	ASN
3	I	465	GLN
3	I	495	ASN
3	I	739	GLN
3	I	777	HIS
3	I	1268	ASN
3	I	1366	HIS
4	J	15	ASN
5	Y	437	GLN
5	Y	455	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	1RL	H	1401	-	68,70,70	3.29	21 (30%)	89,104,104	2.31	32 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1RL	C	1401	-	68,70,70	3.30	20 (29%)	89,104,104	2.18	23 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1RL	H	1401	-	-	31/65/84/84	0/5/6/6
6	1RL	C	1401	-	-	32/65/84/84	0/5/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	1RL	O3-C6	12.53	1.60	1.37
6	H	1401	1RL	O3-C6	12.52	1.60	1.37
6	C	1401	1RL	C6-C7	10.81	1.58	1.39
6	H	1401	1RL	C6-C7	10.71	1.58	1.39
6	C	1401	1RL	C5-C6	-8.19	1.29	1.39
6	H	1401	1RL	C5-C6	-8.15	1.29	1.39
6	H	1401	1RL	C5-C11	-8.07	1.27	1.45
6	C	1401	1RL	C5-C11	-7.97	1.27	1.45
6	H	1401	1RL	C17-C16	7.60	1.55	1.34
6	C	1401	1RL	C17-C16	7.28	1.54	1.34
6	C	1401	1RL	C18-C19	5.51	1.53	1.33
6	H	1401	1RL	C18-C19	5.44	1.53	1.33
6	H	1401	1RL	C12-C11	-5.32	1.33	1.54
6	C	1401	1RL	C12-C11	-5.30	1.33	1.54
6	H	1401	1RL	C15-N1	5.24	1.47	1.37
6	C	1401	1RL	C10-C4	5.23	1.53	1.46
6	C	1401	1RL	C4-N3	5.20	1.38	1.30
6	C	1401	1RL	C15-N1	5.13	1.47	1.37
6	H	1401	1RL	C10-C4	5.02	1.52	1.46
6	H	1401	1RL	C4-N3	5.00	1.38	1.30
6	H	1401	1RL	C10-C5	4.69	1.52	1.41
6	C	1401	1RL	C10-C5	4.66	1.52	1.41
6	C	1401	1RL	O-C06	3.98	1.45	1.37
6	H	1401	1RL	O-C06	3.96	1.45	1.37
6	C	1401	1RL	O7-C35	3.69	1.43	1.35
6	H	1401	1RL	O7-C35	3.50	1.42	1.35
6	H	1401	1RL	C18-C17	3.41	1.53	1.43
6	C	1401	1RL	C18-C17	3.33	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1401	1RL	C34-C26	-2.89	1.47	1.53
6	C	1401	1RL	C34-C26	-2.79	1.47	1.53
6	C	1401	1RL	O2-C8	2.59	1.42	1.36
6	C	1401	1RL	O01-C3	2.38	1.42	1.37
6	C	1401	1RL	C06-C02	2.33	1.44	1.40
6	H	1401	1RL	O01-C3	2.26	1.41	1.37
6	C	1401	1RL	C8-C7	2.23	1.44	1.40
6	H	1401	1RL	O2-C8	2.21	1.41	1.36
6	H	1401	1RL	C06-C02	2.21	1.44	1.40
6	H	1401	1RL	C8-C7	2.21	1.44	1.40
6	H	1401	1RL	O7-C25	-2.18	1.41	1.44
6	H	1401	1RL	O01-C01	2.17	1.41	1.38
6	C	1401	1RL	O01-C01	2.16	1.41	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	1RL	C20-C19-C18	-8.33	108.88	126.11
6	H	1401	1RL	C12-O3-C6	-7.70	94.83	107.69
6	H	1401	1RL	C8-C7-C6	-7.56	106.66	116.86
6	C	1401	1RL	C12-O3-C6	-7.50	95.17	107.69
6	C	1401	1RL	C8-C7-C6	-7.16	107.20	116.86
6	C	1401	1RL	C20-C19-C18	-6.84	111.97	126.11
6	C	1401	1RL	C3-C4-N3	-4.43	116.91	122.59
6	C	1401	1RL	O7-C35-C36	4.38	118.91	111.09
6	H	1401	1RL	C3-C4-N3	-4.34	117.03	122.59
6	H	1401	1RL	C9-C10-C5	-4.26	114.33	119.91
6	C	1401	1RL	C9-C10-C5	-4.22	114.38	119.91
6	H	1401	1RL	O4-C11-C5	-4.05	122.06	130.69
6	C	1401	1RL	O4-C11-C5	-4.01	122.16	130.69
6	H	1401	1RL	C34-C26-C25	-3.92	104.50	111.40
6	H	1401	1RL	C17-C18-C19	-3.91	115.36	124.43
6	H	1401	1RL	O01-C3-C4	3.70	122.66	118.13
6	H	1401	1RL	O7-C35-C36	3.68	117.65	111.09
6	H	1401	1RL	C16-C15-N1	3.65	121.89	115.01
6	C	1401	1RL	O01-C3-C4	3.65	122.60	118.13
6	H	1401	1RL	C18-C17-C16	-3.27	117.41	126.64
6	C	1401	1RL	C16-C15-N1	3.25	121.13	115.01
6	C	1401	1RL	C17-C18-C19	-3.22	116.97	124.43
6	C	1401	1RL	O3-C6-C5	-3.06	112.50	114.34
6	H	1401	1RL	C9-C8-C7	3.01	127.07	122.37
6	C	1401	1RL	C18-C17-C16	-2.91	118.42	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	1RL	O11-C15-N1	-2.84	117.80	122.88
6	C	1401	1RL	C10-C9-C8	2.77	123.64	119.65
6	C	1401	1RL	C02-N3-C4	2.76	122.97	118.00
6	C	1401	1RL	C34-C26-C25	-2.68	106.68	111.40
6	H	1401	1RL	C02-N3-C4	2.68	122.83	118.00
6	C	1401	1RL	O11-C15-N1	-2.68	118.09	122.88
6	H	1401	1RL	O3-C6-C5	-2.66	112.75	114.34
6	H	1401	1RL	C10-C9-C8	2.41	123.11	119.65
6	H	1401	1RL	C14-C7-C8	2.41	124.54	120.52
6	C	1401	1RL	C9-C8-C7	2.39	126.10	122.37
6	C	1401	1RL	C8-C9-C1	-2.36	116.66	120.85
6	H	1401	1RL	C8-C9-C1	-2.33	116.70	120.85
6	C	1401	1RL	C03-C01-C02	2.29	123.74	119.94
6	H	1401	1RL	C03-C01-C02	2.28	123.73	119.94
6	C	1401	1RL	C14-C7-C8	2.27	124.30	120.52
6	C	1401	1RL	C26-C25-C24	-2.25	110.14	114.68
6	C	1401	1RL	O3-C12-C13	2.24	115.75	109.56
6	C	1401	1RL	C13-C12-C11	2.23	119.39	113.90
6	H	1401	1RL	C5-C10-C4	2.19	126.69	122.13
6	H	1401	1RL	C13-C12-C11	2.18	119.28	113.90
6	H	1401	1RL	O3-C12-C13	2.18	115.57	109.56
6	H	1401	1RL	C26-C25-C24	-2.17	110.29	114.68
6	H	1401	1RL	C31-C20-C19	-2.17	105.00	109.91
6	H	1401	1RL	O2-C8-C9	-2.14	116.25	120.95
6	H	1401	1RL	C23-C22-C21	-2.13	108.28	112.55
6	H	1401	1RL	O6-C27-C28	-2.11	104.92	111.05
6	H	1401	1RL	C1-C2-N1	2.05	119.70	115.21
6	H	1401	1RL	C31-C20-C21	2.04	115.82	111.45
6	H	1401	1RL	O7-C25-C24	2.04	112.22	107.52
6	H	1401	1RL	C14-C7-C6	2.01	124.38	121.24

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	1RL	C11-C12-O5-C29
6	C	1401	1RL	C13-C12-O5-C29
6	C	1401	1RL	C16-C17-C18-C19
6	C	1401	1RL	C19-C20-C21-O10
6	C	1401	1RL	C31-C20-C21-C22
6	C	1401	1RL	C21-C22-C23-C24
6	C	1401	1RL	C32-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RL	C26-C27-C28-C29
6	H	1401	1RL	C11-C12-O5-C29
6	H	1401	1RL	C13-C12-O5-C29
6	H	1401	1RL	C30-C16-C17-C18
6	H	1401	1RL	C19-C20-C21-O10
6	H	1401	1RL	C31-C20-C21-C22
6	H	1401	1RL	C21-C22-C23-C24
6	H	1401	1RL	C32-C22-C23-C24
6	H	1401	1RL	C26-C27-C28-C29
6	H	1401	1RL	O8-C35-O7-C25
6	C	1401	1RL	O8-C35-O7-C25
6	C	1401	1RL	C32-C22-C23-O9
6	H	1401	1RL	C32-C22-C23-O9
6	C	1401	1RL	C21-C22-C23-O9
6	H	1401	1RL	C21-C22-C23-O9
6	C	1401	1RL	C17-C18-C19-C20
6	H	1401	1RL	C17-C18-C19-C20
6	C	1401	1RL	C33-C24-C25-C26
6	H	1401	1RL	C33-C24-C25-C26
6	C	1401	1RL	C23-C24-C25-C26
6	C	1401	1RL	C36-C35-O7-C25
6	C	1401	1RL	C31-C20-C21-O10
6	H	1401	1RL	C31-C20-C21-O10
6	C	1401	1RL	C30-C16-C17-C18
6	H	1401	1RL	C36-C35-O7-C25
6	C	1401	1RL	C19-C20-C21-C22
6	H	1401	1RL	C19-C20-C21-C22
6	C	1401	1RL	C33-C24-C25-O7
6	C	1401	1RL	C23-C24-C25-O7
6	H	1401	1RL	C23-C24-C25-O7
6	H	1401	1RL	C23-C24-C25-C26
6	C	1401	1RL	C15-C16-C17-C18
6	H	1401	1RL	C15-C16-C17-C18
6	H	1401	1RL	C33-C24-C25-O7
6	H	1401	1RL	C-C39-N-C09
6	H	1401	1RL	C16-C17-C18-C19
6	C	1401	1RL	C-C39-N-C08
6	C	1401	1RL	C-C39-N-C09
6	C	1401	1RL	O3-C12-O5-C29
6	H	1401	1RL	O3-C12-O5-C29
6	H	1401	1RL	C-C39-N-C08
6	C	1401	1RL	O7-C25-C26-C34

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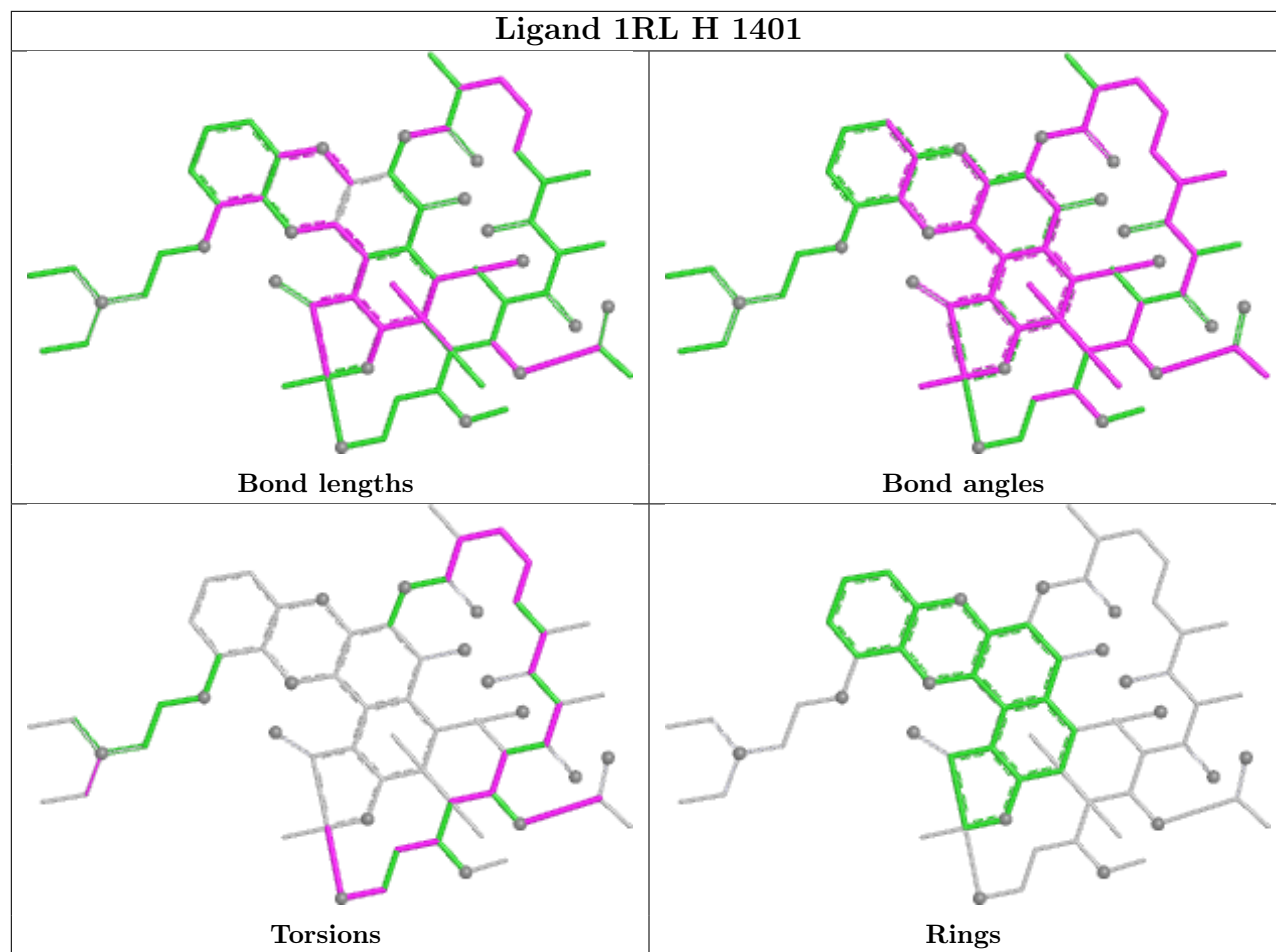
Mol	Chain	Res	Type	Atoms
6	H	1401	1RL	O7-C25-C26-C34
6	C	1401	1RL	N1-C15-C16-C17
6	H	1401	1RL	N1-C15-C16-C17
6	H	1401	1RL	O11-C15-C16-C17
6	C	1401	1RL	O7-C25-C26-C27
6	C	1401	1RL	O11-C15-C16-C17
6	C	1401	1RL	C28-C29-O5-C12
6	H	1401	1RL	C28-C29-O5-C12
6	C	1401	1RL	O6-C27-C28-C29
6	H	1401	1RL	O6-C27-C28-C29
6	C	1401	1RL	O11-C15-C16-C30
6	C	1401	1RL	N1-C15-C16-C30
6	H	1401	1RL	N1-C15-C16-C30
6	H	1401	1RL	O11-C15-C16-C30

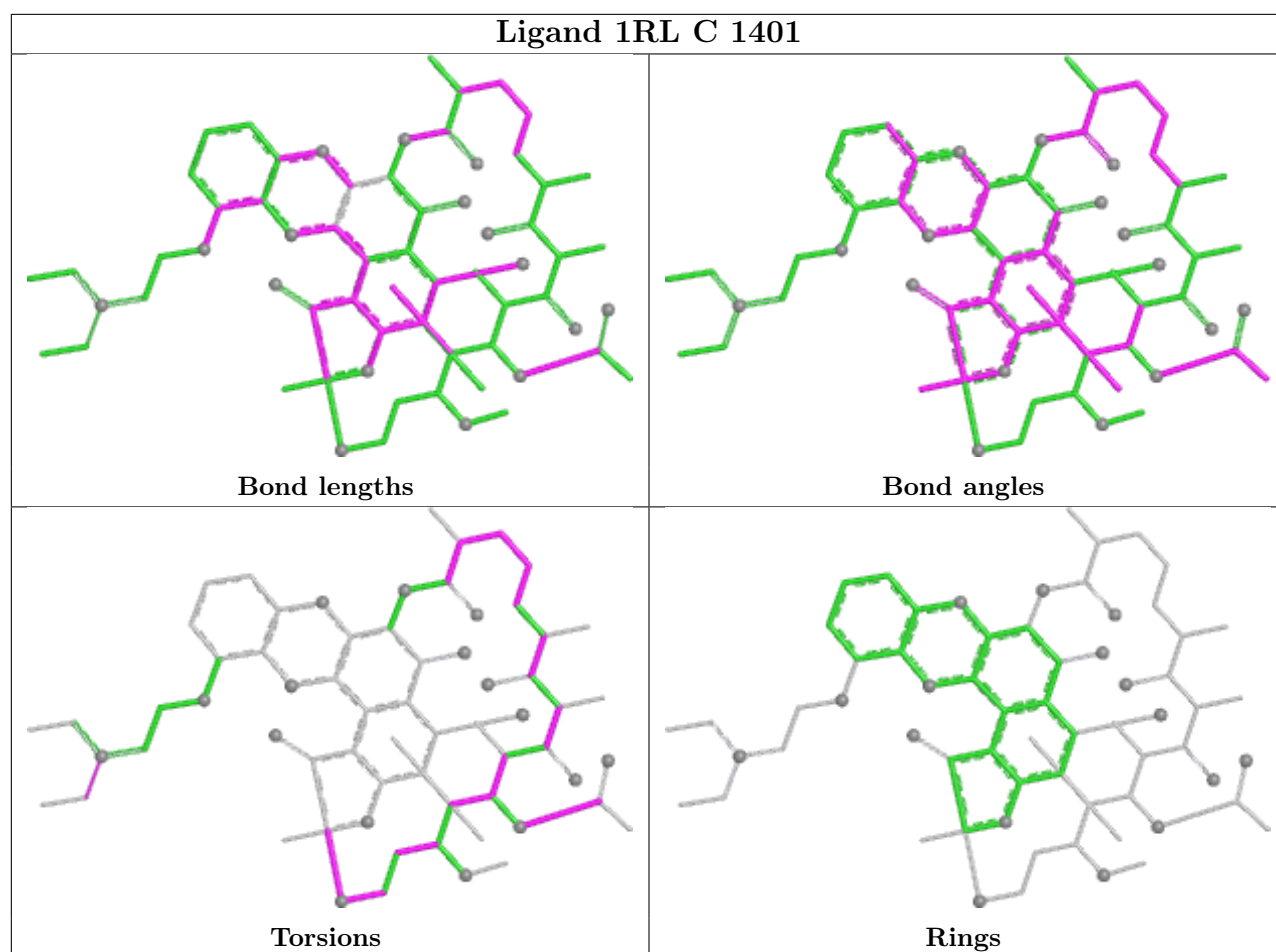
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	1RL	10	0
6	C	1401	1RL	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/329 (98%)	-0.68	0 100 100	0, 68, 172, 270	0
1	B	221/329 (67%)	-0.50	1 (0%) 87 72	6, 90, 201, 277	0
1	F	229/329 (69%)	-0.43	1 (0%) 88 75	9, 123, 209, 249	0
1	G	217/329 (65%)	-0.49	2 (0%) 81 62	34, 112, 176, 230	0
2	C	1335/1342 (99%)	-0.56	5 (0%) 88 75	0, 43, 165, 367	0
2	H	1335/1342 (99%)	-0.63	0 100 100	0, 81, 205, 388	0
3	D	1160/1407 (82%)	-0.59	1 (0%) 92 87	0, 34, 158, 313	0
3	I	1160/1407 (82%)	-0.58	4 (0%) 90 78	0, 50, 190, 338	0
4	E	90/91 (98%)	-0.74	0 100 100	0, 34, 108, 170	0
4	J	76/91 (83%)	-0.75	0 100 100	3, 75, 160, 201	0
5	X	517/613 (84%)	-0.60	4 (0%) 82 64	1, 99, 236, 425	0
5	Y	458/613 (74%)	-0.61	2 (0%) 88 75	1, 102, 234, 374	0
All	All	7121/8222 (86%)	-0.59	20 (0%) 90 78	0, 66, 199, 425	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	1215	GLU	4.2
2	C	194	LEU	3.6
5	X	56	MET	3.5
1	G	39	LEU	3.5
5	X	497	VAL	3.0
3	I	510	LEU	2.6
2	C	206	ALA	2.6
5	Y	221	PHE	2.6
3	D	344	GLY	2.4
1	B	217	ILE	2.4
1	G	59	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	116	ASP	2.4
1	F	131	CYS	2.3
5	Y	337	VAL	2.2
5	X	44	ILE	2.2
5	X	319	ALA	2.1
2	C	251	ALA	2.1
3	I	368	LEU	2.1
3	I	132	LEU	2.0
2	C	52	ALA	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](#)

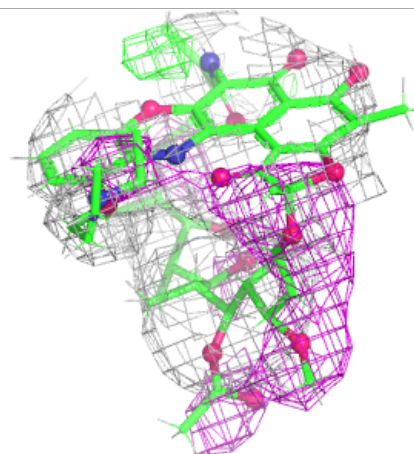
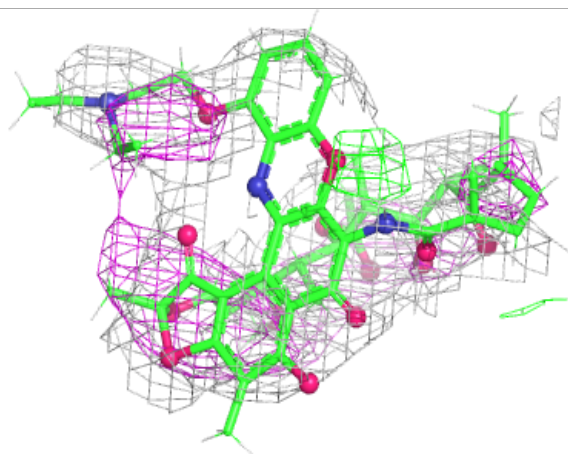
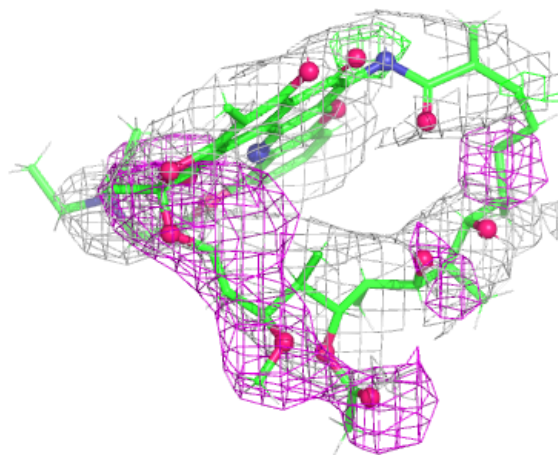
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1RL	H	1401	65/65	0.82	0.09	20,20,20,20	0
6	1RL	C	1401	65/65	0.89	0.07	20,20,20,20	0
8	MG	I	1503	1/1	0.92	0.19	20,20,20,20	0
8	MG	D	1503	1/1	0.96	0.08	24,24,24,24	0
7	ZN	D	1501	1/1	0.98	0.03	54,54,54,54	0
7	ZN	I	1502	1/1	0.99	0.06	49,49,49,49	0
7	ZN	I	1501	1/1	1.00	0.01	60,60,60,60	0
7	ZN	D	1502	1/1	1.00	0.04	8,8,8,8	0

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

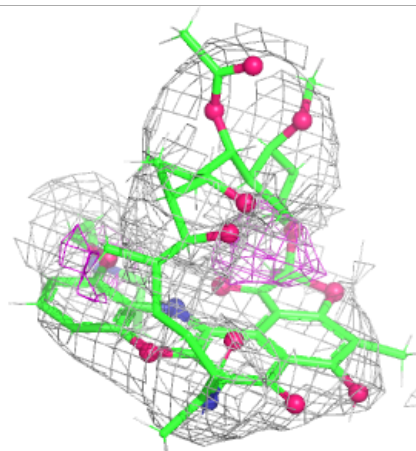
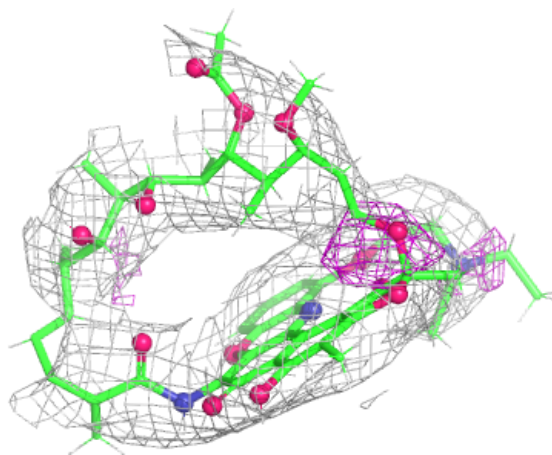
Electron density around 1RL H 1401:

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



Electron density around 1RL C 1401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.