



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2020 – 12:40 PM EDT

PDB ID : 6VJS
Title : Escherichia coli RNA polymerase and ureidothiophene-2-carboxylic acid complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2020-01-17
Resolution : 4.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

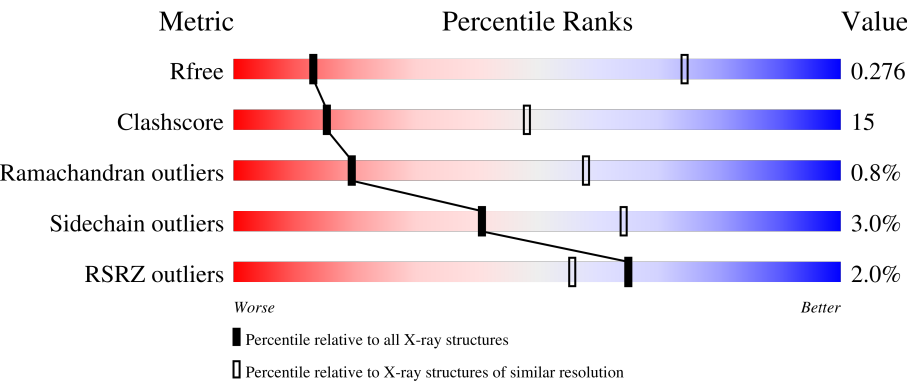
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.02 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div><div></div><div><div></div><div>54%</div><div>17%</div><div>29%</div></div></div>
1	B	329	<div><div>2%</div><div></div><div><div></div><div>58%</div><div>33%</div><div>9%</div></div></div>
1	F	329	<div><div>2%</div><div></div><div><div></div><div>54%</div><div>16%</div><div>29%</div></div></div>
1	G	329	<div><div>5%</div><div></div><div><div></div><div>53%</div><div>16%</div><div>30%</div></div></div>
2	C	1342	<div><div></div><div><div></div><div>66%</div><div>31%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	1342	
3	D	1407	
3	I	1407	
4	E	91	
4	J	91	
5	X	613	
5	Y	613	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	B	301	Total	C	N	O	S	0	0	0
			2337	1462	411	456	8			
1	F	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	G	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			
2	H	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1164	Total	C	N	O	S	0	0	0
			9093	5717	1626	1704	46			
3	I	1160	Total	C	N	O	S	0	0	0
			9061	5698	1619	1698	46			

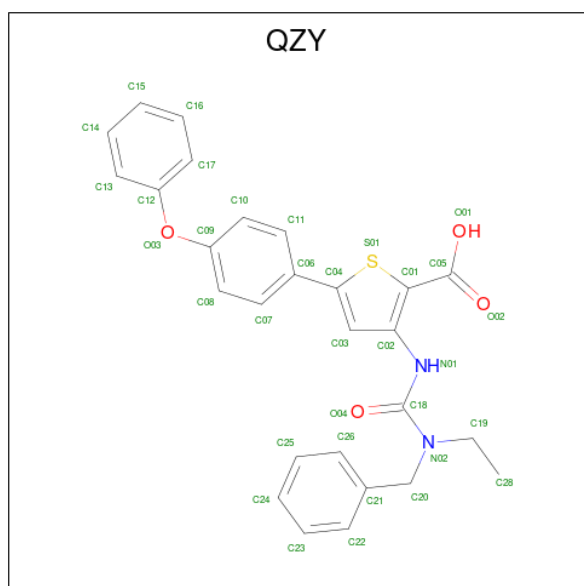
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	471	Total	C	N	O	S	0	0	0
			3832	2398	687	724	23			
5	Y	475	Total	C	N	O	S	0	0	0
			3862	2413	692	734	23			

- Molecule 6 is 3-{[benzyl(ethyl)carbamoyl]amino}-5-(4-phenoxyphenyl)thiophene-2-carboxylic acid (three-letter code: QZY) (formula: C₂₇H₂₄N₂O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			34	27	2	4	1		

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

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

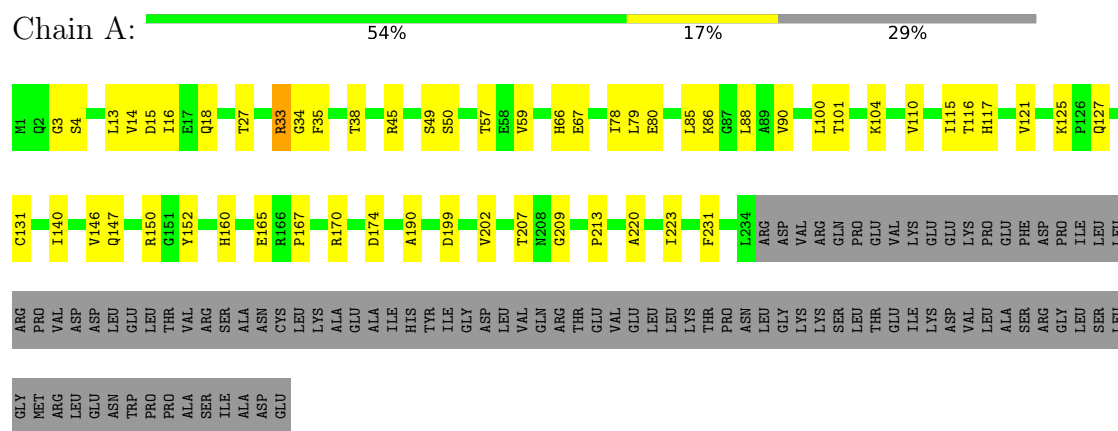
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

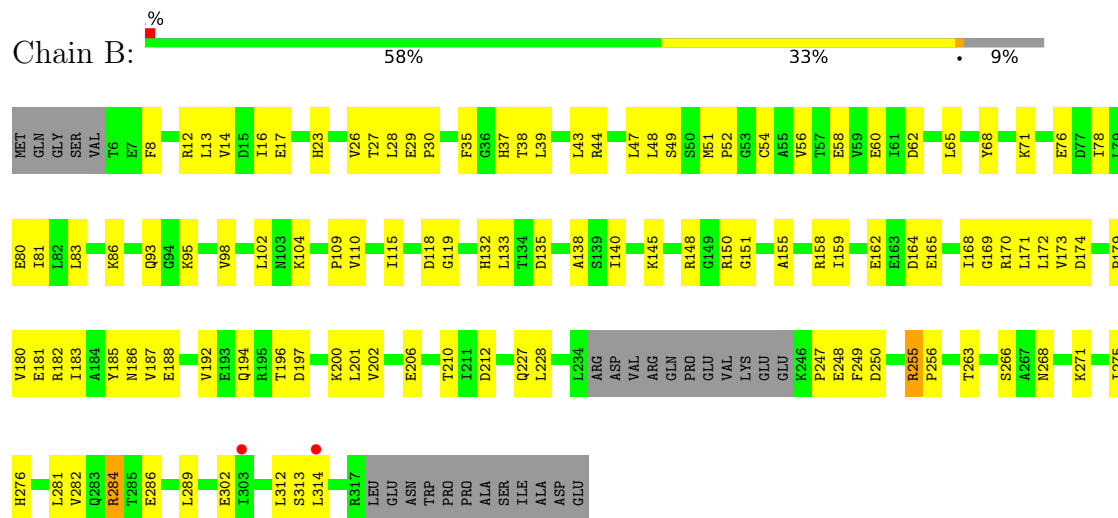
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

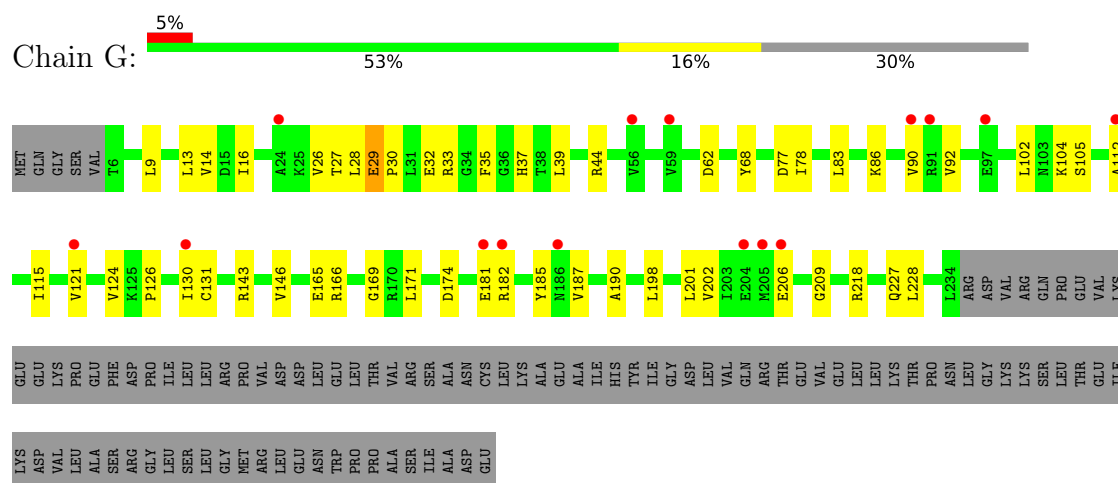


• Molecule 1: DNA-directed RNA polymerase subunit alpha

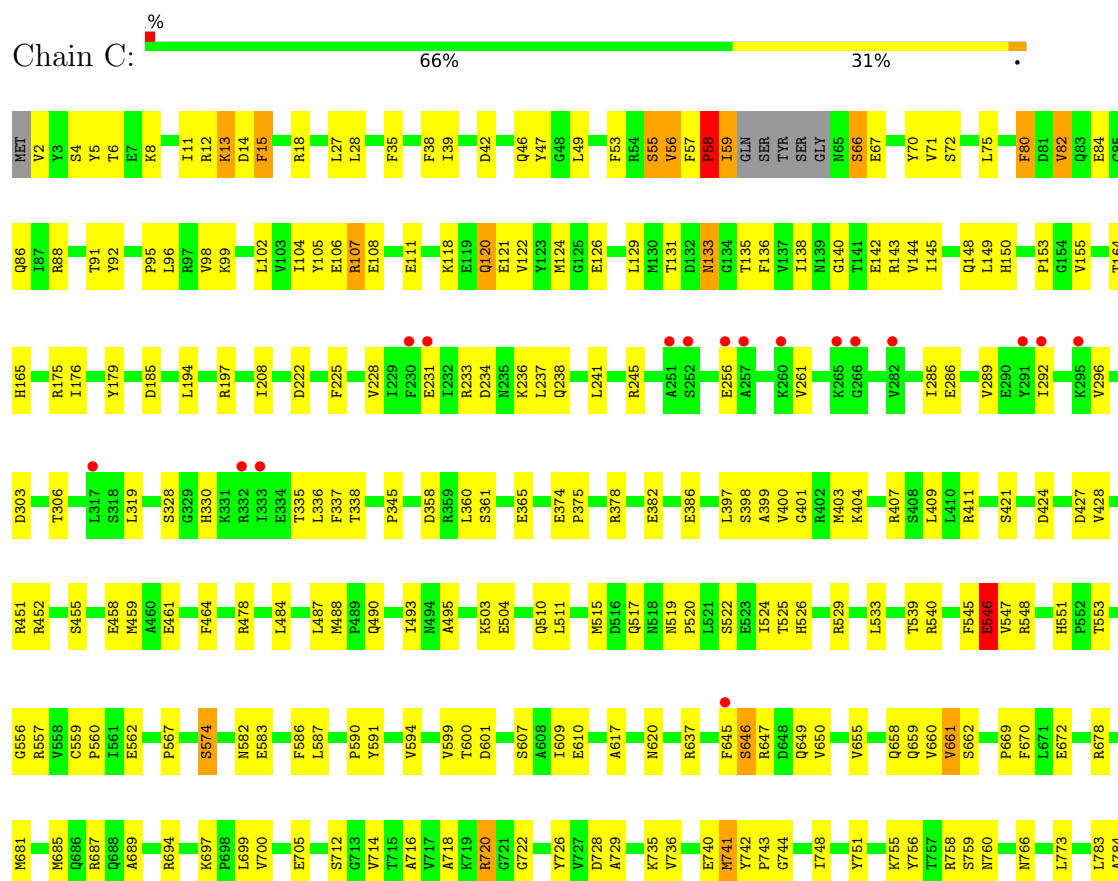


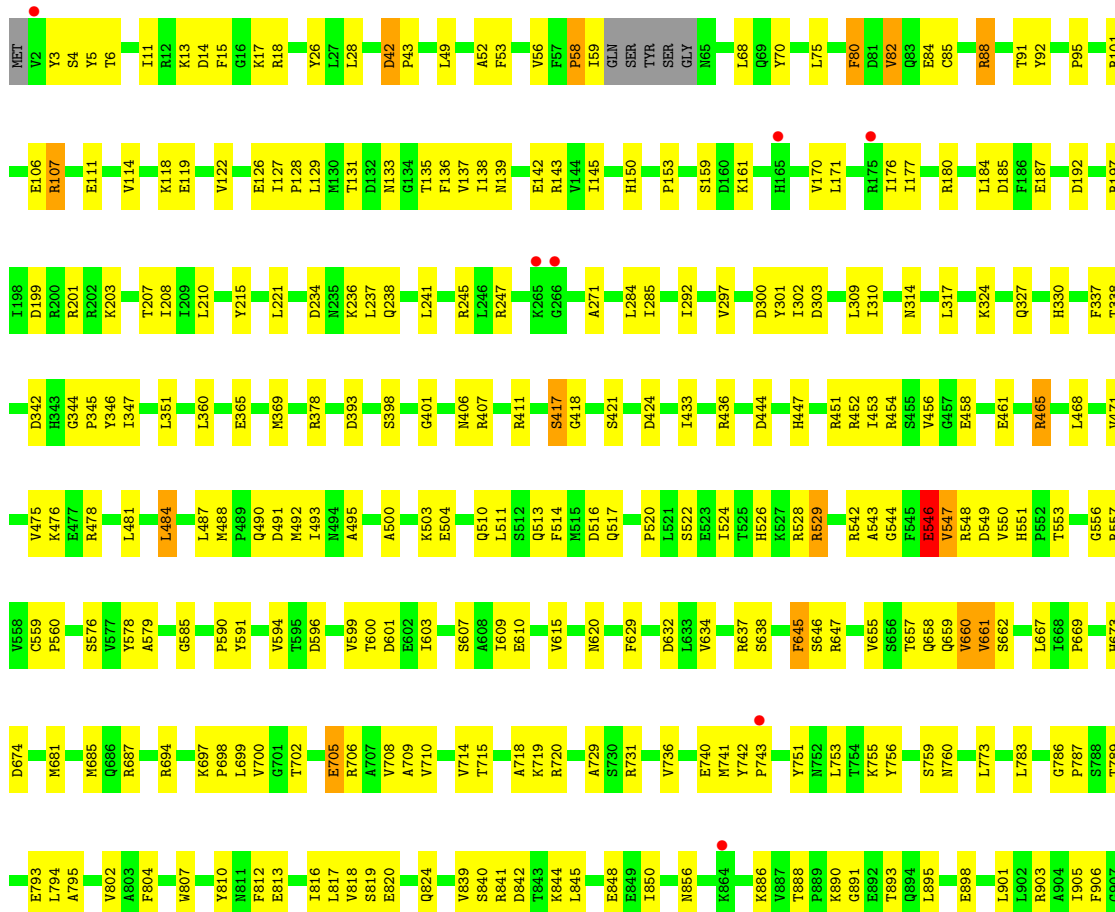


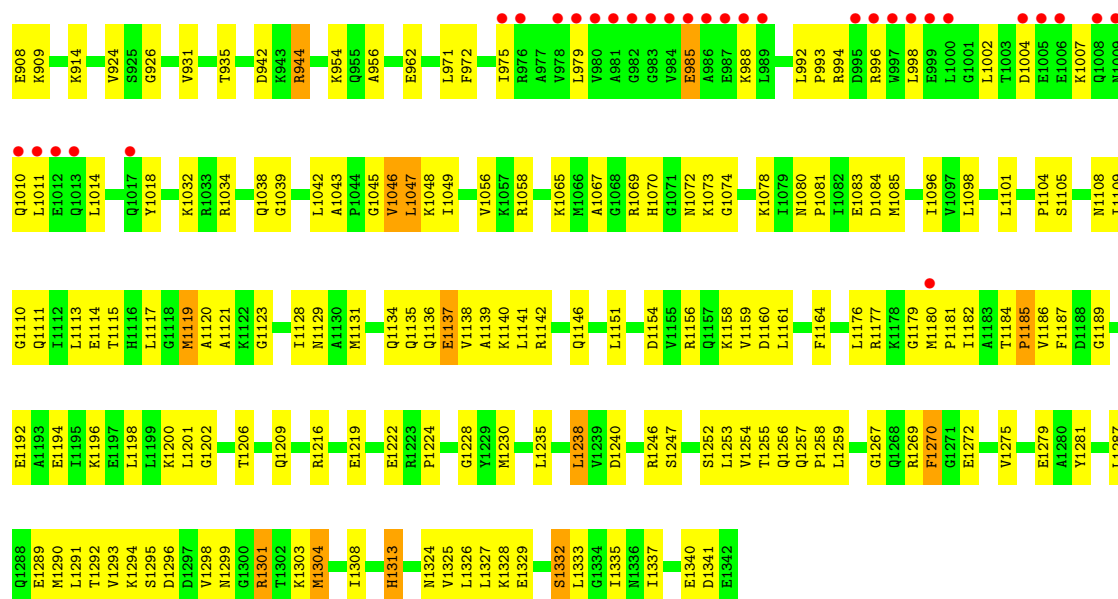
• Molecule 1: DNA-directed RNA polymerase subunit alpha



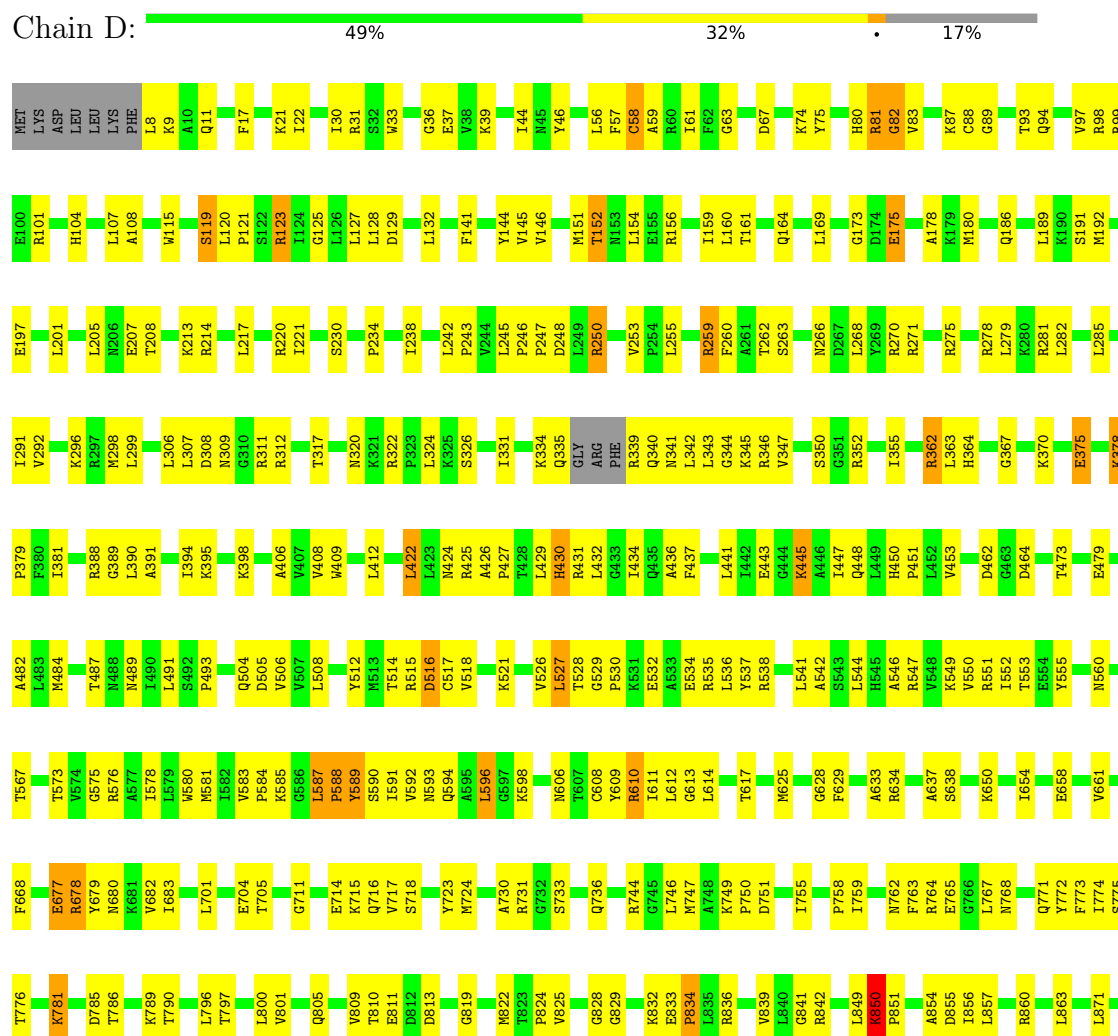
• Molecule 2: DNA-directed RNA polymerase subunit beta

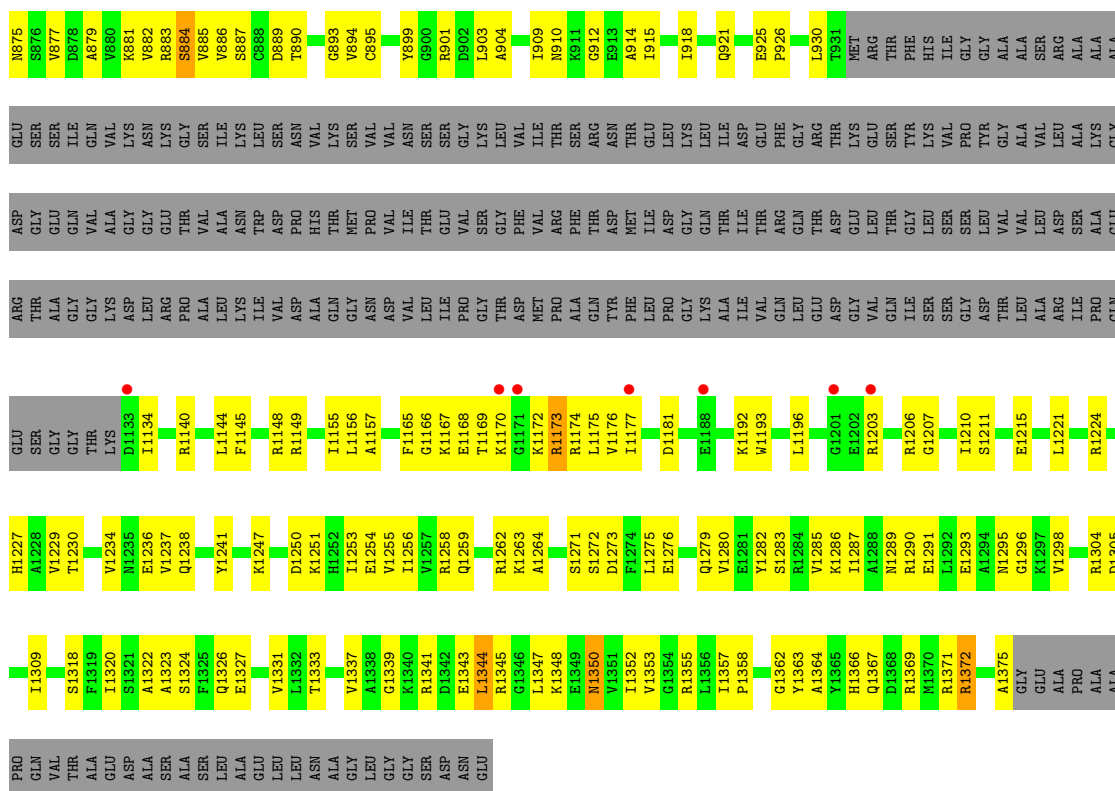




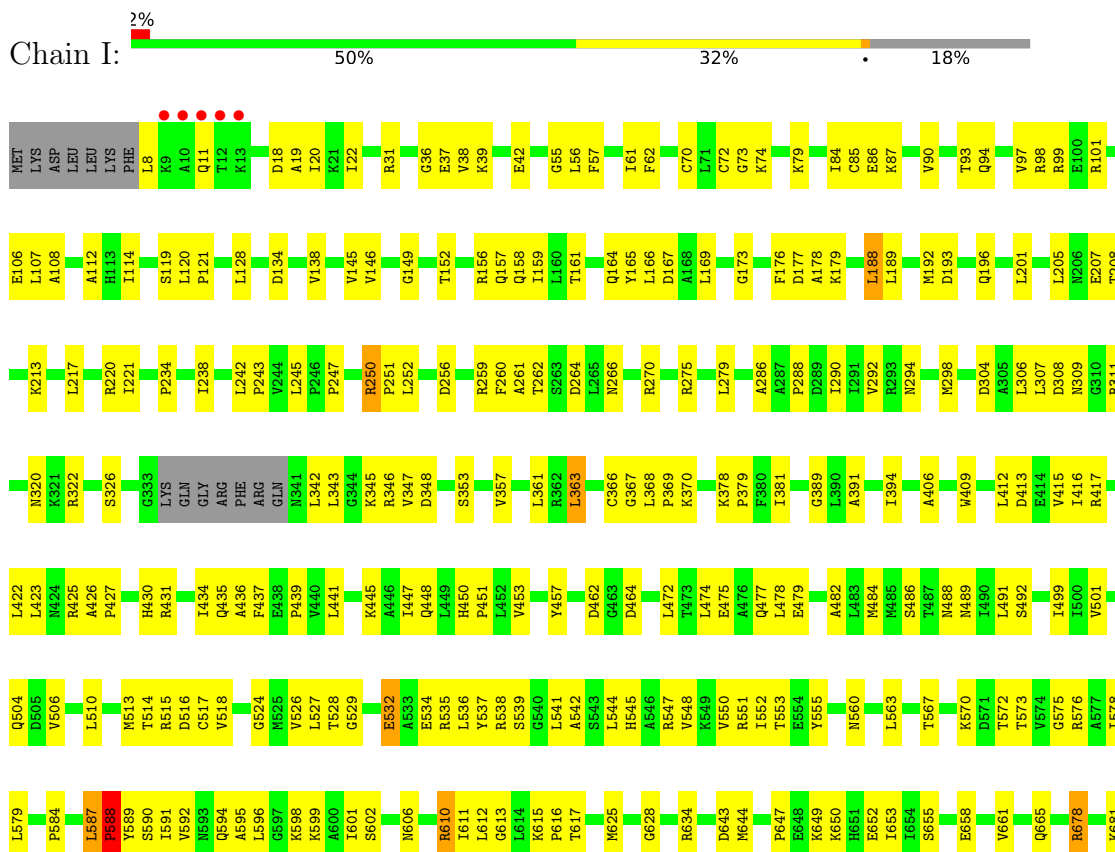


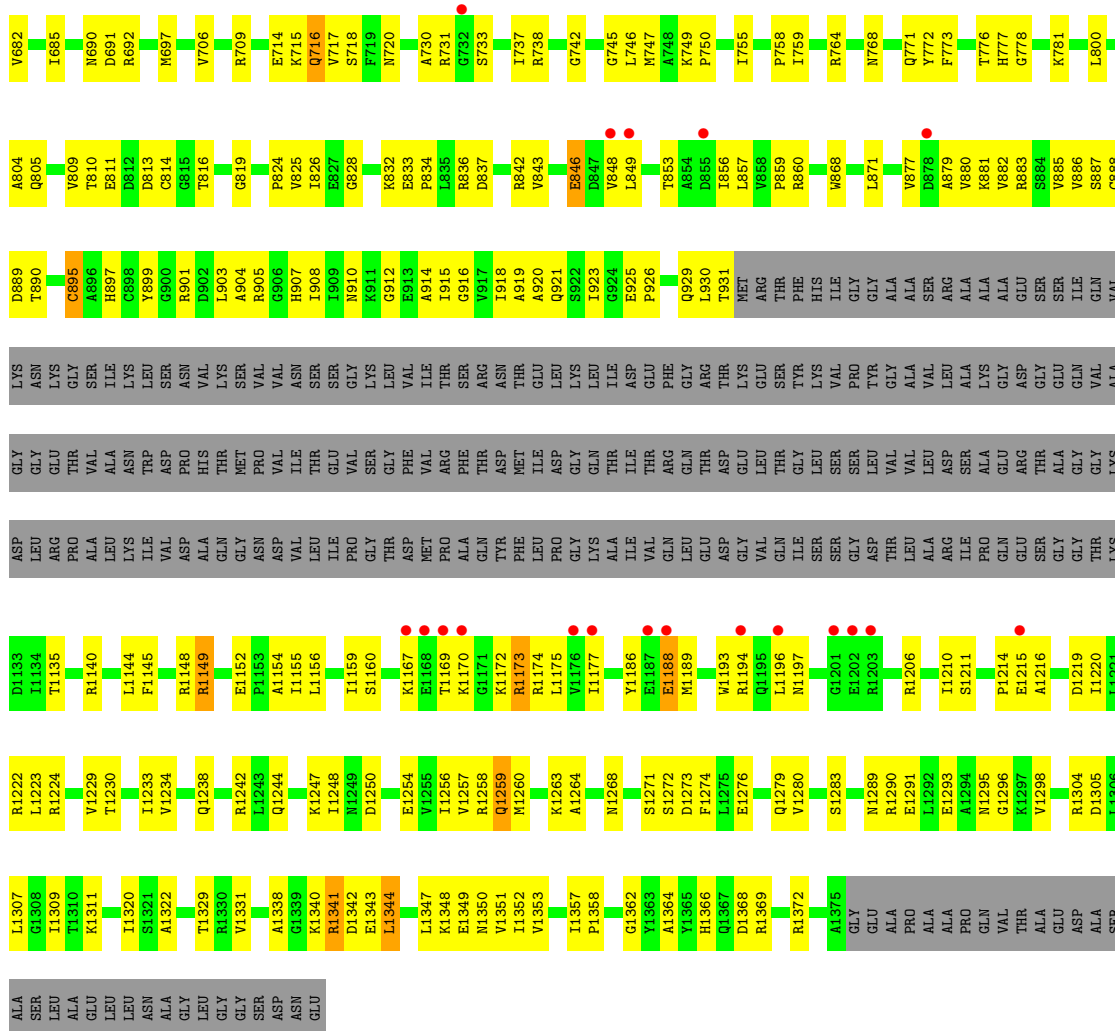
• Molecule 3: DNA-directed RNA polymerase subunit beta'





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





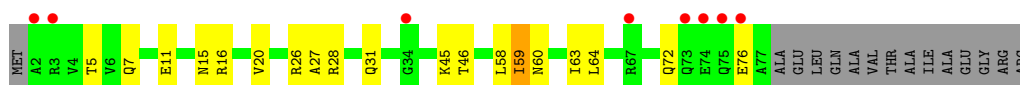
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 87% 12% .



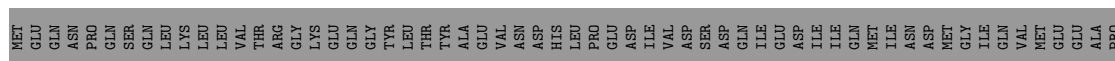
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain J: 9% 63% 20% 16% .



- Molecule 5: RNA polymerase sigma factor RpoD

Chain X: 2% 51% 24% 23% .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.08Å 205.50Å 309.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.09 – 4.02 50.09 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.09-4.02) 99.3 (50.09-4.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.230 , 0.276 0.229 , 0.276	Depositor DCC
R_{free} test set	1999 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	157.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 154.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56011	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: QZY, 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	0.26	0/1831	0.50	0/2481
1	B	0.24	0/2365	0.48	1/3202 (0.0%)
1	F	0.25	0/1830	0.47	0/2478
1	G	0.24	0/1797	0.47	0/2436
2	C	0.27	0/10708	0.55	1/14448 (0.0%)
2	H	0.26	0/10708	0.51	2/14448 (0.0%)
3	D	0.26	0/9231	0.52	2/12459 (0.0%)
3	I	0.25	0/9199	0.50	0/12417
4	E	0.23	0/710	0.46	0/956
4	J	0.22	0/607	0.44	0/817
5	X	0.28	0/3884	0.51	3/5220 (0.1%)
5	Y	0.25	0/3914	0.47	3/5261 (0.1%)
All	All	0.26	0/56784	0.51	12/76623 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	8
2	H	0	5
3	D	0	9
3	I	0	8
5	Y	0	1
All	All	0	31

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	LEU	CA-CB-CG	8.35	134.50	115.30
3	D	711	GLY	N-CA-C	-6.24	97.51	113.10
5	X	259	PHE	CB-CG-CD2	6.21	125.15	120.80
1	B	228	LEU	CA-CB-CG	5.90	128.87	115.30
5	X	503	GLU	C-N-CD	-5.89	107.65	120.60
5	Y	503	GLU	C-N-CD	-5.80	107.83	120.60
2	H	753	LEU	CA-CB-CG	5.67	128.34	115.30
5	Y	259	PHE	N-CA-CB	-5.58	100.56	110.60
5	X	259	PHE	N-CA-CB	-5.46	100.76	110.60
3	D	596	LEU	CA-CB-CG	5.45	127.83	115.30
2	H	1140	LYS	C-N-CA	5.45	135.31	121.70
5	Y	503	GLU	C-N-CA	5.12	143.51	122.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1005	GLU	Peptide
2	C	1137	GLU	Peptide
2	C	13	LYS	Peptide
2	C	42	ASP	Peptide
2	C	546	GLU	Peptide
2	C	55	SER	Peptide
2	C	58	PRO	Peptide
2	C	660	VAL	Peptide
3	D	1172	LYS	Peptide
3	D	119	SER	Peptide
3	D	1343	GLU	Peptide
3	D	1344	LEU	Peptide
3	D	152	THR	Peptide
3	D	588	PRO	Peptide
3	D	832	LYS	Peptide
3	D	833	GLU	Peptide
3	D	850	LYS	Peptide
2	H	1137	GLU	Peptide
2	H	42	ASP	Peptide
2	H	546	GLU	Peptide
2	H	58	PRO	Peptide
2	H	660	VAL	Peptide
3	I	1172	LYS	Peptide
3	I	119	SER	Peptide
3	I	1344	LEU	Peptide
3	I	152	THR	Peptide

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Mol	Chain	Res	Type	Group
3	I	588	PRO	Peptide
3	I	832	LYS	Peptide
3	I	833	GLU	Peptide
3	I	848	VAL	Peptide
5	Y	259	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1837	43	0
1	B	2337	0	2397	75	0
1	F	1809	0	1836	41	0
1	G	1775	0	1800	39	0
2	C	10540	0	10561	357	0
2	H	10540	0	10561	326	0
3	D	9093	0	9290	358	0
3	I	9061	0	9260	350	0
4	E	708	0	719	7	0
4	J	605	0	612	18	0
5	X	3832	0	3907	120	0
5	Y	3862	0	3926	113	0
6	D	34	0	0	2	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	56011	0	56706	1676	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 15.

All (1676) 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:1159:ILE:HD12	3:I:1186:TYR:CE2	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:166:VAL:H	5:X:259:PHE:HA	1.15	1.05
5:X:165:PHE:HB3	5:X:259:PHE:CD2	1.93	1.03
1:A:14:VAL:HG12	1:A:15:ASP:H	1.26	0.96
2:C:841:ARG:HA	2:C:1046:VAL:HG11	1.51	0.93
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.21	0.92
5:Y:165:PHE:HB2	5:Y:259:PHE:HB2	1.53	0.91
2:C:1330:ILE:HG13	6:D:1501:QZY:C16	2.01	0.89
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.54	0.89
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.53	0.89
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.53	0.88
2:H:106:GLU:H	2:H:107:ARG:HA	1.37	0.88
3:D:860:ARG:HE	3:D:883:ARG:HH12	1.20	0.87
3:I:1280:VAL:HA	3:I:1283:SER:HB3	1.56	0.86
5:X:165:PHE:CD1	5:X:259:PHE:HB3	2.11	0.85
2:C:1046:VAL:HG22	2:C:1047:LEU:H	1.40	0.85
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.57	0.85
3:I:1159:ILE:CD1	3:I:1186:TYR:OH	2.25	0.85
2:C:590:PRO:O	2:C:659:GLN:NE2	2.10	0.84
2:H:487:LEU:HA	2:H:488:MET:HB3	1.59	0.84
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.57	0.83
2:C:131:THR:HG23	2:C:133:ASN:H	1.42	0.82
3:I:146:VAL:HA	3:I:178:ALA:HB1	1.62	0.81
5:X:165:PHE:HB3	5:X:259:PHE:HD2	1.39	0.81
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.61	0.81
2:C:487:LEU:HA	2:C:488:MET:HB3	1.62	0.81
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.63	0.80
2:C:490:GLN:HG2	5:X:472:GLN:HB3	1.63	0.80
2:H:560:PRO:HD2	2:H:661:VAL:HG12	1.63	0.80
1:A:104:LYS:HD2	1:A:110:VAL:HG22	1.63	0.80
3:D:81:ARG:HG2	3:D:82:GLY:H	1.47	0.80
3:D:1295:ASN:HB2	3:D:1298:VAL:HG23	1.65	0.79
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.63	0.79
3:I:857:LEU:HD11	3:I:871:LEU:HD21	1.63	0.79
3:I:1159:ILE:HD12	3:I:1186:TYR:CZ	2.18	0.79
2:C:14:ASP:HA	2:C:1158:LYS:HE2	1.63	0.79
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.65	0.79
2:H:493:ILE:O	5:Y:472:GLN:NE2	2.16	0.79
3:D:278:ARG:HG2	3:D:281:ARG:HH21	1.48	0.78
2:C:106:GLU:H	2:C:107:ARG:HA	1.48	0.78
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.66	0.78
2:H:590:PRO:O	2:H:659:GLN:NE2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:824:PRO:HD3	3:I:836:ARG:HE	1.50	0.77
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.64	0.77
3:I:245:LEU:O	3:I:250:ARG:NH1	2.18	0.77
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.33	0.77
3:I:856:ILE:HG23	3:I:857:LEU:HG	1.67	0.77
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.67	0.77
2:H:1324:ASN:HA	2:H:1327:LEU:HD12	1.67	0.77
3:D:406:ALA:HA	3:D:409:TRP:HD1	1.50	0.76
2:H:1269:ARG:HD2	3:I:343:LEU:HB3	1.66	0.76
5:X:165:PHE:HD1	5:X:259:PHE:HB3	1.50	0.76
2:H:176:ILE:HD12	2:H:184:LEU:HD23	1.68	0.75
2:H:520:PRO:HB3	2:H:714:VAL:HG11	1.67	0.75
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.65	0.75
3:D:370:LYS:HG2	3:D:443:GLU:HA	1.69	0.75
1:G:90:VAL:HG11	1:G:146:VAL:HG11	1.68	0.75
1:G:83:LEU:HD11	3:I:527:LEU:HA	1.68	0.75
3:I:809:VAL:HG13	3:I:912:GLY:H	1.51	0.74
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.68	0.74
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.69	0.74
3:D:169:LEU:HD22	3:D:173:GLY:HA2	1.69	0.74
3:D:74:LYS:HD2	3:D:87:LYS:HE3	1.69	0.74
2:C:39:ILE:HD11	2:C:75:LEU:HD11	1.70	0.74
2:H:101:ARG:HG3	2:H:119:GLU:HG2	1.69	0.74
2:H:1291:LEU:HD11	3:I:1351:VAL:HG13	1.70	0.74
5:Y:149:ASP:HA	5:Y:152:GLU:HB2	1.70	0.74
3:D:1177:ILE:HD11	3:D:1196:LEU:HD21	1.69	0.73
2:C:106:GLU:HG2	2:C:111:GLU:HA	1.70	0.73
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.68	0.73
3:D:506:VAL:HG21	3:D:625:MET:HA	1.68	0.73
2:H:1137:GLU:O	2:H:1139:ALA:N	2.21	0.73
1:F:232:VAL:HA	1:G:218:ARG:HG3	1.69	0.73
2:C:546:GLU:O	2:C:548:ARG:N	2.22	0.73
3:D:813:ASP:HB3	3:D:860:ARG:HH22	1.52	0.73
1:A:125:LYS:HE2	1:A:127:GLN:HB2	1.70	0.73
2:C:135:THR:OG1	2:C:142:GLU:O	2.07	0.73
5:X:166:VAL:N	5:X:259:PHE:HA	1.99	0.73
1:A:14:VAL:HG12	1:A:15:ASP:N	2.01	0.72
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.72
3:I:816:THR:HG21	3:I:888:CYS:H	1.54	0.72
3:D:207:GLU:HG2	3:D:208:THR:HG22	1.70	0.72
1:B:159:ILE:HG12	1:B:172:LEU:HD22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HB3	1:B:180:VAL:HG21	1.71	0.72
5:Y:165:PHE:CB	5:Y:259:PHE:HB2	2.19	0.72
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.70	0.72
3:I:517:CYS:H	3:I:545:HIS:HB2	1.53	0.72
3:I:555:TYR:H	3:I:589:TYR:HD2	1.37	0.72
5:Y:231:THR:HG23	5:Y:249:ILE:HG12	1.71	0.72
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.72	0.72
2:H:517:GLN:HE21	2:H:760:ASN:H	1.38	0.72
2:C:1240:ASP:HA	3:D:445:LYS:HE2	1.73	0.71
1:B:181:GLU:HA	3:D:535:ARG:HD3	1.71	0.71
5:X:165:PHE:HA	5:X:260:ARG:H	1.54	0.71
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.23	0.71
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.71	0.71
1:A:14:VAL:CG1	1:A:15:ASP:H	2.03	0.71
2:H:106:GLU:N	2:H:107:ARG:HA	2.05	0.71
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.55	0.71
2:H:1275:VAL:HG12	2:H:1287:LEU:HD11	1.70	0.70
2:H:840:SER:HA	2:H:886:LYS:HD2	1.73	0.70
5:X:166:VAL:HG13	5:X:260:ARG:HG2	1.73	0.70
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.55	0.70
3:I:422:LEU:HA	3:I:436:ALA:HA	1.74	0.70
1:G:9:LEU:HD22	1:G:32:GLU:HG3	1.71	0.70
5:Y:598:LEU:HD12	5:Y:601:PRO:HB3	1.74	0.70
3:I:1159:ILE:HD11	3:I:1186:TYR:OH	1.89	0.70
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.74	0.70
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.24	0.70
2:H:516:ASP:OD1	2:H:522:SER:OG	2.09	0.70
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.74	0.69
3:I:555:TYR:HB2	3:I:589:TYR:HE2	1.55	0.69
3:I:527:LEU:HD13	3:I:532:GLU:HG3	1.73	0.69
2:C:804:PHE:O	3:D:638:SER:OG	2.08	0.69
2:H:546:GLU:O	2:H:548:ARG:N	2.25	0.69
3:I:1264:ALA:HA	3:I:1305:ASP:HB2	1.74	0.69
3:I:814:CYS:O	3:I:860:ARG:NH2	2.26	0.69
1:B:68:TYR:HE1	1:B:171:LEU:HD12	1.58	0.69
2:C:545:PHE:HZ	3:D:781:LYS:HB2	1.57	0.69
2:C:2:VAL:O	2:C:12:ARG:NH1	2.25	0.69
3:I:846:GLU:HA	3:I:859:PRO:HA	1.74	0.69
3:D:260:PHE:HB2	5:X:504:PRO:HG3	1.75	0.69
2:H:58:PRO:HB3	2:H:476:LYS:HA	1.73	0.69
5:X:562:ARG:NH1	5:X:591:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.75	0.68
3:D:1375:ALA:HB2	3:I:849:LEU:HD22	1.74	0.68
3:D:422:LEU:HA	3:D:436:ALA:HA	1.75	0.68
1:B:188:GLU:HB3	1:B:200:LYS:HE3	1.76	0.68
5:X:598:LEU:HD12	5:X:601:PRO:HB3	1.76	0.68
2:H:82:VAL:HA	2:H:85:CYS:HB2	1.76	0.68
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.76	0.68
5:Y:405:ILE:O	5:Y:409:ASN:ND2	2.27	0.68
2:H:971:LEU:HD21	2:H:1014:LEU:HG	1.76	0.67
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.75	0.67
2:H:1046:VAL:HG22	2:H:1047:LEU:H	1.60	0.67
5:X:112:THR:HG22	5:X:113:ARG:H	1.60	0.67
3:I:279:LEU:O	3:I:279:LEU:HD13	1.94	0.67
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.27	0.67
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.74	0.67
5:Y:165:PHE:HB2	5:Y:259:PHE:CB	2.25	0.67
3:D:521:LYS:HB3	3:D:542:ALA:HB1	1.77	0.67
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.77	0.67
3:I:437:PHE:HZ	3:I:453:VAL:HG21	1.60	0.67
5:X:130:VAL:HG13	5:X:365:MET:HG3	1.77	0.67
5:Y:380:VAL:HG23	5:Y:412:LEU:HD23	1.76	0.66
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.76	0.66
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.78	0.66
3:D:1215:GLU:OE1	3:D:1224:ARG:NH2	2.29	0.66
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.76	0.66
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.77	0.66
5:X:111:LEU:HD22	5:X:115:GLY:HA3	1.76	0.66
5:X:165:PHE:HA	5:X:260:ARG:N	2.09	0.66
5:X:234:THR:HB	5:X:245:ALA:HB1	1.78	0.66
3:I:1215:GLU:OE1	3:I:1224:ARG:NH2	2.28	0.66
2:C:720:ARG:HH11	2:C:736:VAL:HG21	1.59	0.66
1:B:37:HIS:HE1	1:B:187:VAL:HG22	1.60	0.66
2:C:840:SER:OG	2:C:1048:LYS:O	2.14	0.66
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.77	0.66
3:I:275:ARG:HD3	3:I:298:MET:HB3	1.77	0.66
2:H:56:VAL:O	2:H:58:PRO:HD3	1.94	0.66
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.78	0.66
3:I:1295:ASN:HB2	3:I:1298:VAL:HG23	1.76	0.66
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.29	0.66
3:I:368:LEU:HD23	3:I:439:PRO:HB3	1.78	0.65
2:C:517:GLN:HE21	2:C:760:ASN:HD22	1.41	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:495:ALA:HB3	5:Y:471:LEU:HD13	1.77	0.65
3:I:482:ALA:O	3:I:488:ASN:ND2	2.30	0.65
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.77	0.65
3:D:81:ARG:CG	3:D:82:GLY:H	2.08	0.65
3:I:492:SER:HB2	3:I:499:ILE:HD13	1.76	0.65
3:I:527:LEU:HD23	3:I:528:THR:H	1.62	0.65
2:H:49:LEU:HG	2:H:461:GLU:HG3	1.76	0.65
2:H:68:LEU:HD22	2:H:475:VAL:HG21	1.79	0.65
3:I:85:CYS:SG	3:I:86:GLU:N	2.69	0.65
2:C:398:SER:O	2:C:401:GLY:N	2.29	0.65
3:I:811:GLU:OE2	3:I:890:THR:OG1	2.12	0.65
1:B:95:LYS:HE3	1:B:98:VAL:HB	1.77	0.65
2:C:1269:ARG:HD2	3:D:343:LEU:HD21	1.77	0.65
2:H:1134:GLN:O	2:H:1137:GLU:N	2.29	0.65
2:H:600:THR:HG22	2:H:601:ASP:H	1.61	0.65
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.28	0.65
1:A:86:LYS:HE2	1:A:174:ASP:HB2	1.77	0.65
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.79	0.65
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	1.79	0.65
3:D:553:THR:HG23	3:D:567:THR:HG22	1.77	0.65
3:I:768:ASN:O	3:I:771:GLN:NE2	2.29	0.65
3:I:474:LEU:HD11	4:J:27:ALA:HB3	1.79	0.65
3:I:70:CYS:HB2	3:I:90:VAL:HB	1.78	0.65
5:Y:562:ARG:NH1	5:Y:591:GLU:OE1	2.30	0.65
2:C:1137:GLU:O	2:C:1139:ALA:N	2.30	0.64
1:G:83:LEU:HD13	3:I:526:VAL:HG23	1.79	0.64
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.79	0.64
2:H:607:SER:HB2	2:H:610:GLU:HG3	1.80	0.64
3:I:114:ILE:HD12	3:I:304:ASP:HB3	1.80	0.64
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.80	0.64
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.79	0.64
2:C:1013:GLN:HA	2:C:1016:GLU:HB2	1.79	0.64
1:F:11:PRO:HG3	1:G:227:GLN:HG3	1.78	0.64
3:I:1159:ILE:CD1	3:I:1186:TYR:CE2	2.74	0.64
2:C:495:ALA:HB3	5:X:471:LEU:HD13	1.79	0.64
3:I:826:ILE:HG13	3:I:828:GLY:H	1.62	0.64
2:C:560:PRO:HD2	2:C:661:VAL:HG12	1.80	0.64
2:H:935:THR:HA	2:H:1048:LYS:HB3	1.78	0.64
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.80	0.64
5:X:240:ARG:HD3	5:X:244:THR:HB	1.79	0.64
3:D:768:ASN:N	3:D:771:GLN:HE22	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HH21	4:J:16:ARG:HG3	1.63	0.64
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.79	0.63
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.63	0.63
1:B:188:GLU:O	1:B:200:LYS:HG2	1.97	0.63
3:D:587:LEU:O	3:D:589:TYR:N	2.32	0.63
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.79	0.63
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.62	0.63
2:H:906:PHE:HZ	5:Y:601:PRO:HB2	1.63	0.63
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.79	0.63
1:G:68:TYR:HE1	1:G:171:LEU:HG	1.64	0.63
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.64	0.63
2:C:138:ILE:HB	2:C:143:ARG:HD2	1.78	0.63
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.80	0.63
3:D:534:GLU:HB2	3:D:578:ILE:HD13	1.80	0.63
2:H:590:PRO:HB2	2:H:655:VAL:HG21	1.81	0.63
2:C:228:VAL:N	2:C:335:THR:O	2.30	0.63
3:D:123:ARG:HD3	3:D:1337:VAL:HG21	1.79	0.63
3:D:205:LEU:HB3	3:D:217:LEU:HD13	1.78	0.63
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.30	0.63
5:X:139:GLU:HA	5:X:142:THR:HG22	1.81	0.63
2:C:1275:VAL:HG12	2:C:1287:LEU:HD11	1.80	0.63
2:H:1156:ARG:NH2	2:H:1194:GLU:OE1	2.27	0.63
3:I:615:LYS:HA	4:J:5:THR:HG21	1.81	0.63
2:C:66:SER:N	2:C:105:TYR:HB2	2.14	0.63
2:C:946:LEU:HA	2:C:949:GLU:HG2	1.81	0.63
3:I:649:LYS:HE2	3:I:652:GLU:HG3	1.80	0.63
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.81	0.62
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.80	0.62
3:I:644:MET:O	3:I:764:ARG:NH1	2.32	0.62
2:H:1073:LYS:HB2	3:I:462:ASP:HB2	1.81	0.62
3:I:406:ALA:HA	3:I:409:TRP:HD1	1.64	0.62
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.79	0.62
3:I:260:PHE:HB2	5:Y:504:PRO:HG2	1.81	0.62
5:X:166:VAL:HG13	5:X:260:ARG:CG	2.29	0.62
2:C:66:SER:H	2:C:105:TYR:HB2	1.65	0.62
2:C:56:VAL:O	2:C:58:PRO:HD3	2.00	0.62
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.81	0.62
2:H:1108:ASN:ND2	2:H:1111:GLN:OE1	2.33	0.62
2:H:844:LYS:HE3	5:Y:496:LYS:HE3	1.81	0.62
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.82	0.62
3:I:709:ARG:NH1	3:I:714:GLU:OE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:THR:HG21	2:H:351:LEU:HG	1.82	0.62
2:H:839:VAL:HA	2:H:1049:ILE:HG22	1.82	0.62
3:I:653:ILE:HD12	3:I:692:ARG:HB3	1.81	0.62
5:Y:234:THR:HB	5:Y:245:ALA:HB1	1.82	0.62
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.82	0.62
2:H:478:ARG:NH2	2:H:491:ASP:O	2.33	0.62
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.82	0.62
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.81	0.62
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.82	0.62
2:H:903:ARG:HB3	2:H:908:GLU:HA	1.80	0.62
1:A:27:THR:HG22	1:A:202:VAL:HG22	1.81	0.61
2:H:706:ARG:NH2	2:H:793:GLU:OE2	2.32	0.61
5:Y:514:ASP:C	5:Y:516:ASP:HA	2.21	0.61
2:H:18:ARG:NH1	2:H:620:ASN:O	2.33	0.61
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.81	0.61
2:C:1005:GLU:O	2:C:1007:LYS:N	2.33	0.61
3:D:613:GLY:O	3:D:617:THR:OG1	2.17	0.61
1:G:86:LYS:NZ	1:G:174:ASP:OD2	2.23	0.61
3:I:36:GLY:HA3	3:I:61:ILE:HG12	1.82	0.61
3:D:36:GLY:HA3	3:D:61:ILE:HG12	1.82	0.61
5:Y:105:MET:HG3	5:Y:384:LEU:HD12	1.82	0.61
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.81	0.61
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.82	0.61
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.61
3:I:506:VAL:HG23	3:I:628:GLY:HA3	1.82	0.61
2:C:328:SER:OG	2:C:330:HIS:ND1	2.34	0.61
3:I:298:MET:SD	5:Y:402:LEU:HB3	2.40	0.61
3:I:650:LYS:NZ	3:I:742:GLY:O	2.26	0.61
5:X:560:ARG:HA	5:X:565:ILE:HG23	1.83	0.61
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.83	0.61
2:C:1287:LEU:HD23	3:D:1357:ILE:HG12	1.81	0.61
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.82	0.61
3:I:431:ARG:N	3:I:921:GLN:OE1	2.34	0.61
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.81	0.61
2:H:221:LEU:HD11	2:H:314:ASN:HB2	1.82	0.61
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.83	0.61
2:C:672:GLU:HB3	2:C:1187:PHE:HD1	1.66	0.61
2:H:131:THR:HG23	2:H:133:ASN:H	1.63	0.61
3:I:555:TYR:HD2	3:I:563:LEU:HB3	1.66	0.61
5:X:303:ILE:O	5:X:307:THR:OG1	2.15	0.61
2:C:1268:GLN:HE22	3:D:352:ARG:HE	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1327:LEU:HB3	2:C:1331:ARG:HH12	1.66	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.33	0.60
2:C:817:LEU:HD21	2:C:1078:LYS:HB3	1.83	0.60
3:D:677:GLU:HB2	3:D:680:ASN:HB2	1.83	0.60
1:F:91:ARG:HB3	1:F:122:GLU:HB3	1.83	0.60
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.83	0.60
2:C:99:LYS:HG2	2:C:121:GLU:HG3	1.82	0.60
2:C:559:CYS:HB2	2:C:662:SER:H	1.66	0.60
5:X:157:ARG:HB3	5:X:160:ASP:OD2	2.01	0.60
3:I:1291:GLU:HA	3:I:1296:GLY:HA2	1.84	0.60
3:I:1159:ILE:CD1	3:I:1186:TYR:CZ	2.84	0.60
2:H:559:CYS:HB2	2:H:662:SER:H	1.67	0.60
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.84	0.60
3:I:146:VAL:HA	3:I:178:ALA:CB	2.31	0.60
2:C:104:ILE:HD12	2:C:484:LEU:HD13	1.84	0.60
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.20	0.60
3:D:389:GLY:O	3:D:391:ALA:N	2.35	0.59
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.84	0.59
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.84	0.59
1:B:58:GLU:HB2	1:B:145:LYS:HB3	1.83	0.59
2:H:1293:VAL:HG21	2:H:1304:MET:HG3	1.83	0.59
3:I:415:VAL:O	4:J:45:LYS:NZ	2.35	0.59
2:C:106:GLU:HB2	2:C:108:GLU:H	1.67	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.37	0.59
2:H:557:ARG:NH2	2:H:607:SER:O	2.35	0.59
1:A:45:ARG:HH12	2:C:1084:ASP:HB3	1.67	0.59
2:C:148:GLN:HB2	2:C:511:LEU:HD21	1.84	0.59
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.18	0.59
3:D:345:LYS:HE3	6:D:1501:QZY:C19	2.32	0.59
2:H:135:THR:OG1	2:H:142:GLU:O	2.20	0.59
4:J:72:GLN:NE2	4:J:76:GLU:OE2	2.36	0.59
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.83	0.59
1:B:110:VAL:HG21	1:B:140:ILE:HD11	1.85	0.59
2:H:1159:VAL:HB	2:H:1160:ASP:HB2	1.84	0.59
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.68	0.59
3:D:517:CYS:HA	3:D:716:GLN:OE1	2.02	0.59
3:D:576:ARG:NH2	3:D:594:GLN:O	2.36	0.59
3:D:849:LEU:O	3:D:850:LYS:HB2	2.02	0.59
3:D:839:VAL:HG12	3:D:863:LEU:HD12	1.84	0.59
2:H:14:ASP:O	2:H:1158:LYS:HD3	2.03	0.59
1:B:104:LYS:HD2	1:B:110:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:615:VAL:HA	2:H:638:SER:HB2	1.85	0.59
2:H:669:PRO:HA	2:H:702:THR:HG22	1.85	0.59
3:D:849:LEU:HA	3:D:856:ILE:H	1.67	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.85	0.59
3:I:514:THR:HG21	3:I:596:LEU:HA	1.85	0.59
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.84	0.58
2:C:1252:SER:HA	5:X:524:GLU:HA	1.85	0.58
2:C:1326:LEU:O	2:C:1330:ILE:HG12	2.03	0.58
3:D:930:LEU:HD11	3:D:1241:TYR:HE2	1.68	0.58
2:C:107:ARG:NE	2:C:107:ARG:O	2.21	0.58
2:C:681:MET:O	2:C:685:MET:HG2	2.04	0.58
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.85	0.58
5:X:165:PHE:CB	5:X:259:PHE:HD2	2.14	0.58
3:D:186:GLN:HG3	3:D:238:ILE:HD11	1.84	0.58
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.85	0.58
3:I:513:MET:O	3:I:575:GLY:HA3	2.02	0.58
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.85	0.58
2:H:1341:ASP:OD1	2:H:1341:ASP:N	2.37	0.58
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.36	0.58
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.67	0.58
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.86	0.58
2:H:95:PRO:HA	2:H:126:GLU:HG2	1.85	0.58
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.84	0.58
1:A:33:ARG:N	1:A:34:GLY:HA3	2.18	0.58
2:C:2:VAL:N	2:C:1158:LYS:HZ2	2.02	0.58
2:H:1252:SER:OG	2:H:1255:THR:O	2.21	0.58
2:H:632:ASP:HA	2:H:647:ARG:HE	1.68	0.58
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.37	0.58
2:H:992:LEU:HB3	2:H:996:ARG:HB3	1.86	0.58
2:C:18:ARG:NH1	2:C:620:ASN:O	2.37	0.58
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.68	0.58
5:Y:248:GLU:HA	5:Y:251:LYS:HB2	1.86	0.58
3:I:584:PRO:HD2	3:I:587:LEU:HD22	1.86	0.57
4:J:60:ASN:H	4:J:63:ILE:HB	1.69	0.57
3:D:527:LEU:HD13	3:D:535:ARG:HH21	1.67	0.57
3:I:207:GLU:HG2	3:I:208:THR:HG22	1.85	0.57
2:H:1308:ILE:HG21	3:I:379:PRO:HB2	1.86	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.86	0.57
2:H:1078:LYS:HD3	2:H:1080:ASN:HD22	1.69	0.57
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.86	0.57
1:B:133:LEU:HD21	1:B:140:ILE:HD13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:151:MET:HB3	3:D:152:THR:HG23	1.86	0.57
5:Y:149:ASP:OD2	5:Y:149:ASP:N	2.32	0.57
3:D:311:ARG:HB3	3:D:312:ARG:HG3	1.86	0.57
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.84	0.57
3:I:1344:LEU:O	3:I:1350:ASN:ND2	2.37	0.57
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.84	0.57
3:D:650:LYS:HE3	3:D:654:ILE:HD11	1.86	0.57
2:H:971:LEU:HD12	2:H:1018:TYR:CD1	2.39	0.57
3:I:587:LEU:O	3:I:589:TYR:N	2.37	0.57
2:C:524:ILE:HG13	2:C:712:SER:HB2	1.86	0.57
1:G:92:VAL:HG22	1:G:121:VAL:HG22	1.87	0.57
3:D:156:ARG:NH2	3:D:191:SER:OG	2.38	0.57
2:H:238:GLN:HB3	2:H:284:LEU:HD11	1.86	0.57
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.87	0.57
1:A:66:HIS:HB3	2:C:874:GLY:HA2	1.86	0.57
2:H:685:MET:HE3	2:H:1235:LEU:HD11	1.87	0.57
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.87	0.57
2:C:1271:GLY:HA2	3:D:344:GLY:N	2.20	0.57
3:D:214:ARG:HD3	3:D:1275:LEU:HD21	1.86	0.57
3:D:81:ARG:O	3:D:83:VAL:N	2.37	0.57
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.87	0.57
5:Y:157:ARG:NH1	5:Y:159:SER:H	2.02	0.57
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.87	0.56
2:H:1253:LEU:HA	5:Y:525:ASP:HB2	1.87	0.56
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.70	0.56
2:H:731:ARG:NH2	2:H:962:GLU:OE2	2.38	0.56
3:I:353:SER:HB3	3:I:447:ILE:HG22	1.87	0.56
3:I:514:THR:HG22	3:I:515:ARG:H	1.70	0.56
2:H:818:VAL:HA	2:H:1096:ILE:HG22	1.86	0.56
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.87	0.56
2:C:80:PHE:CE2	2:C:84:GLU:HG2	2.39	0.56
3:D:849:LEU:HB3	3:D:854:ALA:O	2.05	0.56
3:D:851:PRO:HG3	3:D:875:ASN:HB2	1.86	0.56
3:I:553:THR:HG23	3:I:567:THR:HG22	1.87	0.56
5:Y:157:ARG:HH11	5:Y:159:SER:H	1.53	0.56
1:B:12:ARG:H	1:B:30:PRO:HD2	1.70	0.56
2:C:1140:LYS:HG2	2:C:1142:ARG:HE	1.70	0.56
2:C:886:LYS:HE2	2:C:916:SER:HB3	1.86	0.56
3:D:871:LEU:HB3	3:D:877:VAL:HG21	1.87	0.56
2:H:1072:ASN:HD22	2:H:1111:GLN:NE2	2.03	0.56
1:B:44:ARG:HA	1:B:183:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:145:VAL:HG22	3:D:159:ILE:HG13	1.86	0.56
2:H:159:SER:HB3	2:H:161:LYS:HG3	1.88	0.56
2:H:720:ARG:HD2	2:H:736:VAL:HG22	1.86	0.56
2:H:1117:LEU:HD21	2:H:1182:ILE:HD13	1.88	0.56
2:H:28:LEU:HD21	2:H:524:ILE:HG12	1.87	0.56
3:I:37:GLU:HG2	3:I:39:LYS:HG2	1.87	0.56
3:I:836:ARG:HH22	3:I:880:VAL:HG22	1.71	0.56
2:C:15:PHE:H	2:C:15:PHE:HD2	1.53	0.56
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.87	0.56
3:D:515:ARG:NH2	3:D:718:SER:O	2.36	0.56
1:F:95:LYS:O	1:F:148:ARG:NH2	2.39	0.56
1:G:169:GLY:O	1:G:171:LEU:HD22	2.05	0.56
3:I:416:ILE:HD12	3:I:439:PRO:HB2	1.88	0.56
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.86	0.56
2:C:1002:LEU:HG	2:C:1007:LYS:HB2	1.87	0.56
3:D:125:GLY:O	3:D:129:ASP:N	2.38	0.56
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.88	0.56
2:H:700:VAL:O	2:H:1069:ARG:NH1	2.33	0.56
3:I:1256:ILE:HA	3:I:1259:GLN:NE2	2.21	0.56
5:Y:161:LEU:O	5:Y:262:VAL:HG22	2.06	0.56
3:D:127:LEU:HD21	3:D:234:PRO:HB3	1.88	0.56
5:Y:562:ARG:HH21	5:Y:587:ILE:HG23	1.71	0.56
2:H:52:ALA:HB2	2:H:465:ARG:HE	1.71	0.56
2:H:810:TYR:HB3	2:H:817:LEU:HD23	1.88	0.56
3:I:718:SER:HB3	3:I:720:ASN:HB2	1.88	0.56
5:X:530:LEU:H	5:X:530:LEU:HD12	1.70	0.56
2:C:699:LEU:HB2	2:C:799:ASN:ND2	2.20	0.56
1:G:190:ALA:N	1:G:198:LEU:O	2.35	0.56
2:H:91:THR:HG22	2:H:139:ASN:H	1.71	0.56
2:H:300:ASP:HB2	2:H:309:LEU:HD21	1.87	0.56
1:F:80:GLU:HA	2:H:694:ARG:HH12	1.71	0.56
5:X:101:TYR:OH	5:X:409:ASN:ND2	2.38	0.56
5:X:575:GLU:HA	5:X:578:LYS:HD2	1.87	0.56
2:C:517:GLN:NE2	2:C:760:ASN:HD22	2.03	0.55
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.87	0.55
2:H:347:ILE:HD11	2:H:433:ILE:HD11	1.89	0.55
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.21	0.55
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.72	0.55
3:D:877:VAL:O	3:D:879:ALA:N	2.36	0.55
2:H:517:GLN:HE21	2:H:760:ASN:N	2.03	0.55
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:489:ASN:HA	3:I:904:ALA:HB1	1.89	0.55
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.86	0.55
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.34	0.55
2:C:798:GLN:HB3	2:C:827:ARG:HH21	1.71	0.55
3:D:1165:PHE:CD2	3:D:1168:GLU:HG3	2.42	0.55
3:D:1347:LEU:HD22	3:D:1357:ILE:HG22	1.87	0.55
2:H:1151:LEU:HD12	2:H:1201:LEU:HD22	1.87	0.55
2:H:556:GLY:HA2	2:H:659:GLN:O	2.07	0.55
3:D:169:LEU:O	3:D:169:LEU:HD13	2.06	0.55
1:F:167:PRO:HG2	1:F:170:ARG:HD2	1.87	0.55
2:H:841:ARG:NH1	3:I:256:ASP:HB3	2.21	0.55
1:B:255:ARG:HG2	1:B:256:PRO:HD2	1.89	0.55
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.42	0.55
5:X:469:GLN:NE2	5:X:473:GLU:OE2	2.31	0.55
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.88	0.55
2:H:300:ASP:N	2:H:300:ASP:OD1	2.37	0.55
2:H:755:LYS:HB3	2:H:756:TYR:HD2	1.71	0.55
1:B:159:ILE:HA	1:B:162:GLU:HG2	1.88	0.55
3:D:825:VAL:HB	3:D:834:PRO:HB2	1.88	0.55
4:E:26:ARG:HE	4:E:30:MET:HE3	1.72	0.55
2:H:971:LEU:HD12	2:H:1018:TYR:HD1	1.72	0.55
3:I:1159:ILE:HD12	3:I:1186:TYR:OH	2.01	0.55
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.89	0.55
5:Y:583:THR:HG22	5:Y:584:ARG:H	1.72	0.55
1:B:49:SER:O	1:B:151:GLY:HA2	2.07	0.55
3:D:245:LEU:O	3:D:250:ARG:NH1	2.39	0.55
2:H:80:PHE:CE2	2:H:84:GLU:HG2	2.42	0.55
3:I:931:THR:HG23	3:I:1244:GLN:HE22	1.72	0.55
1:B:155:ALA:N	1:B:174:ASP:OD1	2.39	0.54
5:X:157:ARG:HG3	5:X:159:SER:HB2	1.89	0.54
5:Y:412:LEU:HB2	5:Y:435:ILE:HD11	1.88	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.40	0.54
3:I:1349:GLU:OE1	3:I:1349:GLU:N	2.31	0.54
3:I:612:LEU:HB3	3:I:616:PRO:HB2	1.89	0.54
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.88	0.54
4:J:7:GLN:NE2	4:J:11:GLU:OE1	2.39	0.54
1:A:207:THR:HG23	1:A:209:GLY:H	1.72	0.54
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.22	0.54
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.89	0.54
2:C:231:GLU:HB3	2:C:233:ARG:HG3	1.89	0.54
3:D:285:LEU:HD12	5:X:410:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:856:ILE:HG23	3:D:857:LEU:HG	1.89	0.54
1:G:68:TYR:HB3	1:G:78:ILE:HB	1.89	0.54
2:H:1295:SER:HB2	3:I:347:VAL:HG12	1.89	0.54
2:H:1313:HIS:HD2	3:I:477:GLN:HE22	1.53	0.54
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.88	0.54
2:C:935:THR:HG21	2:C:941:LYS:HG2	1.88	0.54
3:D:771:GLN:HA	3:D:774:ILE:HB	1.88	0.54
3:I:1268:ASN:O	3:I:1274:PHE:HB3	2.07	0.54
3:I:528:THR:HG21	3:I:551:ARG:HE	1.73	0.54
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.43	0.54
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.54
2:C:545:PHE:CZ	3:D:781:LYS:HB2	2.39	0.54
2:H:4:SER:HA	2:H:1159:VAL:HG21	1.88	0.54
2:H:344:GLY:HA3	2:H:346:TYR:CZ	2.42	0.54
2:H:452:ARG:HH11	2:H:585:GLY:HA3	1.71	0.54
2:H:484:LEU:H	2:H:484:LEU:HD23	1.72	0.54
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.89	0.54
5:Y:545:HIS:ND1	5:Y:545:HIS:O	2.40	0.54
2:C:13:LYS:HG2	2:C:1181:PRO:HG2	1.88	0.54
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.36	0.54
3:I:643:ASP:O	3:I:720:ASN:ND2	2.41	0.54
3:D:884:SER:OG	3:D:885:VAL:N	2.41	0.54
2:H:80:PHE:CE2	2:H:88:ARG:HD3	2.42	0.54
3:I:825:VAL:HB	3:I:834:PRO:HB2	1.89	0.54
3:I:843:VAL:HG12	3:I:883:ARG:HD3	1.90	0.54
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.88	0.54
2:C:1159:VAL:HB	2:C:1160:ASP:HB2	1.89	0.54
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.89	0.54
3:I:156:ARG:NH1	3:I:157:GLN:OE1	2.41	0.54
3:I:245:LEU:HD23	3:I:250:ARG:HG2	1.89	0.54
2:H:1281:TYR:CD2	3:I:484:MET:HG2	2.43	0.54
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.88	0.54
2:C:1180:MET:HG3	2:C:1181:PRO:O	2.07	0.54
2:H:444:ASP:HB3	2:H:447:HIS:HB2	1.90	0.54
2:H:591:TYR:OH	2:H:637:ARG:NH2	2.40	0.54
2:H:11:ILE:HD13	2:H:697:LYS:NZ	2.23	0.54
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.72	0.54
5:X:165:PHE:H	5:X:260:ARG:NH1	2.05	0.54
1:B:197:ASP:OD1	1:B:197:ASP:N	2.36	0.53
2:C:1139:ALA:O	2:C:1140:LYS:HB2	2.08	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.89	0.53
3:D:527:LEU:HB2	3:D:532:GLU:CD	2.28	0.53
1:F:118:ASP:OD1	1:F:119:GLY:N	2.40	0.53
2:H:131:THR:HG22	2:H:135:THR:H	1.73	0.53
2:H:13:LYS:HG2	2:H:1181:PRO:HG2	1.90	0.53
3:I:201:LEU:HB3	3:I:221:ILE:HG22	1.89	0.53
1:B:51:MET:H	1:B:150:ARG:HG3	1.73	0.53
1:F:158:ARG:NH1	1:F:173:VAL:O	2.41	0.53
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.90	0.53
2:H:1209:GLN:HB3	2:H:1224:PRO:HB2	1.90	0.53
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.90	0.53
2:C:839:VAL:O	2:C:886:LYS:NZ	2.25	0.53
3:D:1289:ASN:HD22	3:D:1290:ARG:HG3	1.73	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.41	0.53
2:C:150:HIS:HE2	2:C:452:ARG:HE	1.55	0.53
3:I:515:ARG:NH2	3:I:718:SER:O	2.42	0.53
5:X:582:VAL:HG12	5:X:586:ARG:HB2	1.91	0.53
1:B:282:VAL:HG21	1:B:312:LEU:HD23	1.90	0.53
2:C:1073:LYS:HB2	3:D:462:ASP:HB2	1.90	0.53
3:D:516:ASP:H	3:D:576:ARG:HH11	1.55	0.53
3:D:587:LEU:HD12	3:D:611:ILE:HD11	1.91	0.53
3:D:773:PHE:O	3:D:776:THR:HG22	2.09	0.53
1:G:104:LYS:HD3	1:G:105:SER:N	2.24	0.53
1:G:68:TYR:CE1	1:G:171:LEU:HG	2.44	0.53
5:Y:469:GLN:NE2	5:Y:473:GLU:OE2	2.37	0.53
3:D:88:CYS:SG	3:D:89:GLY:N	2.81	0.53
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.74	0.53
2:C:908:GLU:HG2	2:C:909:LYS:H	1.72	0.53
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.42	0.53
2:H:53:PHE:CE1	2:H:68:LEU:HB3	2.43	0.53
2:H:718:ALA:HB2	2:H:783:LEU:HG	1.91	0.53
3:I:18:ASP:OD1	3:I:1369:ARG:NH2	2.40	0.53
3:I:655:SER:HA	3:I:658:GLU:HG2	1.91	0.53
3:I:901:ARG:HB3	3:I:908:ILE:HA	1.90	0.53
5:X:445:ASP:N	5:X:445:ASP:OD1	2.36	0.53
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.91	0.53
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.91	0.53
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.90	0.53
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.44	0.53
5:X:162:ILE:HA	5:X:262:VAL:HG23	1.91	0.53
5:Y:585:GLU:O	5:Y:589:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.91	0.53
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.92	0.53
3:I:1341:ARG:NH2	3:I:1343:GLU:OE1	2.42	0.53
4:J:26:ARG:HD3	4:J:64:LEU:HD21	1.91	0.53
5:X:105:MET:CG	5:X:384:LEU:HD12	2.32	0.53
2:C:510:GLN:O	2:C:511:LEU:HB2	2.09	0.52
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.91	0.52
3:D:871:LEU:HD12	3:D:877:VAL:HG21	1.90	0.52
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.89	0.52
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.90	0.52
1:B:44:ARG:HD2	3:D:538:ARG:HH11	1.74	0.52
2:C:1134:GLN:O	2:C:1137:GLU:N	2.27	0.52
2:C:1238:LEU:H	2:C:1238:LEU:HD23	1.73	0.52
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.09	0.52
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.41	0.52
3:I:871:LEU:HD12	3:I:877:VAL:HG21	1.90	0.52
1:B:268:ASN:HA	1:B:271:LYS:HB3	1.90	0.52
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.73	0.52
2:H:906:PHE:CZ	5:Y:601:PRO:HB2	2.44	0.52
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.91	0.52
2:C:1051:LYS:HB3	2:C:1053:TYR:HE1	1.75	0.52
3:D:1353:VAL:HG13	3:D:1355:ARG:HG3	1.91	0.52
3:D:154:LEU:HD11	3:D:160:LEU:HD21	1.91	0.52
2:H:1238:LEU:HD23	2:H:1238:LEU:H	1.74	0.52
1:B:37:HIS:HD2	2:C:1216:ARG:HB3	1.74	0.52
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.92	0.52
2:H:106:GLU:HG2	2:H:111:GLU:HA	1.91	0.52
2:H:942:ASP:OD1	2:H:944:ARG:N	2.42	0.52
2:C:1330:ILE:HD11	3:D:331:ILE:HG21	1.92	0.52
3:I:584:PRO:O	3:I:589:TYR:OH	2.15	0.52
2:C:898:GLU:HG3	5:X:565:ILE:HD12	1.92	0.52
5:Y:495:ARG:HE	5:Y:495:ARG:HA	1.75	0.52
3:D:849:LEU:H	3:D:856:ILE:HG22	1.74	0.52
3:I:213:LYS:O	3:I:217:LEU:HG	2.09	0.52
1:B:313:SER:OG	1:B:314:LEU:N	2.42	0.52
2:C:980:VAL:HG22	2:C:984:VAL:HG22	1.90	0.52
3:D:146:VAL:HA	3:D:178:ALA:HB1	1.91	0.52
2:H:342:ASP:N	2:H:342:ASP:OD1	2.41	0.52
2:H:452:ARG:NH1	2:H:585:GLY:HA3	2.25	0.52
5:X:166:VAL:H	5:X:259:PHE:CA	2.05	0.52
5:X:602:SER:HA	5:X:605:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.52
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.90	0.52
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.92	0.52
3:I:536:LEU:HG	3:I:541:LEU:O	2.09	0.52
3:I:665:GLN:HG2	3:I:678:ARG:NH1	2.25	0.52
3:I:813:ASP:HA	3:I:895:CYS:SG	2.50	0.52
5:X:167:ASP:HA	5:X:259:PHE:CZ	2.45	0.52
5:Y:597:LYS:O	5:Y:598:LEU:HD13	2.10	0.52
1:A:57:THR:HG21	1:A:147:GLN:HB2	1.90	0.52
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.33	0.52
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.75	0.52
2:C:6:THR:HG22	2:C:12:ARG:HH21	1.75	0.52
2:H:247:ARG:HH12	2:H:271:ALA:HB2	1.75	0.52
2:H:80:PHE:HB3	2:H:85:CYS:SG	2.50	0.52
3:I:1160:SER:H	3:I:1206:ARG:HG2	1.74	0.52
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	1.92	0.51
3:D:1237:VAL:HG11	3:D:1253:ILE:HD12	1.91	0.51
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.92	0.51
2:H:549:ASP:OD1	2:H:550:VAL:N	2.43	0.51
2:H:905:ILE:HG12	5:Y:595:LEU:HD22	1.91	0.51
3:I:527:LEU:HD23	3:I:528:THR:N	2.23	0.51
3:I:57:PHE:HB3	3:I:98:ARG:NH1	2.24	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.10	0.51
5:Y:165:PHE:CA	5:Y:259:PHE:HB2	2.39	0.51
2:C:958:LYS:O	2:C:962:GLU:HG2	2.09	0.51
3:D:515:ARG:HH22	3:D:717:VAL:C	2.14	0.51
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.92	0.51
3:I:79:LYS:HG3	5:Y:569:THR:HG22	1.92	0.51
2:C:814:ASP:OD2	2:C:1106:ARG:NH2	2.43	0.51
1:A:45:ARG:HD2	1:B:38:THR:OG1	2.10	0.51
1:B:186:ASN:HB2	1:B:202:VAL:HB	1.92	0.51
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.75	0.51
2:C:748:ILE:HD11	2:C:967:LEU:HA	1.91	0.51
2:C:785:ASP:OD1	2:C:791:LEU:N	2.39	0.51
3:D:169:LEU:HD13	3:D:169:LEU:C	2.31	0.51
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.93	0.51
3:D:94:GLN:HB2	3:D:97:VAL:HG23	1.93	0.51
3:D:9:LYS:HG3	3:D:11:GLN:HG2	1.92	0.51
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.74	0.51
2:H:819:SER:HB2	2:H:1085:MET:SD	2.50	0.51
3:I:145:VAL:HG22	3:I:159:ILE:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:161:LEU:HG	5:Y:162:ILE:HG23	1.92	0.51
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.93	0.51
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.26	0.51
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.92	0.51
3:D:849:LEU:N	3:D:856:ILE:HG22	2.25	0.51
2:H:1246:ARG:NH2	2:H:1258:PRO:HB3	2.26	0.51
2:H:741:MET:N	2:H:741:MET:SD	2.84	0.51
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.92	0.51
3:I:72:CYS:SG	3:I:73:GLY:N	2.84	0.51
3:I:930:LEU:HD23	3:I:1244:GLN:HG3	1.92	0.51
1:A:100:LEU:HB3	1:A:115:ILE:HD11	1.92	0.51
2:C:697:LYS:HE2	2:C:790:ASP:OD2	2.11	0.51
1:G:112:ALA:HB3	1:G:126:PRO:HA	1.91	0.51
3:I:1271:SER:HB2	3:I:1290:ARG:CZ	2.41	0.51
3:I:589:TYR:O	3:I:590:SER:HB2	2.09	0.51
3:I:843:VAL:HG11	3:I:897:HIS:HB3	1.93	0.51
2:C:1270:PHE:CZ	2:C:1290:MET:HG2	2.45	0.51
3:D:809:VAL:HG13	3:D:912:GLY:H	1.75	0.51
2:H:542:ARG:O	2:H:544:GLY:N	2.44	0.51
3:I:306:LEU:HD23	3:I:307:LEU:HD23	1.91	0.51
3:I:42:GLU:O	3:I:55:GLY:HA3	2.11	0.51
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.92	0.51
5:X:374:ARG:NH2	5:X:377:LYS:HD2	2.25	0.51
2:C:842:ASP:N	2:C:1046:VAL:HG21	2.25	0.51
2:C:539:THR:HG22	2:C:540:ARG:H	1.75	0.51
2:H:118:LYS:HG2	2:H:488:MET:H	1.74	0.51
2:H:75:LEU:HD21	2:H:127:ILE:HD11	1.93	0.51
3:I:1219:ASP:HA	3:I:1222:ARG:HB3	1.93	0.51
3:I:93:THR:O	3:I:94:GLN:HG2	2.11	0.51
2:H:898:GLU:HG3	5:Y:565:ILE:HD12	1.93	0.51
2:C:102:LEU:HD12	2:C:118:LYS:HD3	1.92	0.51
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.93	0.51
1:F:186:ASN:HB3	1:F:188:GLU:HG3	1.93	0.51
2:H:1240:ASP:HA	3:I:445:LYS:HE2	1.93	0.51
3:I:389:GLY:O	3:I:391:ALA:N	2.44	0.51
5:X:452:ILE:HD11	5:X:500:ILE:HG22	1.92	0.51
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.76	0.50
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.92	0.50
2:C:646:SER:O	2:C:647:ARG:HB3	2.11	0.50
3:D:1264:ALA:HA	3:D:1305:ASP:HB2	1.93	0.50
3:D:334:LYS:HE3	3:D:1324:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.92	0.50
3:I:733:SER:O	3:I:737:ILE:HG12	2.11	0.50
5:X:423:ARG:HB3	5:X:425:TYR:HD1	1.75	0.50
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.93	0.50
2:C:517:GLN:HE21	2:C:760:ASN:H	1.58	0.50
3:D:309:ASN:HB2	3:D:326:SER:HB3	1.93	0.50
3:D:530:PRO:HB2	3:D:581:MET:HG2	1.93	0.50
4:E:38:LEU:HD11	4:E:67:ARG:HH12	1.75	0.50
1:F:78:ILE:HD13	1:F:81:ILE:HD12	1.93	0.50
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.76	0.50
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.92	0.50
5:Y:143:TYR:HA	5:Y:146:GLU:HB2	1.94	0.50
1:A:190:ALA:H	1:A:199:ASP:HA	1.77	0.50
2:C:71:VAL:HG12	2:C:72:SER:HB3	1.91	0.50
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.46	0.50
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.93	0.50
1:F:197:ASP:O	1:F:198:LEU:HD23	2.11	0.50
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.92	0.50
2:H:1259:LEU:HD12	3:I:346:ARG:NH1	2.25	0.50
3:I:311:ARG:HH22	3:I:1329:THR:HG21	1.75	0.50
5:Y:511:ILE:HG23	5:Y:517:SER:HB3	1.93	0.50
1:B:17:GLU:HG3	1:B:17:GLU:O	2.10	0.50
2:C:360:LEU:HD11	2:C:378:ARG:HG2	1.92	0.50
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.11	0.50
3:D:914:ALA:O	3:D:918:ILE:HG22	2.11	0.50
3:D:1333:THR:O	3:D:1337:VAL:HG23	2.11	0.50
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.47	0.50
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.93	0.50
2:H:3:TYR:HD2	2:H:6:THR:HG21	1.75	0.50
2:H:594:VAL:HG22	2:H:599:VAL:HG22	1.93	0.50
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.93	0.50
5:X:157:ARG:NH1	5:X:159:SER:H	2.10	0.50
5:Y:157:ARG:HG3	5:Y:159:SER:HB2	1.92	0.50
2:C:1167:GLU:HA	2:C:1170:MET:HB2	1.94	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HB3	1.93	0.50
3:D:381:ILE:HG21	3:D:408:VAL:HG23	1.94	0.50
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.93	0.50
3:D:842:ARG:HB3	3:D:882:VAL:CG2	2.41	0.50
4:J:26:ARG:HB2	4:J:64:LEU:HD11	1.92	0.50
2:C:106:GLU:N	2:C:107:ARG:HA	2.14	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:VAL:HG13	2:C:319:LEU:HD22	1.94	0.50
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.94	0.50
3:D:1280:VAL:HA	3:D:1283:SER:HB3	1.93	0.50
2:H:187:GLU:OE2	2:H:197:ARG:NE	2.38	0.50
2:H:1304:MET:HE1	3:I:472:LEU:HB3	1.94	0.50
1:B:44:ARG:HG3	1:B:183:ILE:HG22	1.93	0.50
2:C:1247:SER:HB3	3:D:375:GLU:O	2.12	0.50
3:D:1372:ARG:HG3	3:I:853:THR:OG1	2.11	0.50
2:H:478:ARG:HA	2:H:481:LEU:HD12	1.94	0.50
3:I:251:PRO:HD2	5:Y:507:MET:HE1	1.94	0.50
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.44	0.50
2:C:1222:GLU:OE1	3:D:537:TYR:OH	2.21	0.50
2:C:890:LYS:HE2	2:C:893:THR:HG21	1.93	0.50
3:D:230:SER:HB2	3:D:1339:GLY:H	1.77	0.50
3:D:308:ASP:OD1	3:D:311:ARG:NH1	2.44	0.50
3:I:205:LEU:HD13	3:I:217:LEU:HB3	1.93	0.50
2:C:1002:LEU:HD13	2:C:1003:THR:N	2.27	0.49
2:C:153:PRO:HG2	2:C:179:TYR:HD1	1.76	0.49
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.47	0.49
2:C:6:THR:HG22	2:C:12:ARG:NH2	2.27	0.49
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.27	0.49
3:I:804:ALA:O	3:I:916:GLY:HA3	2.12	0.49
3:D:46:TYR:HB3	5:X:451:ARG:O	2.12	0.49
2:C:487:LEU:HA	2:C:488:MET:CB	2.37	0.49
2:C:935:THR:HA	2:C:1048:LYS:HB3	1.94	0.49
3:D:282:LEU:HD13	3:D:291:ILE:HG22	1.94	0.49
1:G:13:LEU:O	1:G:28:LEU:HA	2.12	0.49
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.47	0.49
2:H:812:PHE:HB2	3:I:357:VAL:HG21	1.94	0.49
5:X:165:PHE:HB3	5:X:259:PHE:CG	2.45	0.49
2:C:1335:ILE:HD12	3:D:22:ILE:HD11	1.94	0.49
3:D:339:ARG:O	3:D:340:GLN:NE2	2.44	0.49
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.44	0.49
2:H:131:THR:HG21	2:H:135:THR:HG22	1.95	0.49
3:I:1177:ILE:HD11	3:I:1196:LEU:HD11	1.95	0.49
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.93	0.49
1:B:263:THR:HG22	1:B:302:GLU:HG2	1.94	0.49
2:C:144:VAL:HG23	2:C:515:MET:HG3	1.94	0.49
2:C:540:ARG:HD3	2:C:567:PRO:HB2	1.93	0.49
1:G:37:HIS:HE1	1:G:187:VAL:HG22	1.78	0.49
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:ARG:NH1	2:H:201:ARG:O	2.44	0.49
5:X:231:THR:HG23	5:X:249:ILE:HG12	1.94	0.49
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.93	0.49
3:D:1344:LEU:O	3:D:1350:ASN:ND2	2.45	0.49
3:D:262:THR:OG1	3:D:263:SER:N	2.46	0.49
3:D:910:ASN:HB3	4:E:15:ASN:ND2	2.27	0.49
1:F:80:GLU:HB2	2:H:694:ARG:HH22	1.76	0.49
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.95	0.49
2:H:1270:PHE:CE1	2:H:1290:MET:HG2	2.48	0.49
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.47	0.49
3:I:877:VAL:O	3:I:879:ALA:N	2.40	0.49
5:X:96:ASP:O	5:X:100:MET:HB2	2.11	0.49
3:D:1286:LYS:HA	3:D:1289:ASN:HB3	1.94	0.49
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.45	0.49
1:F:195:ARG:O	1:F:198:LEU:HG	2.12	0.49
3:I:714:GLU:HG3	3:I:715:LYS:H	1.77	0.49
5:X:292:VAL:HG11	5:X:299:LYS:HG2	1.94	0.49
1:B:14:VAL:HG22	1:B:28:LEU:HD22	1.93	0.49
2:C:59:ILE:HD12	2:C:59:ILE:H	1.77	0.49
3:D:1250:ASP:O	3:D:1254:GLU:HG3	2.12	0.49
2:H:15:PHE:CE2	2:H:1182:ILE:HD11	2.48	0.49
3:I:128:LEU:HA	3:I:192:MET:HE1	1.95	0.49
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.95	0.49
5:X:163:THR:OG1	5:X:261:LEU:O	2.27	0.49
2:C:493:ILE:O	5:X:472:GLN:NE2	2.46	0.49
5:Y:255:VAL:HA	5:Y:258:GLN:HG3	1.93	0.49
5:Y:290:LEU:HD13	5:Y:336:GLU:HB3	1.94	0.49
2:C:338:THR:HB	2:C:345:PRO:HG3	1.94	0.49
2:C:718:ALA:HA	2:C:751:TYR:CE1	2.48	0.49
2:C:729:ALA:O	2:C:755:LYS:HD2	2.12	0.49
2:C:758:ARG:HA	2:C:833:ILE:HD12	1.94	0.49
2:H:1038:GLN:HG2	2:H:1039:GLY:H	1.77	0.49
3:D:584:PRO:HD2	3:D:587:LEU:HD22	1.94	0.49
3:D:733:SER:OG	3:D:736:GLN:OE1	2.29	0.49
5:X:105:MET:O	5:X:108:VAL:HG13	2.13	0.49
5:X:279:ARG:NH2	5:X:347:ILE:HG12	2.28	0.49
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.94	0.49
3:D:811:GLU:OE2	3:D:890:THR:OG1	2.17	0.49
3:D:890:THR:HG21	3:D:894:VAL:HA	1.94	0.49
3:D:493:PRO:HB3	3:D:918:ILE:HD11	1.94	0.49
1:G:181:GLU:HA	3:I:535:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HG3	2:H:1181:PRO:O	2.12	0.49
2:H:992:LEU:HG	2:H:996:ARG:HG2	1.95	0.49
3:I:205:LEU:HB3	3:I:217:LEU:HD13	1.94	0.49
3:I:615:LYS:HE3	4:J:5:THR:OG1	2.13	0.49
5:X:306:PHE:O	5:X:310:GLU:HG2	2.13	0.49
5:Y:270:VAL:HA	5:Y:273:MET:HE3	1.95	0.49
1:A:167:PRO:HB2	1:A:170:ARG:HG3	1.94	0.48
3:D:1291:GLU:HA	3:D:1296:GLY:HA2	1.95	0.48
3:D:144:TYR:CD2	3:D:180:MET:HB3	2.48	0.48
3:D:744:ARG:HD2	3:D:763:PHE:CZ	2.48	0.48
2:H:1267:GLY:HA3	3:I:347:VAL:O	2.13	0.48
3:I:1362:GLY:C	3:I:1364:ALA:H	2.16	0.48
3:I:262:THR:O	5:Y:507:MET:N	2.34	0.48
3:I:506:VAL:HG21	3:I:625:MET:HA	1.94	0.48
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.94	0.48
1:A:67:GLU:HA	1:A:78:ILE:HG21	1.94	0.48
2:C:975:ILE:HD11	2:C:1011:LEU:HD21	1.95	0.48
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	1.95	0.48
2:C:102:LEU:HB3	2:C:118:LYS:HB2	1.94	0.48
2:C:722:GLY:HA3	2:C:735:LYS:O	2.13	0.48
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.28	0.48
1:G:104:LYS:HD3	1:G:105:SER:H	1.78	0.48
2:H:956:ALA:HB3	2:H:1032:LYS:HE3	1.95	0.48
2:H:1072:ASN:N	2:H:1072:ASN:OD1	2.45	0.48
2:C:672:GLU:HG2	2:C:1186:VAL:O	2.12	0.48
2:C:1299:ASN:HB3	2:C:1303:LYS:HE3	1.95	0.48
3:D:270:ARG:HE	5:X:449:THR:HG22	1.78	0.48
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.95	0.48
1:B:196:THR:HB	3:D:443:GLU:HG3	1.95	0.48
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.16	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.54	0.48
2:C:551:HIS:CE1	2:C:553:THR:HG1	2.30	0.48
2:C:1290:MET:HG3	3:D:347:VAL:HG11	1.95	0.48
1:F:189:ALA:HA	1:F:199:ASP:HA	1.95	0.48
2:H:131:THR:HG22	2:H:135:THR:N	2.28	0.48
3:I:94:GLN:HB2	3:I:97:VAL:HG23	1.94	0.48
3:I:286:ALA:HB2	5:Y:373:ARG:NH2	2.29	0.48
5:X:458:GLU:HA	5:X:461:ASN:HD22	1.79	0.48
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.29	0.48
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.29	0.48
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1339:LEU:HD23	3:D:17:PHE:CD2	2.49	0.48
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	1.96	0.48
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.12	0.48
2:C:856:ASN:ND2	5:X:609:SER:O	2.45	0.48
1:A:50:SER:HA	1:A:150:ARG:HD2	1.96	0.48
2:C:164:THR:HG23	2:C:165:HIS:H	1.79	0.48
2:C:234:ASP:HB2	2:C:236:LYS:HE2	1.95	0.48
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.12	0.48
2:H:153:PRO:HA	2:H:177:ILE:HG22	1.95	0.48
3:I:849:LEU:HD12	3:I:849:LEU:H	1.79	0.48
2:C:685:MET:HE2	2:C:1073:LYS:HG2	1.96	0.48
3:D:701:LEU:HD23	3:D:723:TYR:HB2	1.95	0.48
5:Y:412:LEU:HD13	5:Y:435:ILE:HD11	1.95	0.48
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.48	0.48
2:C:358:ASP:OD1	2:C:361:SER:OG	2.21	0.48
2:C:848:GLU:HG2	2:C:888:THR:HA	1.95	0.48
3:I:837:ASP:HA	3:I:868:TRP:HE1	1.79	0.48
5:Y:151:VAL:HG11	5:Y:158:LEU:HB2	1.96	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	2.29	0.48
1:F:51:MET:HE1	1:F:216:ALA:HA	1.95	0.48
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.79	0.48
3:I:1135:THR:HB	3:I:1140:ARG:HD3	1.96	0.48
5:X:105:MET:HG2	5:X:105:MET:O	2.14	0.48
5:X:287:ILE:HG22	5:X:302:PHE:HZ	1.79	0.48
5:X:511:ILE:HG23	5:X:512:GLY:H	1.78	0.48
2:C:1136:GLN:O	2:C:1139:ALA:HB2	2.14	0.47
3:D:298:MET:SD	5:X:402:LEU:HB3	2.54	0.47
5:X:98:VAL:HB	5:X:402:LEU:HD21	1.96	0.47
2:C:756:TYR:H	2:C:766:ASN:HB2	1.79	0.47
2:C:906:PHE:HZ	5:X:601:PRO:HB2	1.78	0.47
2:C:985:GLU:HG3	2:C:988:LYS:HB2	1.94	0.47
3:D:1289:ASN:ND2	3:D:1293:GLU:OE1	2.47	0.47
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.29	0.47
3:D:596:LEU:HD11	3:D:598:LYS:HZ1	1.80	0.47
1:F:104:LYS:HG3	1:F:110:VAL:HG13	1.95	0.47
2:H:407:ARG:HH22	2:H:609:ILE:HG21	1.79	0.47
2:H:629:PHE:CE2	2:H:634:VAL:HG21	2.49	0.47
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.38	0.47
3:D:201:LEU:HB3	3:D:221:ILE:HG22	1.96	0.47
2:C:1271:GLY:HA2	3:D:344:GLY:H	1.79	0.47
3:D:536:LEU:HG	3:D:541:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:NH1	3:D:717:VAL:HB	2.29	0.47
1:F:152:TYR:CZ	2:H:824:GLN:HA	2.49	0.47
1:F:190:ALA:H	1:F:199:ASP:HA	1.79	0.47
1:G:16:ILE:HG12	1:G:26:VAL:HG13	1.97	0.47
3:I:1289:ASN:ND2	3:I:1293:GLU:OE1	2.47	0.47
3:I:56:LEU:O	3:I:250:ARG:NH2	2.39	0.47
3:I:576:ARG:NH2	3:I:594:GLN:O	2.47	0.47
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.79	0.47
3:D:1247:LYS:H	3:D:1247:LYS:HG2	1.51	0.47
3:D:173:GLY:O	3:D:175:GLU:HG3	2.14	0.47
3:D:747:MET:O	3:D:755:ILE:HG22	2.14	0.47
3:D:860:ARG:HH21	3:D:883:ARG:HH22	1.61	0.47
2:H:490:GLN:NE2	5:Y:472:GLN:O	2.47	0.47
3:I:1197:ASN:HB3	3:I:1210:ILE:HA	1.96	0.47
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.47	0.47
3:D:1362:GLY:C	3:D:1364:ALA:H	2.17	0.47
2:C:808:ASN:H	3:D:633:ALA:HB2	1.79	0.47
2:H:1067:ALA:HB2	2:H:1073:LYS:HA	1.97	0.47
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.46	0.47
2:H:673:HIS:O	2:H:1109:ILE:HG22	2.15	0.47
2:H:170:VAL:HG23	2:H:171:LEU:H	1.80	0.47
2:H:82:VAL:HG23	2:H:137:VAL:HG21	1.97	0.47
3:I:1152:GLU:HG3	3:I:1214:PRO:HD2	1.97	0.47
3:I:1358:PRO:HB3	3:I:1366:HIS:CG	2.49	0.47
3:I:161:THR:O	3:I:165:TYR:N	2.43	0.47
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.96	0.47
5:Y:166:VAL:HG13	5:Y:260:ARG:HG2	1.97	0.47
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.15	0.47
3:D:1369:ARG:HA	3:D:1372:ARG:HB2	1.95	0.47
2:H:360:LEU:HD11	2:H:378:ARG:HG2	1.95	0.47
1:A:35:PHE:HA	1:A:38:THR:HB	1.96	0.47
2:C:818:VAL:HA	2:C:1096:ILE:HG22	1.96	0.47
2:C:1200:LYS:C	2:C:1202:GLY:H	2.18	0.47
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.50	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
1:F:164:ASP:C	1:F:166:ARG:H	2.16	0.47
1:G:44:ARG:HD3	1:G:185:TYR:HE2	1.79	0.47
2:H:1110:GLY:HA2	2:H:1113:LEU:HD13	1.97	0.47
3:I:518:VAL:HA	3:I:547:ARG:HH12	1.78	0.47
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.97	0.47
2:C:587:LEU:HD12	2:C:587:LEU:HA	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1166:GLY:N	3:D:1176:VAL:O	2.35	0.47
3:D:514:THR:HG21	3:D:596:LEU:HA	1.96	0.47
2:H:1131:MET:SD	2:H:1141:LEU:HD12	2.55	0.47
2:H:314:ASN:ND2	2:H:314:ASN:O	2.48	0.47
2:H:551:HIS:CE1	2:H:553:THR:HG1	2.32	0.47
3:I:528:THR:HA	3:I:529:GLY:HA2	1.59	0.47
3:I:716:GLN:O	3:I:717:VAL:HG23	2.14	0.47
2:C:672:GLU:O	3:D:767:LEU:HB2	2.15	0.47
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.95	0.47
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.96	0.47
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.97	0.47
2:C:8:LYS:HE3	2:C:8:LYS:HB3	1.54	0.47
3:D:1175:LEU:HD12	3:D:1175:LEU:H	1.80	0.47
2:H:1200:LYS:C	2:H:1202:GLY:H	2.18	0.47
2:H:187:GLU:OE2	2:H:203:LYS:HD3	2.14	0.47
2:H:303:ASP:OD1	2:H:310:ILE:HD11	2.15	0.47
2:H:513:GLN:OE1	2:H:526:HIS:NE2	2.48	0.47
3:I:1350:ASN:HA	3:I:1353:VAL:HG12	1.97	0.47
3:I:537:TYR:CE1	3:I:544:LEU:HG	2.49	0.47
3:I:528:THR:HG22	3:I:551:ARG:HB2	1.97	0.47
5:X:134:VAL:HG22	5:X:273:MET:HE1	1.97	0.47
5:X:383:ASN:HB3	5:X:386:LEU:HD12	1.97	0.47
3:D:394:ILE:HG21	5:X:536:THR:HA	1.96	0.47
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.97	0.47
2:C:718:ALA:HA	2:C:751:TYR:HE1	1.80	0.47
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.97	0.47
3:D:819:GLY:H	3:D:881:LYS:HE2	1.79	0.47
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.50	0.47
2:H:180:ARG:CZ	2:H:465:ARG:HD2	2.45	0.47
2:H:91:THR:HG21	2:H:503:LYS:HE3	1.96	0.47
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.15	0.47
2:C:55:SER:O	2:C:67:GLU:HB3	2.16	0.46
3:D:268:LEU:HD22	3:D:324:LEU:HD23	1.98	0.46
3:D:678:ARG:O	3:D:682:VAL:HG13	2.14	0.46
2:H:135:THR:HG21	2:H:142:GLU:OE1	2.15	0.46
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.15	0.46
3:I:1167:LYS:HB3	3:I:1170:LYS:HB2	1.97	0.46
3:I:156:ARG:HD3	3:I:157:GLN:HG3	1.96	0.46
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.97	0.46
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.15	0.46
5:Y:599:ARG:C	5:Y:601:PRO:HD3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.80	0.46
2:C:803:ALA:HB2	2:C:1094:VAL:HG11	1.97	0.46
2:C:1106:ARG:HE	3:D:731:ARG:HH22	1.63	0.46
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.49	0.46
2:H:1007:LYS:HA	2:H:1010:GLN:HE21	1.80	0.46
3:I:1238:GLN:HE22	3:I:1248:ILE:HG23	1.81	0.46
3:I:149:GLY:HA2	3:I:176:PHE:HB2	1.96	0.46
3:I:62:PHE:CD1	3:I:247:PRO:HD3	2.50	0.46
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.97	0.46
2:C:1337:ILE:HG22	3:D:22:ILE:HG13	1.97	0.46
2:C:407:ARG:HH22	2:C:609:ILE:CD1	2.28	0.46
2:H:14:ASP:HA	2:H:1158:LYS:HE2	1.96	0.46
2:H:529:ARG:HH22	2:H:687:ARG:NH2	2.12	0.46
2:H:646:SER:O	2:H:647:ARG:HB3	2.14	0.46
2:H:759:SER:OG	2:H:760:ASN:N	2.46	0.46
3:I:261:ALA:HA	5:Y:505:ILE:O	2.15	0.46
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.98	0.46
5:X:555:GLU:HG2	5:X:590:ILE:HG23	1.97	0.46
3:D:161:THR:HB	3:D:164:GLN:HG3	1.97	0.46
3:D:292:VAL:O	3:D:296:LYS:HG3	2.16	0.46
3:D:555:TYR:H	3:D:589:TYR:HD2	1.64	0.46
3:D:75:TYR:HD2	3:D:80:HIS:CG	2.34	0.46
2:H:1313:HIS:CE1	4:J:31:GLN:HE22	2.32	0.46
3:I:1156:LEU:HB2	3:I:1223:LEU:HD23	1.98	0.46
2:C:1243:MET:SD	3:D:445:LYS:HG2	2.55	0.46
2:C:672:GLU:HB3	2:C:1187:PHE:CD1	2.50	0.46
2:C:678:ARG:HH21	2:C:1106:ARG:HG2	1.80	0.46
2:C:687:ARG:HE	2:C:687:ARG:HB2	1.60	0.46
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.97	0.46
2:C:75:LEU:HD23	2:C:96:LEU:HD13	1.96	0.46
2:C:826:ASP:OD1	2:C:829:THR:HG21	2.15	0.46
2:C:897:PRO:HB3	5:X:563:PHE:O	2.15	0.46
3:D:1322:ALA:O	3:D:1326:GLN:HG2	2.16	0.46
3:D:255:LEU:HB2	3:D:259:ARG:O	2.16	0.46
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.98	0.46
3:D:813:ASP:HA	3:D:895:CYS:HB2	1.96	0.46
2:H:324:LYS:HA	2:H:327:GLN:HB3	1.97	0.46
3:I:590:SER:O	3:I:594:GLN:HB2	2.16	0.46
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.96	0.46
5:Y:148:TYR:HE2	5:Y:152:GLU:HG2	1.80	0.46
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:HB2	1:B:30:PRO:HG2	1.98	0.46
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.30	0.46
3:D:805:GLN:OE1	3:D:1348:LYS:HE2	2.15	0.46
2:H:302:ILE:HG22	2:H:309:LEU:HA	1.96	0.46
3:I:169:LEU:HD22	3:I:173:GLY:HA2	1.98	0.46
3:I:423:LEU:O	3:I:434:ILE:HA	2.16	0.46
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.97	0.46
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.81	0.46
2:C:1330:ILE:CG2	2:C:1335:ILE:HD11	2.46	0.46
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.49	0.46
2:C:756:TYR:H	2:C:766:ASN:CB	2.29	0.46
2:C:82:VAL:HB	2:C:92:TYR:CD2	2.50	0.46
1:G:165:GLU:O	1:G:165:GLU:CD	2.54	0.46
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.98	0.46
2:H:122:VAL:HG21	2:H:493:ILE:CG2	2.46	0.46
3:I:1272:SER:HB3	3:I:1276:GLU:OE1	2.16	0.46
2:C:1278:LEU:HD21	2:C:1286:THR:HG22	1.98	0.46
2:C:4:SER:O	2:C:5:TYR:HB2	2.16	0.46
3:D:885:VAL:O	3:D:1258:ARG:HD3	2.16	0.46
3:D:530:PRO:HG3	3:D:580:TRP:CE3	2.51	0.46
3:D:93:THR:O	3:D:94:GLN:HG2	2.15	0.46
2:H:1222:GLU:OE1	3:I:537:TYR:OH	2.27	0.46
2:H:710:VAL:HA	2:H:715:THR:HG21	1.97	0.46
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.98	0.46
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.51	0.46
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.45	0.46
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.80	0.46
3:D:21:LYS:HG2	3:D:22:ILE:N	2.31	0.46
2:H:106:GLU:O	2:H:114:VAL:HG23	2.16	0.46
2:H:131:THR:CG2	2:H:135:THR:HG22	2.45	0.46
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.98	0.46
2:H:660:VAL:HG22	2:H:661:VAL:H	1.81	0.46
3:I:363:LEU:O	3:I:486:SER:OG	2.24	0.46
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.15	0.46
3:D:1206:ARG:NH1	3:I:1298:VAL:HG11	2.31	0.46
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.98	0.46
3:I:11:GLN:HB3	3:I:11:GLN:HE21	1.62	0.46
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	1.97	0.46
3:I:572:THR:OG1	3:I:573:THR:N	2.49	0.46
3:I:706:VAL:HA	3:I:714:GLU:O	2.16	0.46
3:I:931:THR:OG1	3:I:931:THR:O	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.51	0.46
2:C:1135:GLN:HA	2:C:1136:GLN:HA	1.64	0.45
3:D:1156:LEU:HD11	3:D:1224:ARG:HH21	1.81	0.45
3:D:1262:ARG:HD3	3:D:1279:GLN:OE1	2.16	0.45
3:D:427:PRO:O	3:D:429:LEU:HD22	2.15	0.45
3:D:512:TYR:HD2	3:D:724:MET:HE1	1.81	0.45
1:G:130:ILE:HG22	1:G:131:CYS:SG	2.55	0.45
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.98	0.45
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.98	0.45
3:I:475:GLU:OE2	4:J:28:ARG:NH2	2.49	0.45
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.49	0.45
5:Y:112:THR:HG22	5:Y:113:ARG:HG2	1.97	0.45
1:B:52:PRO:O	1:B:179:PRO:HD3	2.16	0.45
2:C:1270:PHE:CE2	2:C:1290:MET:HG2	2.51	0.45
2:C:409:LEU:HD12	2:C:427:ASP:HB3	1.99	0.45
2:C:705:GLU:HB2	2:C:794:LEU:H	1.82	0.45
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.97	0.45
2:C:914:LYS:HG2	2:C:915:ASP:H	1.81	0.45
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.98	0.45
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.52	0.45
3:D:514:THR:HG22	3:D:515:ARG:H	1.80	0.45
3:D:583:VAL:HG21	3:D:593:ASN:OD1	2.16	0.45
1:F:111:THR:HG22	1:F:129:VAL:HG22	1.99	0.45
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.98	0.45
2:H:700:VAL:HA	2:H:1182:ILE:HG22	1.98	0.45
3:I:1170:LYS:O	3:I:1173:ARG:HD2	2.17	0.45
3:I:1247:LYS:H	3:I:1247:LYS:HG2	1.56	0.45
3:D:1157:ALA:O	3:D:1207:GLY:N	2.49	0.45
3:D:146:VAL:HA	3:D:178:ALA:CB	2.45	0.45
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.50	0.45
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.98	0.45
2:H:234:ASP:HB2	2:H:236:LYS:HE2	1.99	0.45
2:H:804:PHE:HE1	2:H:1115:THR:HG21	1.80	0.45
3:I:413:ASP:O	3:I:417:ARG:HG2	2.16	0.45
5:X:457:ILE:O	5:X:461:ASN:ND2	2.49	0.45
5:Y:105:MET:O	5:Y:108:VAL:HG13	2.16	0.45
5:Y:448:ARG:HD2	5:Y:452:ILE:HB	1.98	0.45
1:B:13:LEU:O	1:B:28:LEU:HA	2.16	0.45
2:C:582:ASN:HB3	2:C:586:PHE:N	2.32	0.45
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.16	0.45
3:D:1258:ARG:HG3	3:D:1259:GLN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:ARG:CG	3:D:82:GLY:N	2.76	0.45
1:B:35:PHE:O	1:B:39:LEU:HG	2.17	0.45
2:C:600:THR:HG22	2:C:601:ASP:H	1.81	0.45
2:C:886:LYS:HE2	2:C:916:SER:CB	2.46	0.45
3:D:849:LEU:HA	3:D:856:ILE:N	2.31	0.45
2:H:1115:THR:HG22	2:H:1228:GLY:HA3	1.97	0.45
3:I:518:VAL:HA	3:I:547:ARG:NH1	2.30	0.45
3:I:74:LYS:HD2	3:I:87:LYS:HE3	1.97	0.45
1:A:90:VAL:HG11	1:A:146:VAL:HG11	1.99	0.45
1:A:3:GLY:HA3	1:A:4:SER:HA	1.59	0.45
2:C:814:ASP:OD1	2:C:1106:ARG:NH1	2.50	0.45
2:C:744:GLY:HA2	2:C:974:ARG:HH11	1.82	0.45
3:D:437:PHE:HZ	3:D:453:VAL:HG21	1.81	0.45
2:H:1292:THR:OG1	2:H:1293:VAL:N	2.49	0.45
2:H:145:ILE:HG22	2:H:456:VAL:HG22	1.98	0.45
2:H:510:GLN:O	2:H:511:LEU:HB2	2.16	0.45
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.52	0.45
1:G:181:GLU:O	3:I:535:ARG:NH1	2.48	0.45
3:I:587:LEU:H	3:I:611:ILE:HD11	1.81	0.45
3:I:914:ALA:O	3:I:918:ILE:HG22	2.17	0.45
5:Y:157:ARG:NH1	5:Y:159:SER:N	2.65	0.45
2:C:105:TYR:HA	2:C:106:GLU:HA	1.47	0.45
2:H:1135:GLN:HA	2:H:1136:GLN:HA	1.62	0.45
5:Y:311:THR:O	5:Y:345:GLN:NE2	2.49	0.45
2:C:88:ARG:NH2	2:C:1040:ASP:HA	2.31	0.45
2:C:685:MET:CE	2:C:1073:LYS:HG2	2.47	0.45
2:C:28:LEU:HD21	2:C:524:ILE:HG12	1.98	0.45
3:D:1134:ILE:O	3:D:1134:ILE:HD12	2.16	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.30	0.45
3:D:704:GLU:O	3:D:705:THR:OG1	2.32	0.45
2:H:53:PHE:CZ	2:H:68:LEU:HB3	2.52	0.45
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	1.99	0.45
2:H:901:LEU:O	2:H:905:ILE:HG13	2.17	0.45
3:I:193:ASP:HB3	3:I:196:GLN:HB2	1.98	0.45
3:I:370:LYS:HA	3:I:441:LEU:CD1	2.46	0.45
3:I:479:GLU:HG3	4:J:20:VAL:HG11	1.98	0.45
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.16	0.45
1:B:65:LEU:HB3	1:B:168:ILE:HG21	1.98	0.45
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.98	0.45
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.52	0.45
4:J:59:ILE:HG23	4:J:64:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.79	0.45
3:D:1323:ALA:HA	3:D:1331:VAL:HG11	1.97	0.45
3:D:343:LEU:HG	3:D:344:GLY:N	2.31	0.45
3:D:504:GLN:HA	3:D:730:ALA:HA	1.99	0.45
2:H:393:ASP:OD1	2:H:393:ASP:N	2.46	0.45
2:H:985:GLU:HG3	2:H:988:LYS:HB2	1.99	0.45
3:I:1169:THR:HA	3:I:1173:ARG:O	2.17	0.45
3:I:1175:LEU:H	3:I:1175:LEU:HD12	1.82	0.45
3:I:538:ARG:HA	3:I:539:SER:HA	1.64	0.45
3:I:777:HIS:NE2	3:I:781:LYS:HD3	2.32	0.45
3:I:819:GLY:H	3:I:881:LYS:HE2	1.81	0.45
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.99	0.45
5:Y:562:ARG:HD3	5:Y:573:LEU:HG	1.99	0.45
2:C:1289:GLU:HA	2:C:1293:VAL:HG12	1.98	0.44
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.52	0.44
2:C:844:LYS:HD3	2:C:844:LYS:HA	1.77	0.44
2:C:943:LYS:O	2:C:947:GLU:HG2	2.17	0.44
3:D:186:GLN:CG	3:D:238:ILE:HD11	2.46	0.44
3:D:841:GLY:HA3	3:D:901:ARG:HD3	2.00	0.44
2:H:1247:SER:O	3:I:348:ASP:HB3	2.17	0.44
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.82	0.44
2:H:338:THR:HB	2:H:345:PRO:HG3	1.99	0.44
2:H:417:SER:OG	2:H:418:GLY:N	2.50	0.44
5:X:151:VAL:HG22	5:X:156:ALA:HB3	1.99	0.44
5:Y:105:MET:SD	5:Y:384:LEU:HD12	2.57	0.44
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.82	0.44
3:D:527:LEU:H	3:D:550:VAL:HG12	1.82	0.44
3:D:528:THR:HA	3:D:529:GLY:HA2	1.55	0.44
3:D:796:LEU:HG	3:D:800:LEU:HD23	1.99	0.44
2:H:1011:LEU:HA	2:H:1014:LEU:HB3	1.99	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.82	0.44
2:H:895:LEU:HD13	2:H:895:LEU:HA	1.79	0.44
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.99	0.44
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.82	0.44
3:I:516:ASP:OD1	3:I:516:ASP:N	2.49	0.44
5:X:108:VAL:HG23	5:X:110:LEU:HG	1.99	0.44
5:X:222:ALA:O	5:X:226:ALA:N	2.45	0.44
5:X:165:PHE:C	5:X:259:PHE:HD2	2.20	0.44
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.97	0.44
2:C:726:TYR:OH	2:C:728:ASP:OD1	2.35	0.44
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1315:MET:HE2	3:D:473:THR:HG21	1.98	0.44
3:D:608:CYS:O	3:D:612:LEU:HB2	2.17	0.44
1:F:152:TYR:O	1:F:152:TYR:CG	2.70	0.44
2:H:1004:ASP:OD1	2:H:1004:ASP:N	2.50	0.44
2:H:1272:GLU:HG2	3:I:342:LEU:H	1.83	0.44
2:H:136:PHE:CE1	2:H:456:VAL:HG11	2.52	0.44
3:I:1280:VAL:HG21	3:I:1304:ARG:CZ	2.46	0.44
3:I:366:CYS:HB3	3:I:437:PHE:CD2	2.52	0.44
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.99	0.44
3:I:544:LEU:HD22	3:I:575:GLY:HA2	1.99	0.44
3:I:690:ASN:OD1	3:I:738:ARG:NH1	2.50	0.44
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.98	0.44
5:Y:277:MET:HE1	5:Y:359:LYS:HD3	1.99	0.44
2:C:759:SER:OG	2:C:760:ASN:N	2.50	0.44
3:D:515:ARG:HH12	3:D:717:VAL:HB	1.83	0.44
3:I:524:GLY:HA2	3:I:548:VAL:HA	1.99	0.44
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.52	0.44
2:C:1106:ARG:O	2:C:1108:ASN:N	2.46	0.44
2:C:382:GLU:O	2:C:386:GLU:HG2	2.17	0.44
2:C:38:PHE:CE2	2:C:46:GLN:HG2	2.53	0.44
3:D:828:GLY:HA2	3:D:829:GLY:HA2	1.52	0.44
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	2.00	0.44
2:H:848:GLU:HG2	2:H:888:THR:HA	2.00	0.44
2:H:972:PHE:HE1	2:H:998:LEU:HD23	1.82	0.44
3:I:1188:GLU:HG3	3:I:1189:MET:H	1.83	0.44
3:I:1320:ILE:HD12	3:I:1342:ASP:OD2	2.17	0.44
5:X:138:PRO:HD2	5:X:353:LEU:HD11	2.00	0.44
5:X:439:ILE:O	5:X:443:ILE:HG13	2.18	0.44
2:C:122:VAL:HG23	5:X:472:GLN:HG2	2.00	0.44
5:Y:166:VAL:HG22	5:Y:259:PHE:HA	1.99	0.44
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.53	0.44
3:D:431:ARG:N	3:D:921:GLN:OE1	2.50	0.44
2:C:1286:THR:N	3:D:479:GLU:OE2	2.48	0.44
3:D:591:ILE:HG13	3:D:592:VAL:N	2.33	0.44
3:D:63:GLY:O	3:D:98:ARG:NH2	2.51	0.44
2:H:645:PHE:HA	2:H:646:SER:HA	1.61	0.44
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.99	0.44
5:X:166:VAL:N	5:X:259:PHE:CD2	2.86	0.44
1:B:275:ILE:HG21	1:B:281:LEU:HB2	1.99	0.44
2:C:1069:ARG:H	2:C:1069:ARG:HG2	1.38	0.44
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:VAL:HB	2:C:176:ILE:HG12	2.00	0.44
3:D:1169:THR:HA	3:D:1173:ARG:O	2.17	0.44
3:D:37:GLU:HG2	3:D:39:LYS:HG2	2.00	0.44
2:H:301:TYR:HD1	2:H:330:HIS:CD2	2.36	0.44
2:H:755:LYS:HE3	2:H:756:TYR:CE2	2.52	0.44
3:I:1260:MET:HG3	3:I:1307:LEU:O	2.18	0.44
3:I:161:THR:HB	3:I:164:GLN:HG3	2.00	0.44
3:I:309:ASN:HB2	3:I:326:SER:HB3	1.99	0.44
3:I:596:LEU:HD11	3:I:598:LYS:NZ	2.32	0.44
3:D:1371:ARG:HG2	3:I:849:LEU:CD2	2.48	0.44
1:B:62:ASP:O	1:B:71:LYS:HE2	2.17	0.44
2:C:118:LYS:HG2	2:C:488:MET:H	1.83	0.44
2:C:1212:LEU:HD21	2:C:1227:VAL:HG21	1.99	0.44
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	2.00	0.44
3:D:266:ASN:O	3:D:270:ARG:HB2	2.18	0.44
3:D:544:LEU:HD22	3:D:575:GLY:HA2	1.99	0.44
3:D:789:LYS:HD2	3:D:930:LEU:O	2.18	0.44
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.99	0.44
2:H:802:VAL:HG11	2:H:1230:MET:HB2	1.99	0.44
2:H:720:ARG:HD2	2:H:736:VAL:CG2	2.46	0.44
2:H:740:GLU:HB2	2:H:741:MET:SD	2.58	0.44
5:X:140:ALA:HB1	5:X:269:LEU:HD13	1.99	0.44
2:C:1073:LYS:H	2:C:1073:LYS:HG3	1.57	0.44
2:C:556:GLY:HA2	2:C:659:GLN:O	2.17	0.44
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.53	0.44
2:H:192:ASP:OD2	2:H:436:ARG:NH2	2.51	0.44
2:H:908:GLU:HG2	2:H:909:LYS:H	1.82	0.44
3:I:504:GLN:HA	3:I:730:ALA:HA	1.99	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44
5:X:537:THR:O	5:X:541:ARG:HG3	2.18	0.44
5:X:561:MET:O	5:X:571:TYR:HB2	2.18	0.44
5:Y:483:LEU:O	5:Y:487:MET:HG2	2.18	0.44
2:C:645:PHE:HA	2:C:646:SER:HA	1.65	0.43
1:G:27:THR:HG22	1:G:202:VAL:HG22	2.00	0.43
3:I:1173:ARG:HA	3:I:1174:ARG:C	2.38	0.43
3:I:412:LEU:HA	3:I:415:VAL:HG22	2.00	0.43
3:I:925:GLU:HB3	3:I:926:PRO:HD3	2.00	0.43
5:X:402:LEU:HD13	5:X:405:ILE:HD11	2.00	0.43
5:X:407:GLU:O	5:X:410:ILE:HG22	2.18	0.43
1:B:192:VAL:HG12	1:B:194:GLN:HG2	2.00	0.43
2:C:1007:LYS:O	2:C:1011:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.18	0.43
3:D:370:LYS:HD3	3:D:443:GLU:CD	2.39	0.43
2:C:1101:LEU:HD21	3:D:508:LEU:HD13	2.00	0.43
3:D:555:TYR:HB2	3:D:585:LYS:O	2.18	0.43
3:D:781:LYS:NZ	3:D:785:ASP:OD1	2.51	0.43
3:D:822:MET:HG2	3:D:839:VAL:HG23	2.00	0.43
1:F:74:VAL:HG12	1:F:76:GLU:H	1.83	0.43
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.00	0.43
2:H:842:ASP:CB	2:H:1046:VAL:HG21	2.48	0.43
4:J:58:LEU:HA	4:J:58:LEU:HD12	1.79	0.43
5:Y:220:LYS:HB3	5:Y:259:PHE:CE2	2.53	0.43
5:Y:379:MET:HB3	5:Y:416:VAL:HG21	2.00	0.43
1:A:13:LEU:HD11	1:A:16:ILE:HD11	2.01	0.43
1:B:284:ARG:HA	1:B:284:ARG:HD2	1.73	0.43
2:C:91:THR:HG21	2:C:503:LYS:HE3	2.01	0.43
2:H:1151:LEU:HD23	2:H:1151:LEU:HA	1.90	0.43
3:I:738:ARG:NH2	3:I:745:GLY:H	2.16	0.43
2:C:1046:VAL:CG2	2:C:1047:LEU:H	2.20	0.43
2:C:1106:ARG:HE	3:D:731:ARG:NH2	2.16	0.43
2:C:1141:LEU:C	2:C:1141:LEU:HD12	2.39	0.43
2:C:1293:VAL:HG23	2:C:1300:GLY:C	2.38	0.43
2:C:38:PHE:CG	2:C:38:PHE:O	2.71	0.43
2:C:120:GLN:CD	2:C:490:GLN:HB2	2.39	0.43
3:D:1173:ARG:HA	3:D:1174:ARG:C	2.39	0.43
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.83	0.43
2:H:143:ARG:HA	2:H:513:GLN:O	2.18	0.43
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.19	0.43
3:I:716:GLN:HB3	3:I:716:GLN:HE21	1.59	0.43
5:Y:96:ASP:O	5:Y:100:MET:HB2	2.18	0.43
5:Y:231:THR:OG1	5:Y:248:GLU:O	2.37	0.43
5:Y:303:ILE:O	5:Y:307:THR:OG1	2.21	0.43
1:B:135:ASP:OD1	1:B:138:ALA:HB2	2.17	0.43
2:C:409:LEU:HD21	2:C:428:VAL:HG22	1.99	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.01	0.43
2:C:756:TYR:CE2	2:C:766:ASN:ND2	2.87	0.43
2:C:898:GLU:N	2:C:898:GLU:OE1	2.41	0.43
2:C:885:GLY:HA2	2:C:917:SER:HB3	2.01	0.43
3:D:145:VAL:CG2	3:D:159:ILE:HG13	2.48	0.43
2:C:1106:ARG:HH21	3:D:731:ARG:HH22	1.65	0.43
1:F:50:SER:HG	1:G:35:PHE:HZ	1.64	0.43
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:603:ILE:HD12	2:H:603:ILE:O	2.19	0.43
3:I:513:MET:SD	3:I:579:LEU:HD23	2.59	0.43
3:I:682:VAL:HA	3:I:685:ILE:HD12	2.00	0.43
1:A:165:GLU:O	1:A:165:GLU:HG3	2.18	0.43
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.82	0.43
2:C:1124:ILE:O	2:C:1128:ILE:HD13	2.19	0.43
2:C:1305:TYR:CZ	3:D:379:PRO:HG3	2.54	0.43
2:C:421:SER:H	2:C:424:ASP:HB2	1.83	0.43
2:C:455:SER:O	2:C:459:MET:HG3	2.19	0.43
2:C:607:SER:HB2	2:C:610:GLU:HG3	1.99	0.43
2:C:678:ARG:HD3	2:C:681:MET:HG3	2.00	0.43
2:C:47:TYR:HD1	2:C:70:TYR:HH	1.64	0.43
3:D:1181:ASP:OD2	3:D:1203:ARG:NH2	2.52	0.43
3:D:141:PHE:CZ	3:D:296:LYS:HD2	2.53	0.43
3:I:810:THR:O	3:I:811:GLU:HG2	2.18	0.43
3:I:489:ASN:HA	3:I:904:ALA:CB	2.48	0.43
3:I:905:ARG:NH2	4:J:16:ARG:HG3	2.32	0.43
5:Y:165:PHE:HA	5:Y:259:PHE:HB2	1.99	0.43
5:Y:162:ILE:C	5:Y:262:VAL:HG13	2.39	0.43
2:C:1042:LEU:HD11	2:C:1047:LEU:O	2.18	0.43
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.00	0.43
2:C:303:ASP:HB2	2:C:306:THR:OG1	2.19	0.43
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.34	0.43
4:E:58:LEU:HD12	4:E:58:LEU:HA	1.77	0.43
2:H:890:LYS:HB2	2:H:914:LYS:HB2	2.01	0.43
3:I:84:ILE:HG13	3:I:84:ILE:H	1.61	0.43
3:I:910:ASN:OD1	4:J:15:ASN:HA	2.19	0.43
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.34	0.43
2:C:669:PRO:HG2	2:C:670:PHE:H	1.83	0.43
3:D:1173:ARG:HA	3:D:1174:ARG:O	2.19	0.43
3:D:128:LEU:HD12	3:D:192:MET:HE3	2.00	0.43
3:D:253:VAL:HG11	5:X:523:ILE:HG21	1.99	0.43
3:D:355:ILE:HG12	3:D:464:ASP:O	2.18	0.43
1:G:37:HIS:CE1	1:G:187:VAL:HG22	2.54	0.43
2:H:1154:ASP:HB2	2:H:1156:ARG:HE	1.83	0.43
2:H:890:LYS:HG2	2:H:891:GLY:H	1.84	0.43
1:B:78:ILE:HA	1:B:81:ILE:HD12	2.00	0.43
3:D:213:LYS:O	3:D:217:LEU:HG	2.18	0.43
3:D:334:LYS:HG3	3:D:335:GLN:N	2.33	0.43
3:D:716:GLN:HG2	3:D:717:VAL:H	1.84	0.43
2:H:1200:LYS:HE2	2:H:1206:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:179:LYS:HB2	3:I:179:LYS:HE2	1.80	0.43
3:I:294:ASN:ND2	3:I:298:MET:SD	2.92	0.43
3:I:527:LEU:H	3:I:550:VAL:HG12	1.82	0.43
5:X:343:LYS:O	5:X:347:ILE:HG13	2.18	0.43
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.01	0.43
5:X:390:ILE:HD13	5:X:436:ARG:HG3	2.01	0.43
5:Y:105:MET:CG	5:Y:384:LEU:HD12	2.48	0.43
5:Y:540:LEU:HB2	5:Y:607:LEU:HD12	2.01	0.43
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.80	0.43
2:C:399:ALA:O	2:C:403:MET:N	2.46	0.43
2:C:714:VAL:HG23	2:C:787:PRO:HD2	2.00	0.43
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	2.01	0.43
3:D:518:VAL:HA	3:D:547:ARG:HH12	1.82	0.43
3:D:521:LYS:HD2	3:D:542:ALA:O	2.19	0.43
3:D:903:LEU:HG	3:D:909:ILE:HG22	2.00	0.43
2:H:210:LEU:O	2:H:215:TYR:HB2	2.19	0.43
2:H:500:ALA:O	2:H:504:GLU:HB2	2.19	0.43
2:H:578:TYR:CE2	2:H:658:GLN:HG3	2.50	0.43
5:X:274:ARG:O	5:X:278:ASP:N	2.50	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
5:Y:399:LEU:HD12	5:Y:399:LEU:HA	1.84	0.43
1:B:56:VAL:HG12	1:B:173:VAL:HG11	2.01	0.42
1:B:60:GLU:HA	1:B:169:GLY:O	2.19	0.42
2:C:1333:LEU:HD13	3:D:115:TRP:CH2	2.54	0.42
2:C:237:LEU:O	2:C:286:GLU:HG3	2.19	0.42
2:C:296:VAL:HB	2:C:336:LEU:HD12	2.01	0.42
2:C:740:GLU:HB2	2:C:741:MET:SD	2.59	0.42
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.35	0.42
3:D:317:THR:O	3:D:324:LEU:HD11	2.19	0.42
3:I:62:PHE:O	3:I:101:ARG:HG3	2.19	0.42
3:I:363:LEU:HD12	3:I:450:HIS:CE1	2.54	0.42
3:I:647:PRO:HG3	3:I:697:MET:HB2	2.02	0.42
3:I:747:MET:O	3:I:755:ILE:HG22	2.19	0.42
5:X:213:ASP:HB2	5:X:216:LEU:HB3	2.01	0.42
5:X:448:ARG:HD2	5:X:452:ILE:HD12	2.00	0.42
5:Y:390:ILE:HD11	5:Y:435:ILE:CG2	2.48	0.42
5:Y:407:GLU:O	5:Y:410:ILE:HG22	2.19	0.42
1:A:101:THR:OG1	1:A:116:THR:OG1	2.29	0.42
1:B:109:PRO:HB3	1:B:132:HIS:NE2	2.34	0.42
2:C:1146:GLN:HA	2:C:1161:LEU:HD13	2.00	0.42
2:C:225:PHE:CD2	2:C:336:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.52	0.42
3:D:197:GLU:O	3:D:201:LEU:HD23	2.19	0.42
3:D:506:VAL:HG23	3:D:628:GLY:HA3	2.02	0.42
3:D:849:LEU:HA	3:D:855:ASP:HA	2.01	0.42
3:I:1140:ARG:NH2	3:I:1144:LEU:HD21	2.34	0.42
3:I:1173:ARG:HA	3:I:1174:ARG:O	2.20	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
5:X:570:ASP:OD1	5:X:570:ASP:N	2.52	0.42
2:C:256:GLU:HB3	2:C:261:VAL:HG22	2.01	0.42
2:C:720:ARG:HD2	2:C:736:VAL:HG21	2.00	0.42
3:D:381:ILE:HD11	3:D:412:LEU:HD13	2.01	0.42
3:D:521:LYS:HB3	3:D:542:ALA:CB	2.49	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.54	0.42
2:H:660:VAL:HG22	2:H:661:VAL:N	2.34	0.42
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.20	0.42
3:I:901:ARG:CB	3:I:908:ILE:HA	2.48	0.42
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.18	0.42
2:C:948:ILE:HG13	2:C:949:GLU:N	2.33	0.42
3:D:154:LEU:HD23	3:D:154:LEU:HA	1.72	0.42
2:C:1268:GLN:H	3:D:350:SER:HB2	1.84	0.42
2:H:956:ALA:CB	2:H:1032:LYS:HE3	2.50	0.42
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.01	0.42
2:H:714:VAL:HG22	2:H:787:PRO:HD2	2.00	0.42
3:I:361:LEU:HD21	3:I:366:CYS:HA	2.02	0.42
1:B:48:LEU:HD22	3:D:535:ARG:HA	2.00	0.42
2:C:11:ILE:CD1	2:C:697:LYS:HD3	2.49	0.42
2:C:407:ARG:HH22	2:C:609:ILE:HD12	1.84	0.42
2:C:985:GLU:HB3	2:C:989:LEU:HD22	2.01	0.42
3:D:526:VAL:HG12	3:D:549:LYS:O	2.19	0.42
1:F:228:LEU:HD23	1:F:231:PHE:HE2	1.83	0.42
2:H:1252:SER:HA	5:Y:524:GLU:HA	2.02	0.42
2:H:1299:ASN:HB3	2:H:1303:LYS:HE3	2.00	0.42
2:H:453:ILE:HG23	2:H:453:ILE:O	2.18	0.42
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.20	0.42
3:I:681:LYS:HE3	3:I:681:LYS:HB2	1.86	0.42
3:I:264:ASP:OD1	5:Y:506:SER:HB2	2.20	0.42
1:B:54:CYS:SG	1:B:148:ARG:HD3	2.59	0.42
1:B:93:GLN:HG3	1:B:276:HIS:HB3	2.01	0.42
3:D:1238:GLN:O	3:D:1241:TYR:N	2.52	0.42
3:D:546:ALA:N	3:D:573:THR:OG1	2.52	0.42
4:E:12:LYS:HA	4:E:12:LYS:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1326:LEU:HD23	2:H:1326:LEU:HA	1.76	0.42
2:H:687:ARG:HB2	2:H:687:ARG:HE	1.49	0.42
2:H:1313:HIS:CD2	3:I:477:GLN:HE22	2.35	0.42
3:I:534:GLU:HB2	3:I:578:ILE:HD13	2.02	0.42
2:H:844:LYS:HE2	5:Y:499:LYS:NZ	2.35	0.42
1:A:100:LEU:HD11	1:A:121:VAL:HG11	2.00	0.42
2:C:1082:ILE:H	2:C:1082:ILE:HG13	1.59	0.42
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	2.01	0.42
3:D:1372:ARG:HE	3:I:853:THR:HG23	1.85	0.42
3:D:514:THR:HG23	3:D:576:ARG:HG2	2.01	0.42
3:D:714:GLU:HG3	3:D:715:LYS:N	2.35	0.42
1:G:83:LEU:HD12	1:G:83:LEU:HA	1.83	0.42
2:H:122:VAL:HG21	2:H:493:ILE:HG23	2.01	0.42
2:H:719:LYS:HE2	2:H:751:TYR:HE2	1.83	0.42
3:I:85:CYS:SG	3:I:87:LYS:N	2.93	0.42
1:A:220:ALA:HA	1:A:223:ILE:HD12	2.01	0.42
2:C:1083:GLU:H	2:C:1083:GLU:HG2	1.63	0.42
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.01	0.42
2:C:646:SER:HB3	2:C:649:GLN:HG3	2.02	0.42
2:C:525:THR:HG21	2:C:687:ARG:HD2	2.02	0.42
3:D:1362:GLY:O	3:D:1364:ALA:N	2.51	0.42
2:H:1279:GLU:OE2	3:I:1347:LEU:HB3	2.19	0.42
2:H:4:SER:O	2:H:5:TYR:HB2	2.19	0.42
2:H:91:THR:HG22	2:H:139:ASN:N	2.35	0.42
3:I:805:GLN:OE1	3:I:1348:LYS:HE2	2.20	0.42
1:B:76:GLU:HB2	1:B:80:GLU:HB2	2.01	0.42
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.87	0.42
3:D:1272:SER:HB3	3:D:1276:GLU:OE1	2.20	0.42
3:D:521:LYS:O	3:D:542:ALA:HB3	2.20	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HG23	2.55	0.42
1:F:13:LEU:HD21	1:F:16:ILE:HD11	2.00	0.42
3:I:1167:LYS:HE3	3:I:1167:LYS:HB2	1.78	0.42
3:I:1272:SER:H	3:I:1290:ARG:HH12	1.67	0.42
3:I:288:PRO:O	3:I:292:VAL:HG12	2.20	0.42
5:X:396:ASN:O	5:X:396:ASN:ND2	2.52	0.42
1:B:16:ILE:HG12	1:B:26:VAL:HG13	2.02	0.42
1:B:263:THR:HG23	1:B:266:SER:H	1.84	0.42
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.00	0.42
2:C:1268:GLN:H	3:D:350:SER:CB	2.33	0.42
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.55	0.42
3:D:1271:SER:HB2	3:D:1290:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:809:VAL:HG23	3:D:894:VAL:O	2.20	0.42
3:D:825:VAL:O	3:D:834:PRO:HB2	2.20	0.42
2:H:128:PRO:O	2:H:129:LEU:HD23	2.20	0.42
2:H:421:SER:H	2:H:424:ASP:HB2	1.84	0.42
2:H:528:ARG:NH2	2:H:576:SER:O	2.52	0.42
5:X:112:THR:HG22	5:X:113:ARG:N	2.29	0.42
5:Y:354:THR:O	5:Y:358:VAL:HG13	2.20	0.42
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.19	0.42
5:Y:585:GLU:O	5:Y:588:ARG:N	2.53	0.42
2:C:1099:ASN:OD1	2:C:1100:PRO:HD2	2.19	0.41
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.53	0.41
2:C:35:PHE:CE1	2:C:136:PHE:HE2	2.37	0.41
2:C:478:ARG:HE	2:C:487:LEU:HD11	1.85	0.41
2:C:583:GLU:H	2:C:583:GLU:HG3	1.69	0.41
2:C:741:MET:SD	2:C:741:MET:N	2.93	0.41
3:D:762:ASN:OD1	3:D:765:GLU:HG3	2.20	0.41
1:F:48:LEU:HD23	1:F:180:VAL:HG12	2.01	0.41
1:G:182:ARG:HG2	1:G:206:GLU:HB3	2.02	0.41
2:H:1146:GLN:HA	2:H:1161:LEU:HD13	2.02	0.41
3:I:146:VAL:HG12	3:I:158:GLN:O	2.20	0.41
3:I:57:PHE:HZ	3:I:266:ASN:ND2	2.18	0.41
5:Y:257:LYS:HE2	5:Y:257:LYS:HB3	1.82	0.41
1:B:247:PRO:HA	1:B:248:GLU:HA	1.75	0.41
2:C:1069:ARG:HD3	2:C:1114:GLU:OE1	2.21	0.41
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.85	0.41
2:C:49:LEU:HD12	2:C:461:GLU:HB2	2.01	0.41
2:C:404:LYS:HD3	2:C:586:PHE:HZ	1.85	0.41
2:C:856:ASN:HD21	5:X:609:SER:C	2.24	0.41
1:F:97:GLU:HA	1:F:146:VAL:O	2.19	0.41
2:H:542:ARG:H	2:H:542:ARG:HG3	1.50	0.41
2:H:839:VAL:HG11	2:H:841:ARG:NH2	2.35	0.41
3:I:20:ILE:O	3:I:20:ILE:HG13	2.20	0.41
5:X:431:ALA:O	5:X:435:ILE:HG13	2.20	0.41
3:D:388:ARG:HB2	3:D:390:LEU:HD13	2.02	0.41
2:H:1332:SER:O	3:I:243:PRO:HG2	2.20	0.41
2:H:17:LYS:HD3	2:H:1154:ASP:OD2	2.21	0.41
2:H:406:ASN:HB3	2:H:411:ARG:HB2	2.02	0.41
2:H:931:VAL:HG21	2:H:944:ARG:NH2	2.34	0.41
2:H:954:LYS:HB3	2:H:954:LYS:HE3	1.90	0.41
3:I:134:ASP:O	3:I:138:VAL:HG23	2.19	0.41
5:X:558:VAL:HG21	5:X:587:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:NZ	1:B:170:ARG:HH21	2.18	0.41
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.01	0.41
3:D:527:LEU:HD13	3:D:535:ARG:NH2	2.33	0.41
2:H:1119:MET:O	2:H:1123:GLY:N	2.52	0.41
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	2.03	0.41
2:H:1254:VAL:O	3:I:99:ARG:NH1	2.53	0.41
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.56	0.41
2:H:398:SER:O	2:H:401:GLY:N	2.53	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.30	0.41
3:I:1311:LYS:HB3	3:I:1311:LYS:HE3	1.90	0.41
3:I:510:LEU:HD12	3:I:601:ILE:HD13	2.02	0.41
3:I:901:ARG:HA	3:I:908:ILE:HA	2.03	0.41
5:Y:139:GLU:HG3	5:Y:351:THR:HA	2.02	0.41
2:C:398:SER:O	2:C:400:VAL:N	2.54	0.41
2:C:38:PHE:CD2	2:C:46:GLN:HG2	2.56	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.95	0.41
3:D:271:ARG:HD2	3:D:275:ARG:NH2	2.35	0.41
2:H:697:LYS:HE2	2:H:697:LYS:HB3	1.77	0.41
2:H:667:LEU:HD11	2:H:708:VAL:HG21	2.01	0.41
3:I:576:ARG:HG3	3:I:576:ARG:H	1.64	0.41
3:I:856:ILE:O	3:I:857:LEU:HD23	2.21	0.41
5:X:507:MET:HB3	5:X:520:GLY:HA3	2.02	0.41
1:B:289:LEU:HD12	1:B:314:LEU:HD21	2.01	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:HB3	2.03	0.41
2:C:374:GLU:H	2:C:374:GLU:HG3	1.74	0.41
3:D:1167:LYS:HB2	3:D:1167:LYS:HE3	1.80	0.41
3:D:1167:LYS:HE3	3:D:1173:ARG:NH1	2.33	0.41
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.21	0.41
3:D:1327:GLU:H	3:D:1327:GLU:HG3	1.61	0.41
3:D:30:ILE:HD13	3:D:33:TRP:CZ3	2.56	0.41
3:D:584:PRO:O	3:D:589:TYR:OH	2.38	0.41
1:F:100:LEU:HB3	1:F:115:ILE:HD11	2.01	0.41
2:H:1184:THR:OG1	2:H:1189:GLY:HA3	2.21	0.41
2:H:176:ILE:HB	2:H:184:LEU:HB3	2.03	0.41
2:H:576:SER:HB3	2:H:579:ALA:HB2	2.02	0.41
2:H:709:ALA:HB2	2:H:794:LEU:HB2	2.03	0.41
3:I:813:ASP:OD1	3:I:897:HIS:ND1	2.53	0.41
3:I:903:LEU:HB2	3:I:905:ARG:O	2.20	0.41
5:X:407:GLU:HA	5:X:410:ILE:HG22	2.03	0.41
1:A:49:SER:OG	1:A:50:SER:N	2.53	0.41
1:B:23:HIS:HD2	1:B:206:GLU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:HB3	1:B:8:PHE:CE2	2.56	0.41
2:C:1051:LYS:HB3	2:C:1053:TYR:CE1	2.53	0.41
2:C:562:GLU:HG3	2:C:562:GLU:O	2.21	0.41
1:F:11:PRO:HD3	1:G:227:GLN:NE2	2.35	0.41
1:F:221:ALA:HB1	1:G:228:LEU:HD13	2.03	0.41
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	2.03	0.41
2:H:1294:LYS:HE2	3:I:348:ASP:O	2.21	0.41
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.03	0.41
3:I:416:ILE:HD13	3:I:441:LEU:CD2	2.50	0.41
2:C:948:ILE:O	2:C:952:GLN:HG3	2.21	0.41
3:D:343:LEU:HG	3:D:344:GLY:H	1.84	0.41
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.02	0.41
3:D:857:LEU:HD11	3:D:871:LEU:HD21	2.01	0.41
1:F:192:VAL:HG21	1:F:198:LEU:HD12	2.02	0.41
2:H:1043:ALA:C	2:H:1045:GLY:H	2.24	0.41
2:H:1128:ILE:HG21	2:H:1176:LEU:HB2	2.02	0.41
3:I:166:LEU:HD12	3:I:167:ASP:N	2.36	0.41
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	2.03	0.41
1:B:14:VAL:HA	1:B:28:LEU:HD23	2.03	0.41
1:B:37:HIS:CD2	2:C:1216:ARG:HH21	2.38	0.41
2:C:736:VAL:HG11	2:C:740:GLU:HB3	2.03	0.41
3:D:362:ARG:HG2	3:D:364:HIS:CE1	2.56	0.41
3:D:355:ILE:HG22	3:D:447:ILE:HG23	2.01	0.41
3:D:552:ILE:HG23	3:D:580:TRP:CZ2	2.56	0.41
3:D:58:CYS:SG	3:D:59:ALA:N	2.94	0.41
3:D:786:THR:O	3:D:790:THR:OG1	2.26	0.41
2:H:729:ALA:O	2:H:755:LYS:HD2	2.20	0.41
3:I:437:PHE:CZ	3:I:453:VAL:HG21	2.48	0.41
5:X:157:ARG:HH11	5:X:159:SER:H	1.68	0.41
2:C:1004:ASP:O	2:C:1005:GLU:O	2.39	0.41
2:C:801:ARG:HD2	2:C:1229:TYR:OH	2.20	0.41
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.02	0.41
1:F:228:LEU:HD23	1:F:231:PHE:CE2	2.56	0.41
1:F:31:LEU:HD22	1:F:35:PHE:HB2	2.03	0.41
2:H:150:HIS:CE1	2:H:454:ARG:HB2	2.56	0.41
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.56	0.41
2:H:719:LYS:HG3	2:H:751:TYR:CE2	2.55	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.21	0.41
3:I:541:LEU:HA	3:I:542:ALA:HA	1.85	0.41
5:X:484:ALA:HB1	5:X:490:PRO:O	2.21	0.41
5:X:506:SER:O	5:X:509:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:240:ARG:O	5:Y:242:HIS:N	2.53	0.41
5:Y:140:ALA:HB1	5:Y:269:LEU:HD13	2.03	0.41
2:C:817:LEU:CD2	2:C:1078:LYS:HB3	2.49	0.41
3:D:129:ASP:HB2	3:D:220:ARG:CZ	2.51	0.41
3:D:268:LEU:HB3	3:D:306:LEU:HD12	2.01	0.41
2:H:1069:ARG:H	2:H:1069:ARG:HG3	1.61	0.41
2:H:681:MET:O	2:H:685:MET:HG2	2.21	0.41
2:H:786:GLY:H	2:H:789:THR:CG2	2.34	0.41
3:I:1338:ALA:O	3:I:1340:LYS:N	2.48	0.41
3:I:308:ASP:OD1	3:I:311:ARG:NH1	2.54	0.41
3:I:613:GLY:O	3:I:617:THR:OG1	2.17	0.41
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.55	0.41
5:X:562:ARG:HD3	5:X:573:LEU:HG	2.01	0.41
5:Y:162:ILE:HD12	5:Y:162:ILE:C	2.42	0.41
1:B:179:PRO:HB3	1:B:210:THR:HB	2.02	0.40
2:C:1184:THR:HG23	2:C:1184:THR:O	2.22	0.40
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.56	0.40
2:C:136:PHE:CE1	2:C:145:ILE:HD12	2.56	0.40
2:C:519:ASN:OD1	2:C:522:SER:N	2.48	0.40
2:C:699:LEU:HD23	2:C:799:ASN:OD1	2.22	0.40
3:D:123:ARG:HD2	3:D:1333:THR:HG22	2.01	0.40
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.56	0.40
2:C:1106:ARG:NE	3:D:731:ARG:HH22	2.19	0.40
3:D:759:ILE:HG12	3:D:771:GLN:HB2	2.03	0.40
1:F:166:ARG:O	1:F:167:PRO:C	2.60	0.40
2:H:1101:LEU:O	2:H:1104:PRO:HD2	2.21	0.40
2:H:237:LEU:HD13	2:H:292:ILE:HD12	2.04	0.40
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.36	0.40
3:I:773:PHE:O	3:I:776:THR:HG22	2.20	0.40
1:B:286:GLU:HA	1:B:289:LEU:HB2	2.02	0.40
2:C:1100:PRO:HG3	3:D:637:ALA:O	2.21	0.40
2:C:646:SER:O	2:C:646:SER:OG	2.31	0.40
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.21	0.40
3:D:1363:TYR:O	3:D:1367:GLN:HB2	2.22	0.40
2:H:1289:GLU:O	2:H:1294:LYS:HB2	2.21	0.40
2:H:1296:ASP:OD1	3:I:345:LYS:HD3	2.21	0.40
3:I:108:ALA:HB1	3:I:279:LEU:HD12	2.03	0.40
3:I:846:GLU:HA	3:I:859:PRO:CA	2.48	0.40
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.86	0.40
5:X:120:ALA:HA	5:X:123:ILE:HD12	2.02	0.40
5:Y:394:TYR:CD2	5:Y:439:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.21	0.40
2:C:122:VAL:HG21	2:C:493:ILE:CG2	2.52	0.40
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.55	0.40
2:C:557:ARG:HD3	2:C:587:LEU:HB3	2.02	0.40
2:C:817:LEU:HA	2:C:817:LEU:HD23	1.82	0.40
2:H:1328:LYS:O	2:H:1332:SER:N	2.54	0.40
2:H:451:ARG:NH2	2:H:547:VAL:HG11	2.36	0.40
2:H:840:SER:HB3	2:H:850:ILE:HD11	2.03	0.40
2:H:844:LYS:HE2	5:Y:499:LYS:HZ3	1.86	0.40
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	2.03	0.40
1:B:119:GLY:HA3	1:B:271:LYS:HD3	2.03	0.40
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.56	0.40
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.93	0.40
2:C:1259:LEU:HA	2:C:1260:GLY:HA3	1.87	0.40
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.04	0.40
1:F:155:ALA:HA	1:F:158:ARG:HB2	2.03	0.40
2:H:1142:ARG:NH2	2:H:1164:PHE:O	2.29	0.40
2:H:1255:THR:O	2:H:1257:GLN:N	2.49	0.40
3:I:149:GLY:CA	3:I:176:PHE:HB2	2.52	0.40
5:X:133:SER:HA	5:X:136:GLU:OE2	2.21	0.40
5:X:363:ARG:O	5:X:367:ILE:HG12	2.21	0.40
5:Y:311:THR:HB	5:Y:345:GLN:HG2	2.03	0.40
2:C:27:LEU:HD12	2:C:524:ILE:HD13	2.03	0.40
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.96	0.40
2:C:617:ALA:HB2	2:C:650:VAL:HG11	2.03	0.40
2:C:841:ARG:HB2	2:C:848:GLU:CD	2.42	0.40
2:C:977:ALA:O	2:C:980:VAL:HG12	2.21	0.40
3:D:128:LEU:HD13	3:D:189:LEU:HD23	2.02	0.40
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.57	0.40
1:G:14:VAL:HG22	1:G:28:LEU:HD22	2.04	0.40
2:H:468:LEU:O	2:H:471:VAL:HG22	2.22	0.40
3:I:290:ILE:HD12	5:Y:381:GLU:HG2	2.03	0.40
3:I:825:VAL:O	3:I:834:PRO:HB2	2.21	0.40
3:I:929:GLN:HG2	3:I:929:GLN:H	1.63	0.40
5:Y:111:LEU:HD22	5:Y:115:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/329 (70%)	201 (87%)	31 (13%)	0	100	100
1	B	297/329 (90%)	269 (91%)	28 (9%)	0	100	100
1	F	230/329 (70%)	203 (88%)	27 (12%)	0	100	100
1	G	227/329 (69%)	201 (88%)	26 (12%)	0	100	100
2	C	1334/1342 (99%)	1130 (85%)	186 (14%)	18 (1%)	12	48
2	H	1334/1342 (99%)	1127 (84%)	192 (14%)	15 (1%)	14	51
3	D	1158/1407 (82%)	983 (85%)	166 (14%)	9 (1%)	19	58
3	I	1154/1407 (82%)	955 (83%)	192 (17%)	7 (1%)	25	63
4	E	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	14	51
4	J	74/91 (81%)	64 (86%)	9 (12%)	1 (1%)	11	46
5	X	467/613 (76%)	425 (91%)	39 (8%)	3 (1%)	25	63
5	Y	471/613 (77%)	431 (92%)	37 (8%)	3 (1%)	25	63
All	All	7066/8222 (86%)	6064 (86%)	945 (13%)	57 (1%)	19	58

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	15	PHE
2	C	66	SER
2	C	547	VAL
2	C	661	VAL
2	C	1005	GLU
2	C	1006	GLU
2	C	1138	VAL
2	H	547	VAL
2	H	661	VAL
2	H	1047	LEU
2	H	1138	VAL
2	C	546	GLU

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Mol	Chain	Res	Type
2	C	993	PRO
2	C	1185	PRO
3	D	82	GLY
3	D	1273	ASP
2	H	993	PRO
3	I	588	PRO
3	I	889	ASP
3	I	1273	ASP
5	X	490	PRO
2	C	1137	GLU
3	D	588	PRO
3	D	889	ASP
3	D	1173	ARG
2	H	543	ALA
2	H	546	GLU
2	H	893	THR
2	H	1185	PRO
3	I	1173	ARG
5	Y	259	PHE
5	Y	490	PRO
3	D	887	SER
2	H	82	VAL
2	H	813	GLU
3	I	887	SER
2	C	59	ILE
2	C	82	VAL
2	C	1047	LEU
2	H	59	ILE
3	I	587	LEU
5	X	258	GLN
5	Y	503	GLU
3	D	587	LEU
3	D	850	LYS
2	H	42	ASP
2	H	43	PRO
3	I	595	ALA
2	C	1046	VAL
4	J	59	ILE
5	X	503	GLU
2	C	56	VAL
2	C	58	PRO
2	C	1186	VAL

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Mol	Chain	Res	Type
2	H	1046	VAL
3	D	834	PRO
4	E	59	ILE

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	201/286 (70%)	198 (98%)	3 (2%)	65	80
1	B	261/286 (91%)	251 (96%)	10 (4%)	33	59
1	F	201/286 (70%)	195 (97%)	6 (3%)	41	64
1	G	197/286 (69%)	194 (98%)	3 (2%)	65	80
2	C	1152/1157 (100%)	1121 (97%)	31 (3%)	44	67
2	H	1152/1157 (100%)	1122 (97%)	30 (3%)	46	67
3	D	975/1168 (84%)	928 (95%)	47 (5%)	25	53
3	I	972/1168 (83%)	944 (97%)	28 (3%)	42	65
4	E	74/75 (99%)	73 (99%)	1 (1%)	67	81
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	418/540 (77%)	409 (98%)	9 (2%)	52	71
5	Y	422/540 (78%)	409 (97%)	13 (3%)	40	63
All	All	6090/7024 (87%)	5909 (97%)	181 (3%)	41	64

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	117	HIS
1	A	160	HIS
1	B	118	ASP
1	B	164	ASP
1	B	165	GLU
1	B	182	ARG

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Mol	Chain	Res	Type
1	B	212	ASP
1	B	227	GLN
1	B	249	PHE
1	B	250	ASP
1	B	255	ARG
1	B	284	ARG
2	C	53	PHE
2	C	57	PHE
2	C	80	PHE
2	C	107	ARG
2	C	120	GLN
2	C	133	ASN
2	C	222	ASP
2	C	397	LEU
2	C	504	GLU
2	C	529	ARG
2	C	533	LEU
2	C	574	SER
2	C	646	SER
2	C	720	ARG
2	C	741	MET
2	C	773	LEU
2	C	785	ASP
2	C	817	LEU
2	C	994	ARG
2	C	1006	GLU
2	C	1027	LYS
2	C	1032	LYS
2	C	1034	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1180	MET
2	C	1211	ARG
2	C	1236	ASN
2	C	1270	PHE
2	C	1272	GLU
2	C	1276	TRP
3	D	8	LEU
3	D	31	ARG
3	D	58	CYS
3	D	67	ASP
3	D	81	ARG

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Mol	Chain	Res	Type
3	D	101	ARG
3	D	119	SER
3	D	123	ARG
3	D	132	LEU
3	D	175	GLU
3	D	248	ASP
3	D	250	ARG
3	D	259	ARG
3	D	341	ASN
3	D	342	LEU
3	D	362	ARG
3	D	375	GLU
3	D	378	LYS
3	D	422	LEU
3	D	430	HIS
3	D	445	LYS
3	D	505	ASP
3	D	516	ASP
3	D	527	LEU
3	D	560	ASN
3	D	589	TYR
3	D	590	SER
3	D	610	ARG
3	D	629	PHE
3	D	668	PHE
3	D	677	GLU
3	D	678	ARG
3	D	751	ASP
3	D	764	ARG
3	D	772	TYR
3	D	775	SER
3	D	781	LYS
3	D	884	SER
3	D	1148	ARG
3	D	1149	ARG
3	D	1193	TRP
3	D	1227	HIS
3	D	1318	SER
3	D	1341	ARG
3	D	1345	ARG
3	D	1350	ASN
3	D	1372	ARG

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Mol	Chain	Res	Type
4	E	80	LEU
1	F	77	ASP
1	F	117	HIS
1	F	143	ARG
1	F	152	TYR
1	F	158	ARG
1	F	164	ASP
1	G	29	GLU
1	G	77	ASP
1	G	166	ARG
2	H	70	TYR
2	H	80	PHE
2	H	88	ARG
2	H	107	ARG
2	H	199	ASP
2	H	369	MET
2	H	417	SER
2	H	465	ARG
2	H	484	LEU
2	H	514	PHE
2	H	529	ARG
2	H	596	ASP
2	H	645	PHE
2	H	705	GLU
2	H	773	LEU
2	H	807	TRP
2	H	845	LEU
2	H	856	ASN
2	H	944	ARG
2	H	985	GLU
2	H	994	ARG
2	H	1034	ARG
2	H	1042	LEU
2	H	1119	MET
2	H	1238	LEU
2	H	1270	PHE
2	H	1301	ARG
2	H	1304	MET
2	H	1313	HIS
2	H	1332	SER
3	I	8	LEU
3	I	107	LEU

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Mol	Chain	Res	Type
3	I	177	ASP
3	I	188	LEU
3	I	220	ARG
3	I	250	ARG
3	I	259	ARG
3	I	363	LEU
3	I	430	HIS
3	I	532	GLU
3	I	560	ASN
3	I	610	ARG
3	I	678	ARG
3	I	691	ASP
3	I	716	GLN
3	I	772	TYR
3	I	846	GLU
3	I	895	CYS
3	I	1148	ARG
3	I	1149	ARG
3	I	1188	GLU
3	I	1193	TRP
3	I	1194	ARG
3	I	1250	ASP
3	I	1259	GLN
3	I	1341	ARG
3	I	1368	ASP
3	I	1372	ARG
5	X	100	MET
5	X	266	PHE
5	X	400	GLN
5	X	401	PHE
5	X	471	LEU
5	X	489	MET
5	X	495	ARG
5	X	529	GLU
5	X	580	PHE
5	Y	99	ARG
5	Y	136	GLU
5	Y	148	TYR
5	Y	159	SER
5	Y	213	ASP
5	Y	266	PHE
5	Y	385	ARG

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Mol	Chain	Res	Type
5	Y	400	GLN
5	Y	403	ASP
5	Y	471	LEU
5	Y	503	GLU
5	Y	514	ASP
5	Y	580	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	GLN
1	A	127	GLN
1	A	137	ASN
1	B	37	HIS
1	B	268	ASN
1	B	276	HIS
2	C	20	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	688	GLN
2	C	1237	HIS
2	C	1256	GLN
2	C	1268	GLN
3	D	164	GLN
3	D	209	ASN
3	D	465	GLN
3	D	469	HIS
3	D	519	ASN
3	D	545	HIS
3	D	690	ASN
3	D	768	ASN
3	D	771	GLN
3	D	1289	ASN
4	E	15	ASN
1	F	84	ASN
1	G	37	HIS
1	G	84	ASN
1	G	117	HIS
1	G	227	GLN
2	H	517	GLN

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Mol	Chain	Res	Type
2	H	554	HIS
2	H	582	ASN
2	H	688	GLN
2	H	760	ASN
2	H	766	ASN
2	H	834	GLN
2	H	1010	GLN
2	H	1080	ASN
2	H	1108	ASN
2	H	1111	GLN
2	H	1313	HIS
3	I	11	GLN
3	I	153	ASN
3	I	164	GLN
3	I	309	ASN
3	I	488	ASN
3	I	560	ASN
3	I	720	ASN
3	I	768	ASN
3	I	771	GLN
3	I	1197	ASN
3	I	1227	HIS
3	I	1244	GLN
3	I	1289	ASN
4	J	31	GLN
5	X	406	GLN
5	X	446	GLN
5	X	461	ASN
5	Y	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	QZY	D	1501	-	31,37,37	4.21	5 (16%)	36,50,50	1.77	6 (16%)

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	QZY	D	1501	-	-	4/20/26/26	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1501	QZY	C03-C02	21.50	1.59	1.39
6	D	1501	QZY	C03-C04	5.19	1.44	1.37
6	D	1501	QZY	C18-N02	4.83	1.45	1.36
6	D	1501	QZY	C18-N01	4.56	1.45	1.37
6	D	1501	QZY	O04-C18	-2.22	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1501	QZY	C03-C02-N01	-6.10	122.34	130.12
6	D	1501	QZY	N01-C18-N02	4.57	121.12	115.89
6	D	1501	QZY	C02-N01-C18	-4.37	114.21	125.52
6	D	1501	QZY	C09-O03-C12	-3.24	111.23	118.80
6	D	1501	QZY	C20-N02-C19	3.15	120.22	116.54
6	D	1501	QZY	O04-C18-N01	-2.19	118.77	123.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

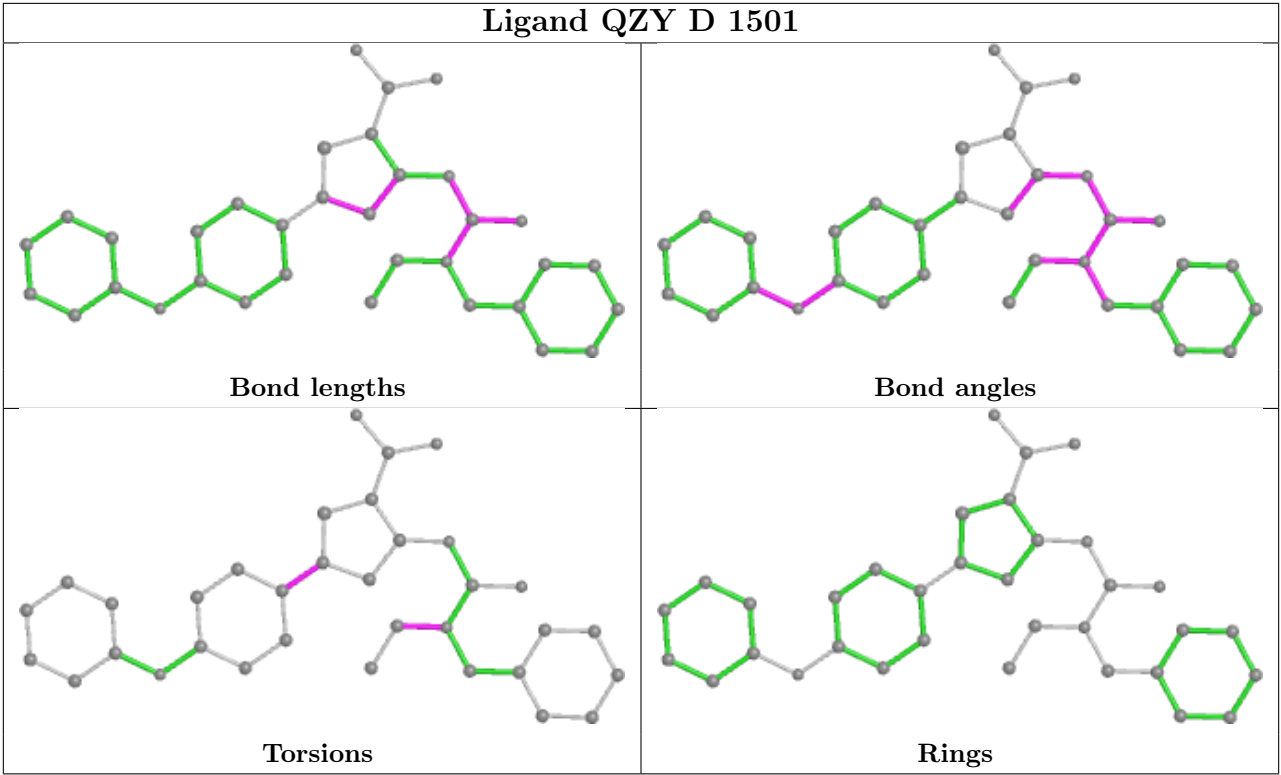
Mol	Chain	Res	Type	Atoms
6	D	1501	QZY	C03-C04-C06-C11
6	D	1501	QZY	C03-C04-C06-C07
6	D	1501	QZY	C28-C19-N02-C18
6	D	1501	QZY	C28-C19-N02-C20

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1501	QZY	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	2:GLN	C	3:GLY	N	3.61

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	234/329 (71%)	-0.30	0 100 100	118, 170, 244, 287	0
1	B	301/329 (91%)	-0.20	2 (0%) 87 82	127, 224, 319, 341	0
1	F	234/329 (71%)	-0.00	6 (2%) 56 45	188, 241, 284, 351	0
1	G	229/329 (69%)	0.36	15 (6%) 18 14	199, 303, 339, 363	0
2	C	1336/1342 (99%)	-0.22	17 (1%) 77 68	95, 160, 263, 327	0
2	H	1336/1342 (99%)	-0.13	38 (2%) 53 42	137, 195, 310, 420	0
3	D	1164/1407 (82%)	-0.25	7 (0%) 89 84	90, 154, 258, 314	0
3	I	1160/1407 (82%)	-0.06	24 (2%) 63 54	130, 203, 302, 360	0
4	E	90/91 (98%)	-0.16	0 100 100	141, 198, 256, 300	0
4	J	76/91 (83%)	0.93	8 (10%) 6 6	277, 333, 432, 451	0
5	X	471/613 (76%)	-0.07	12 (2%) 57 47	135, 226, 364, 410	0
5	Y	475/613 (77%)	-0.05	11 (2%) 60 51	149, 240, 364, 395	0
All	All	7106/8222 (86%)	-0.12	140 (1%) 65 56	90, 194, 319, 451	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	GLN	6.9
2	H	982	GLY	5.9
3	I	11	GLN	5.8
1	F	3	GLY	5.7
2	H	981	ALA	5.5
2	H	999	GLU	5.5
4	J	2	ALA	5.2
2	H	987	GLU	5.2
2	H	998	LEU	4.8
3	I	10	ALA	4.7
1	F	4	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	206	GLU	4.7
2	C	266	GLY	4.6
2	H	983	GLY	4.5
3	I	1203	ARG	4.5
3	I	12	THR	4.5
5	Y	241	SER	4.4
3	I	1169	THR	4.4
1	G	182	ARG	4.3
2	C	645	PHE	3.9
2	C	257	ALA	3.9
1	F	1	MET	3.9
2	H	986	ALA	3.8
1	G	204	GLU	3.8
2	C	282	VAL	3.8
3	I	1168	GLU	3.8
1	G	56	VAL	3.8
2	C	292	ILE	3.7
1	G	181	GLU	3.7
2	H	979	LEU	3.7
5	X	305	LEU	3.5
3	I	13	LYS	3.4
1	G	112	ALA	3.3
2	C	251	ALA	3.2
3	I	1167	LYS	3.2
4	J	75	GLN	3.2
3	I	9	LYS	3.2
2	H	1005	GLU	3.2
5	Y	239	GLY	3.1
1	G	186	ASN	3.1
3	I	1177	ILE	3.1
2	H	1006	GLU	3.1
3	I	1188	GLU	3.1
2	H	996	ARG	3.1
1	B	303	ILE	3.1
2	H	988	LYS	3.0
3	D	1201	GLY	2.9
2	H	266	GLY	2.9
3	D	1203	ARG	2.9
2	H	980	VAL	2.9
2	H	1000	LEU	2.9
2	H	976	ARG	2.9
3	I	855	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
5	X	283	GLN	2.8
2	C	291	TYR	2.8
5	Y	337	VAL	2.8
2	C	265	LYS	2.8
1	G	97	GLU	2.8
2	H	2	VAL	2.8
3	I	732	GLY	2.8
2	C	295	LYS	2.8
3	D	1170	LYS	2.8
3	I	1201	GLY	2.8
2	H	165	HIS	2.8
2	C	260	LYS	2.7
3	D	1133	ASP	2.7
2	C	230	PHE	2.7
1	F	55	ALA	2.7
5	X	239	GLY	2.7
1	G	130	ILE	2.7
5	X	260	ARG	2.7
5	Y	305	LEU	2.7
3	I	1170	LYS	2.7
2	H	985	GLU	2.7
5	Y	315	TRP	2.6
5	X	167	ASP	2.6
5	X	285	ARG	2.6
2	C	252	SER	2.6
2	C	231	GLU	2.6
1	G	90	VAL	2.5
2	H	975	ILE	2.5
2	H	1008	GLN	2.5
4	J	67	ARG	2.5
1	G	24	ALA	2.4
2	H	984	VAL	2.4
4	J	73	GLN	2.4
3	I	1202	GLU	2.4
5	X	315	TRP	2.4
5	Y	319	ALA	2.4
2	H	1180	MET	2.4
2	H	1004	ASP	2.4
2	C	333	ILE	2.4
2	H	995	ASP	2.4
2	H	1017	GLN	2.4
3	D	1177	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
5	Y	165	PHE	2.3
2	C	256	GLU	2.3
2	C	317	LEU	2.3
4	J	74	GLU	2.3
1	G	121	VAL	2.3
5	X	287	ILE	2.3
2	H	1009	ASN	2.3
5	X	325	PRO	2.3
1	B	314	LEU	2.3
1	G	59	VAL	2.3
3	I	1176	VAL	2.3
5	X	328	GLU	2.3
4	J	3	ARG	2.3
2	H	978	VAL	2.3
3	I	1194	ARG	2.3
2	H	265	LYS	2.2
2	H	989	LEU	2.2
5	Y	294	GLN	2.2
2	H	997	TRP	2.2
1	G	205	MET	2.2
4	J	34	GLY	2.2
2	H	1012	GLU	2.2
3	I	1196	LEU	2.2
2	H	1011	LEU	2.2
4	J	76	GLU	2.2
2	H	743	PRO	2.1
5	Y	562	ARG	2.1
5	X	301	ASN	2.1
3	I	848	VAL	2.1
3	D	1171	GLY	2.1
3	I	849	LEU	2.1
1	F	21	SER	2.1
3	I	1187	GLU	2.1
3	D	1188	GLU	2.1
3	I	878	ASP	2.1
2	C	332	ARG	2.1
2	H	175	ARG	2.1
5	X	240	ARG	2.1
5	Y	260	ARG	2.0
1	G	91	ARG	2.0
2	H	1010	GLN	2.0
5	Y	321	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	1013	GLN	2.0
3	I	1215	GLU	2.0
2	H	864	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

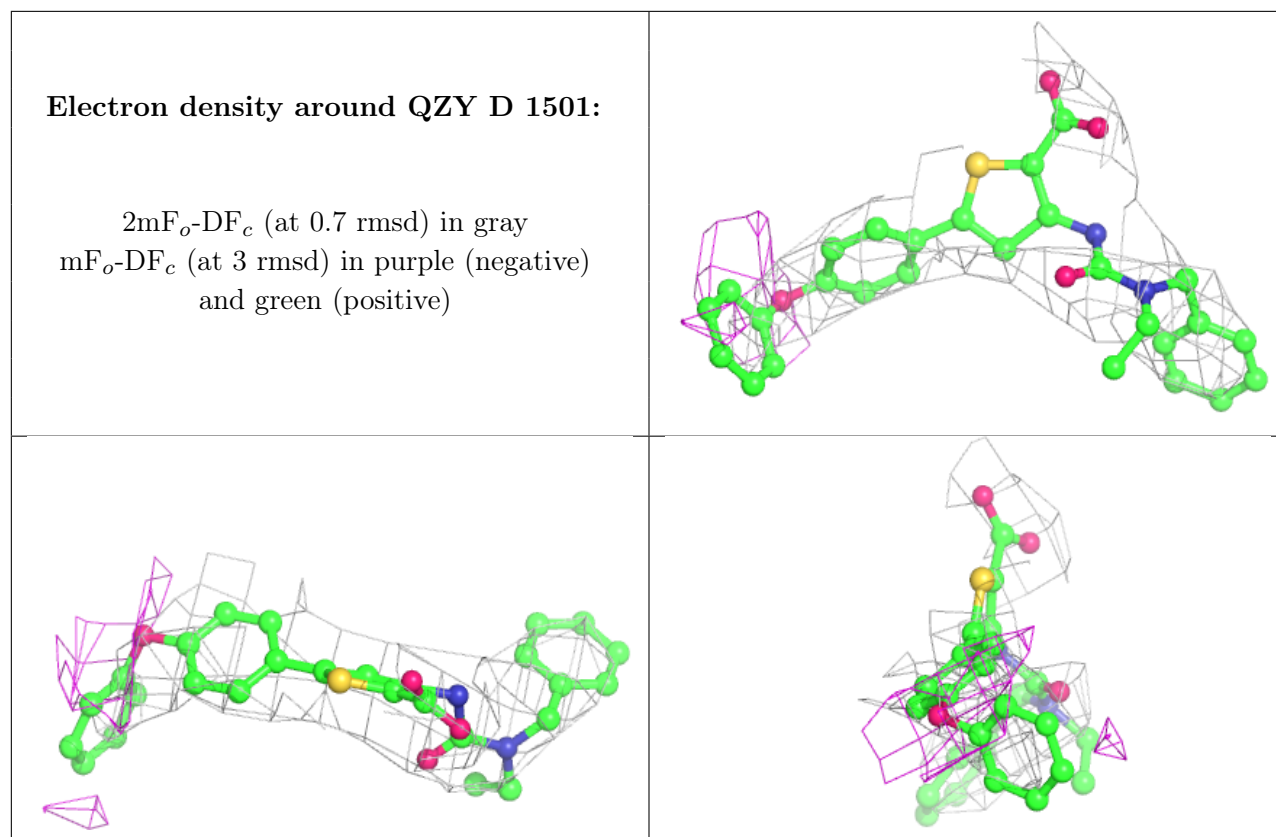
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	QZY	D	1501	34/34	0.84	0.44	112,133,149,170	0
8	MG	I	1503	1/1	0.84	0.33	135,135,135,135	0
7	ZN	D	1503	1/1	0.96	0.37	179,179,179,179	0
7	ZN	I	1502	1/1	0.96	0.20	149,149,149,149	0
8	MG	D	1504	1/1	0.97	0.28	58,58,58,58	0
7	ZN	D	1502	1/1	0.97	0.12	171,171,171,171	0
7	ZN	I	1501	1/1	0.97	0.12	168,168,168,168	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.