



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:25 am BST

PDB ID : 4KN4  
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Benzoxazinorifamycin-2b  
Authors : Murakami, K.S.  
Deposited on : 2013-05-08  
Resolution : 3.96 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

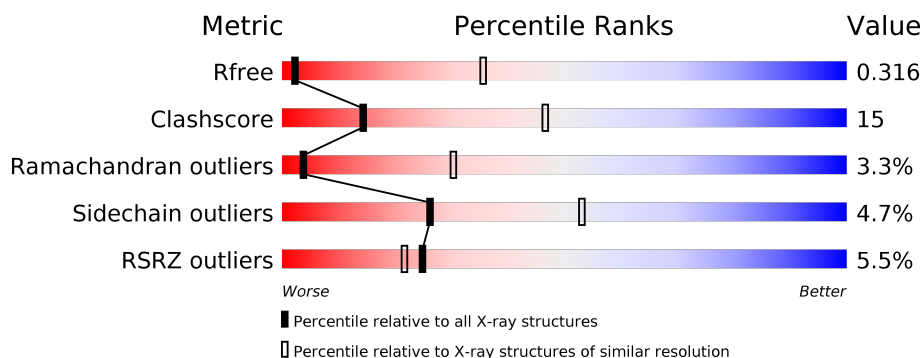
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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  $\geq 3$ , 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	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	
2	H	1342	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1RL	H	1401	-	-	-	X

## 2 Entry composition

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

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

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

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

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

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

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

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

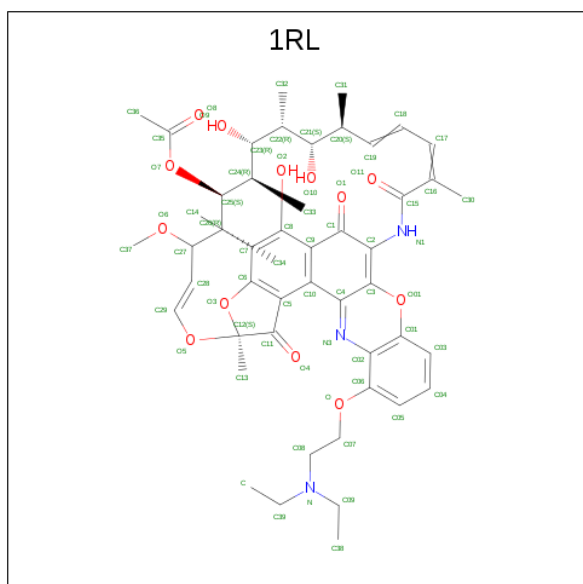
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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

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

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

- Molecule 6 is Benzoxazinorifamycin-2b (three-letter code: 1RL) (formula: C<sub>49</sub>H<sub>61</sub>N<sub>3</sub>O<sub>13</sub>).



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

- Molecule 7 is ZINC ION (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		

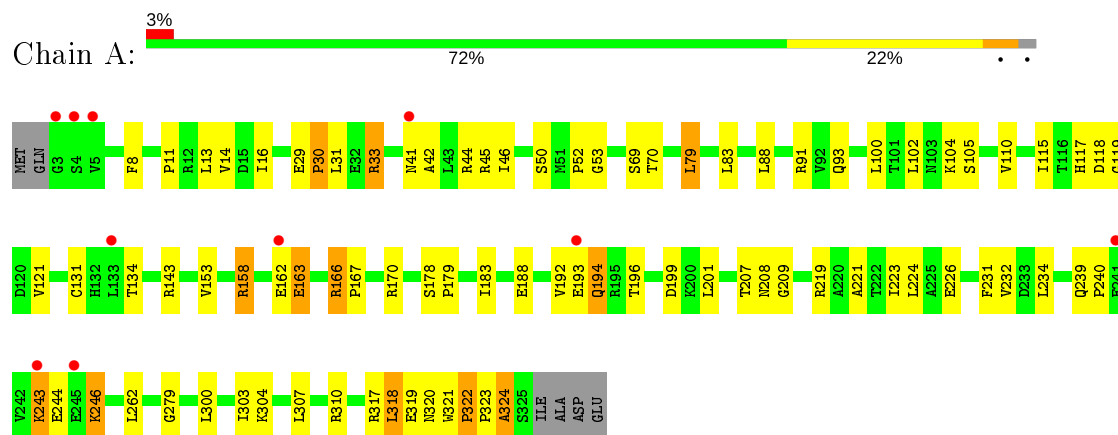
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

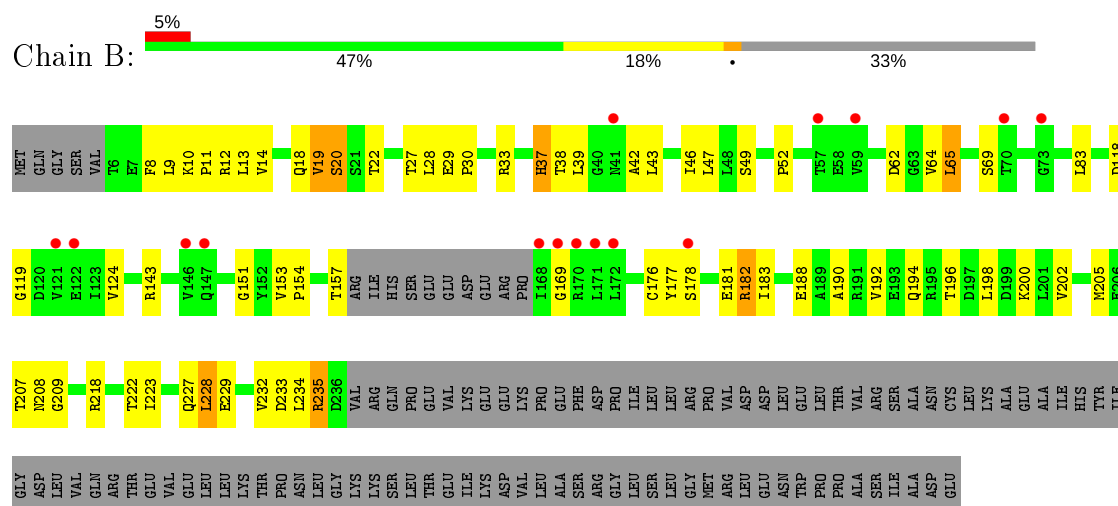
### 3 Residue-property plots [i](#)

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

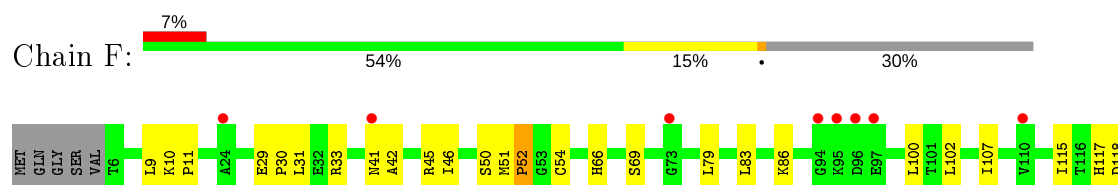
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

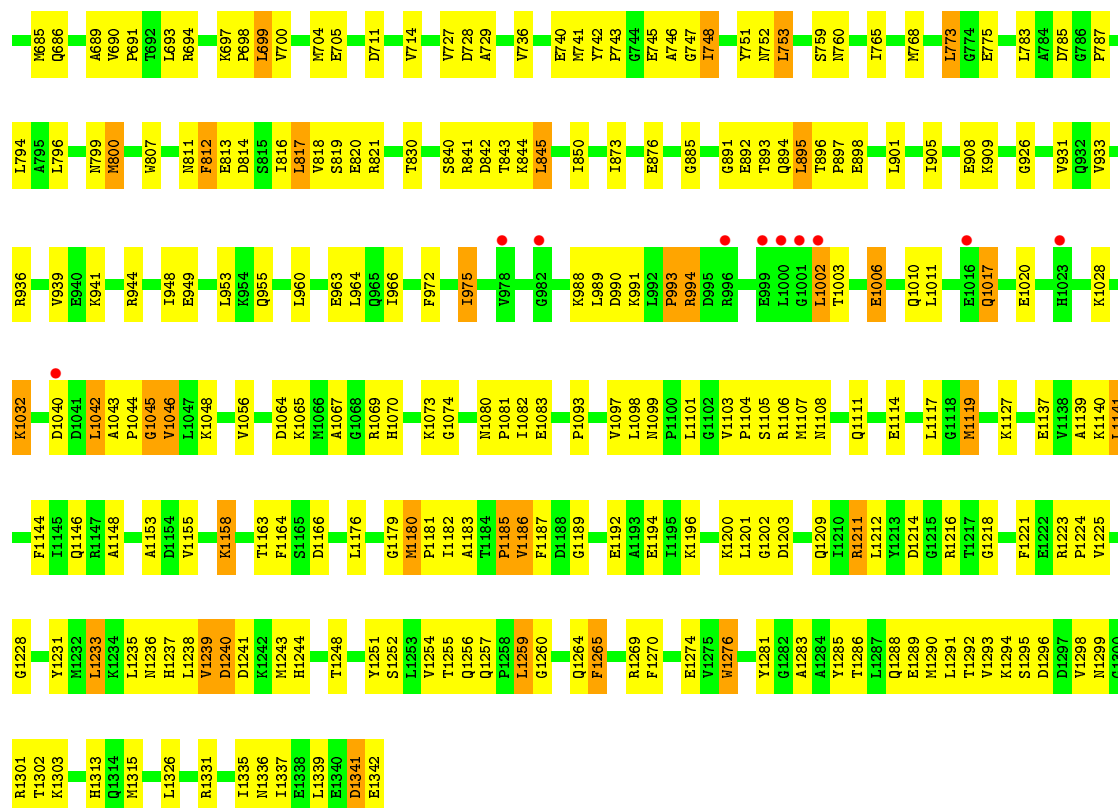


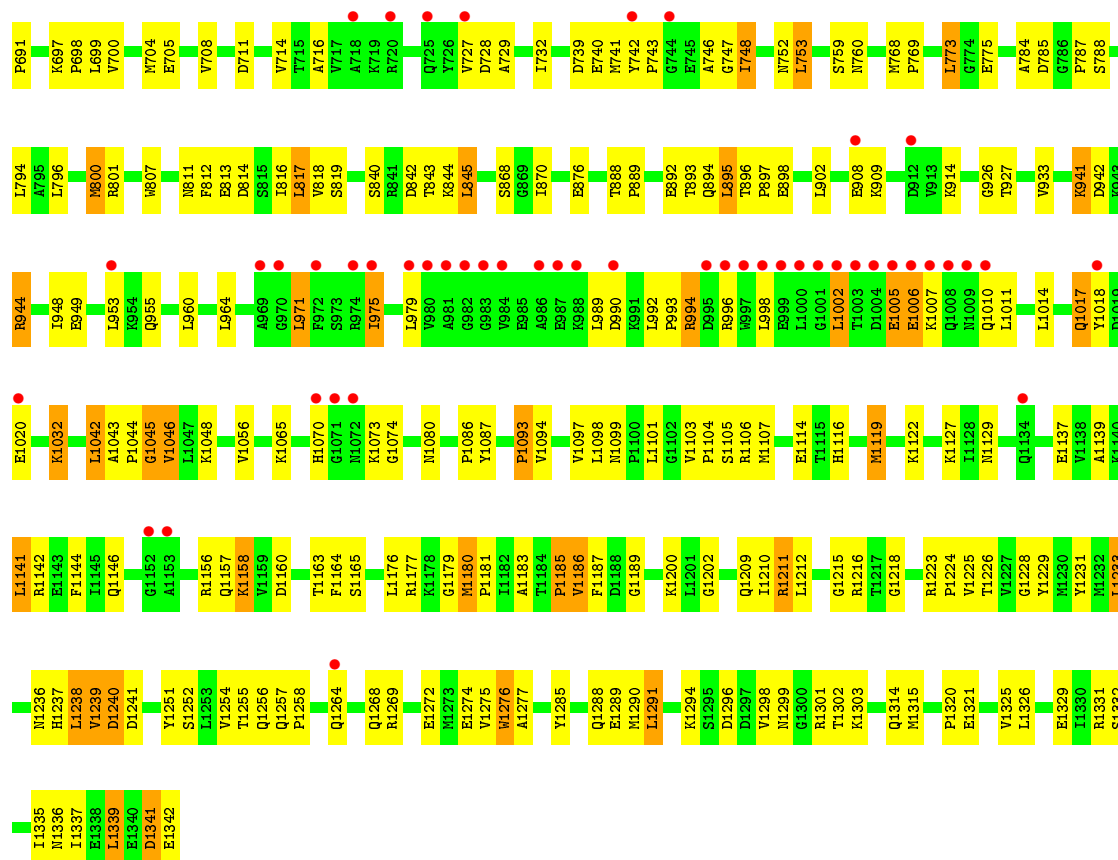
- Molecule 1: DNA-directed RNA polymerase subunit alpha



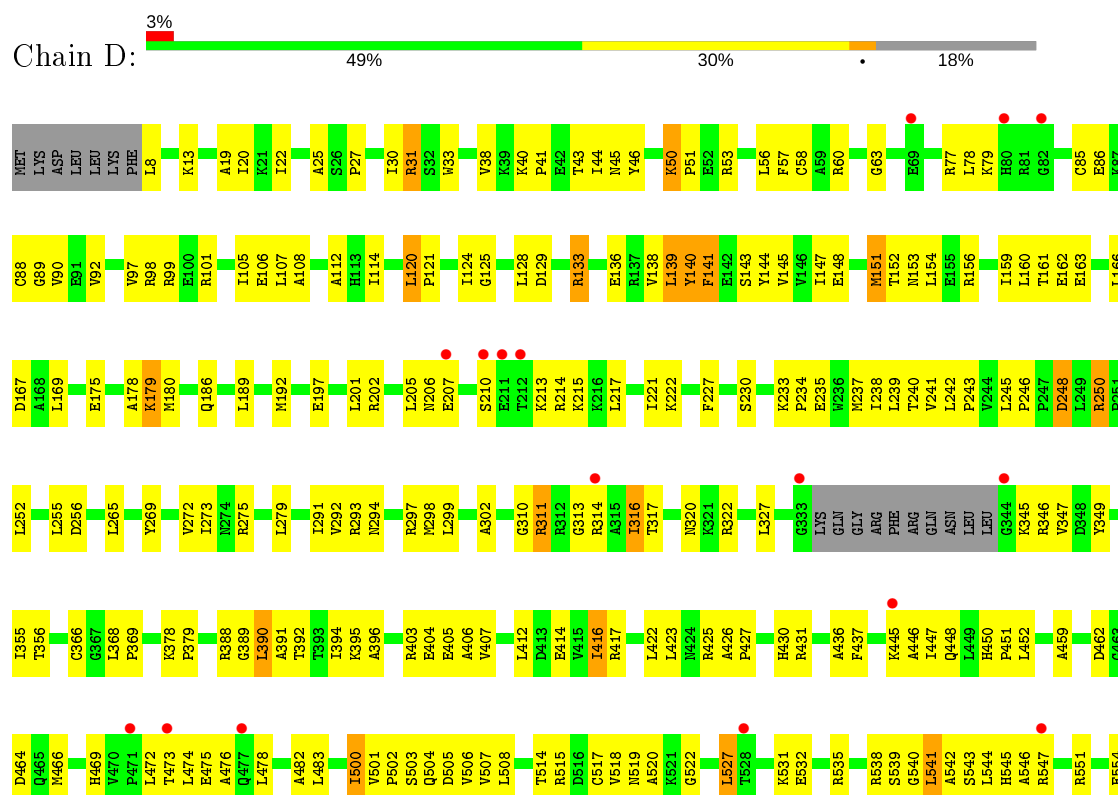


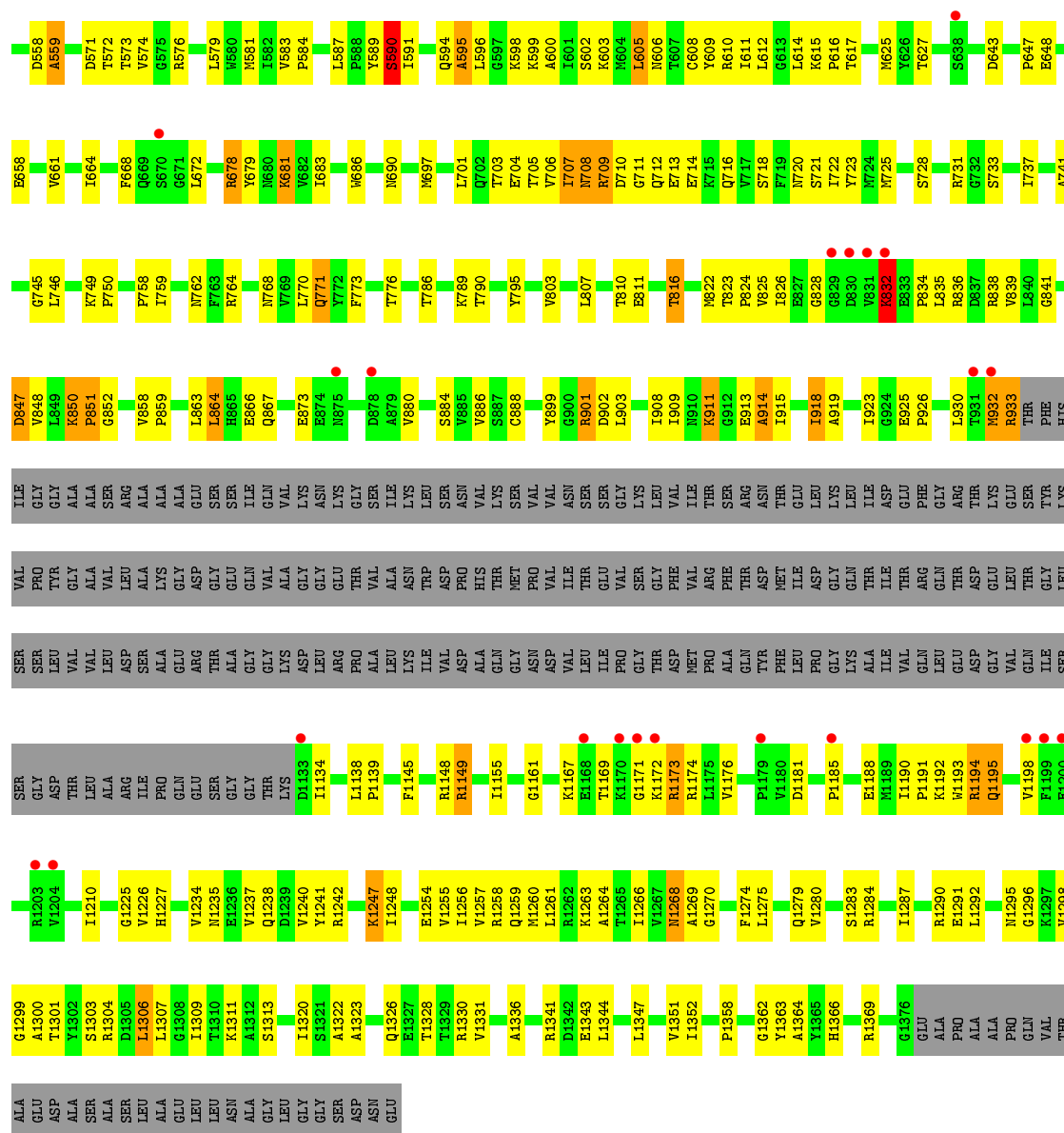




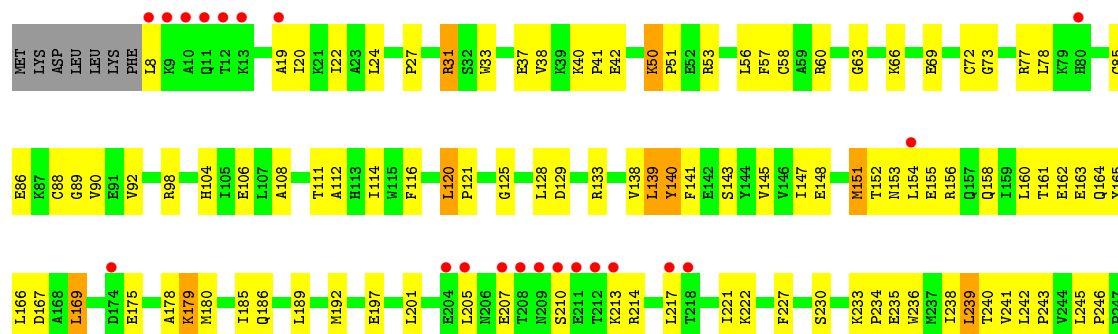


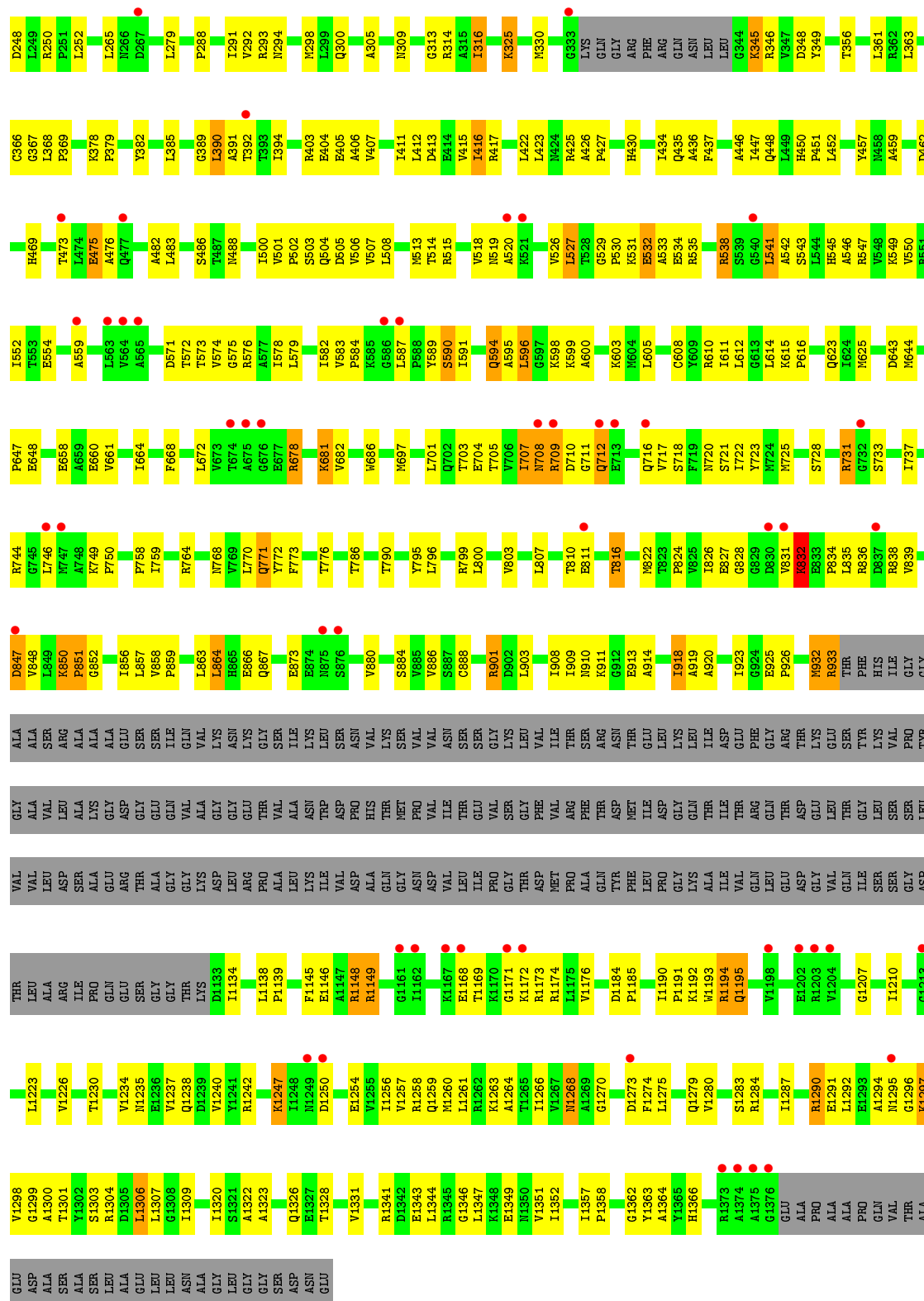
• Molecule 3: DNA-directed RNA polymerase subunit beta'



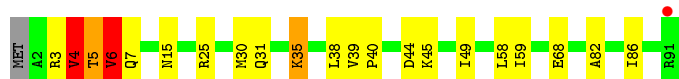


- Molecule 3: DNA-directed RNA polymerase subunit beta'

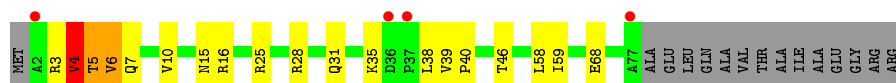




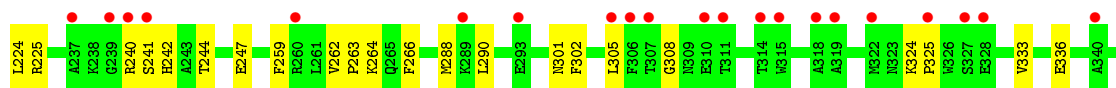
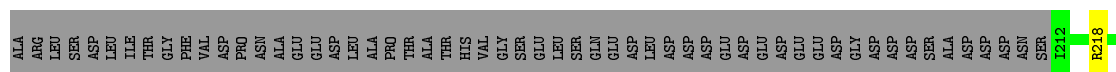
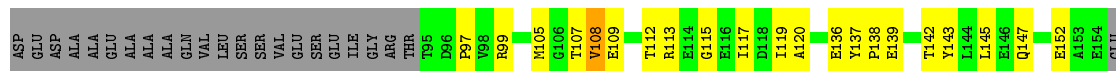
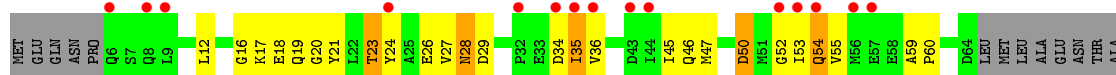
• Molecule 4: DNA-directed RNA polymerase subunit omega



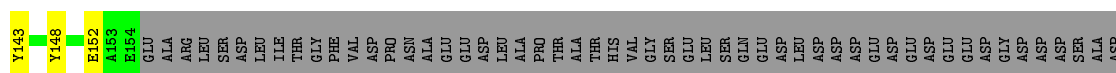
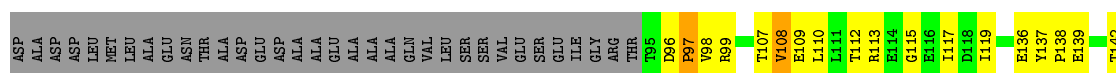
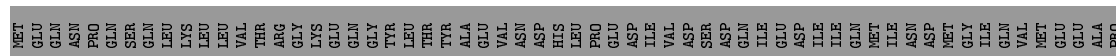
- Molecule 4: DNA-directed RNA polymerase subunit omega

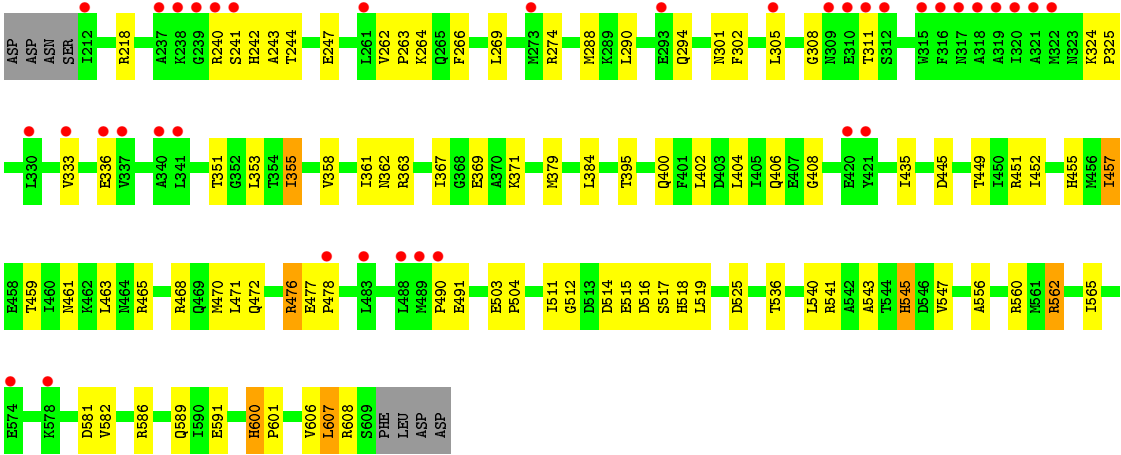


- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.68Å 203.97Å 307.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 3.96 29.77 – 3.96	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.77-3.96) 90.0 (29.77-3.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.251 , 0.315 0.251 , 0.316	Depositor DCC
$R_{free}$ test set	4761 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	151.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	56333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 1RL, 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	0.19	0/2548	0.37	0/3454
1	B	0.19	0/1725	0.40	0/2337
1	F	0.20	0/1797	0.40	0/2436
1	G	0.19	0/1690	0.40	1/2290 (0.0%)
2	C	0.20	0/10690	0.39	0/14423
2	H	0.20	0/10690	0.39	0/14423
3	D	0.20	0/9198	0.40	0/12413
3	I	0.20	0/9198	0.40	0/12413
4	E	0.19	0/710	0.36	0/956
4	J	0.19	0/607	0.36	0/817
5	X	0.20	0/4253	0.37	0/5719
5	Y	0.20	0/3783	0.36	0/5083
All	All	0.20	0/56889	0.39	1/76764 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	228	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	66	0
1	B	1706	0	1738	62	0
1	F	1775	0	1800	40	0
1	G	1671	0	1706	45	0
2	C	10523	0	10546	373	0
2	H	10523	0	10546	344	0
3	D	9060	0	9256	382	0
3	I	9060	0	9255	346	0
4	E	708	0	719	20	0
4	J	605	0	612	16	0
5	X	4198	0	4250	109	0
5	Y	3732	0	3809	74	0
6	C	65	61	61	6	0
6	H	65	61	61	10	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56211	122	56925	1751	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 (1751) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.48	0.92
4:E:5:THR:HA	4:E:6:VAL:CB	2.00	0.90
6:C:1401:1RL:H313	6:C:1401:1RL:H322	1.53	0.90
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.55	0.88
4:J:5:THR:HA	4:J:6:VAL:CB	2.02	0.87
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.03	0.87
2:H:488:MET:HB2	2:H:490:GLN:N	1.89	0.87
2:C:54:ARG:H	2:C:55:SER:HB2	1.38	0.87
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.55	0.86
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.57	0.86
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.56	0.86
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.56	0.85
2:H:487:LEU:CB	2:H:488:MET:HA	2.06	0.84
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.08	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.05	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.60	0.82
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.62	0.82
4:J:5:THR:CA	4:J:6:VAL:HB	2.09	0.82
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.08	0.81
2:H:908:GLU:HG2	2:H:909:LYS:H	1.43	0.81
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.63	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.61	0.80
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.62	0.79
3:D:643:ASP:O	3:D:720:ASN:ND2	2.16	0.79
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.63	0.78
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.64	0.78
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.14	0.78
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.63	0.78
2:H:487:LEU:HB3	2:H:488:MET:CA	2.13	0.77
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.77
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.66	0.77
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.65	0.76
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.67	0.76
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.68	0.76
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.50	0.75
4:E:5:THR:CA	4:E:6:VAL:HB	2.15	0.75
1:G:45:ARG:O	3:I:538:ARG:NH2	2.20	0.75
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.69	0.75
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.75
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:THR:HG21	2:C:135:THR:HG22	1.67	0.74
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.68	0.74
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.69	0.74
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.68	0.74
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.18	0.74
2:H:99:LYS:N	2:H:99:LYS:HD3	2.02	0.73
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.68	0.73
2:H:142:GLU:HG2	2:H:515:MET:SD	2.27	0.73
2:H:54:ARG:N	2:H:55:SER:HB2	2.01	0.73
3:I:850:LYS:O	3:I:852:GLY:N	2.21	0.73
5:X:35:ILE:HG13	5:X:36:VAL:H	1.52	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.54	0.73
2:C:131:THR:CG2	2:C:135:THR:HG22	2.19	0.72
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.71	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.19	0.72
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.25	0.72
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.19	0.72
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.70	0.72
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.71	0.72
1:B:29:GLU:HA	1:B:200:LYS:CB	2.18	0.72
3:D:822:MET:SD	3:D:838:ARG:NH1	2.63	0.72
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.72	0.72
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.23	0.71
3:D:151:MET:N	3:D:151:MET:SD	2.63	0.71
1:G:65:LEU:H	1:G:65:LEU:HD23	1.55	0.71
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.70	0.71
3:D:850:LYS:O	3:D:852:GLY:N	2.22	0.71
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.72	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.72	0.71
2:H:516:ASP:HB2	6:H:1401:1RL:H201	1.73	0.71
2:C:55:SER:CB	2:C:56:VAL:HG22	2.17	0.71
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.72	0.71
2:H:131:THR:CG2	2:H:135:THR:HG22	2.21	0.70
3:D:1362:GLY:O	3:D:1364:ALA:N	2.24	0.70
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.74	0.70
2:C:134:GLY:O	2:C:527:LYS:NZ	2.24	0.70
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.55	0.70
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.27	0.70
2:H:55:SER:CB	2:H:56:VAL:HG22	2.22	0.70
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.57	0.70
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.74	0.69
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.74	0.69
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.22	0.69
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.56	0.69
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.58	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.75	0.69
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.73	0.69
2:C:20:GLN:O	2:C:22:LEU:N	2.25	0.69
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.75	0.69
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.69
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.73	0.69
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.76	0.69
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.57	0.68
3:D:1191:PRO:O	3:D:1193:TRP:N	2.26	0.68
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.57	0.68
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.75	0.68
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.75	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.58	0.68
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.68
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.76	0.68
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.75	0.68
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.68
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.76	0.68
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.75	0.68
3:D:405:GLU:O	3:D:407:VAL:N	2.27	0.68
2:H:664:GLY:O	2:H:686:GLN:NE2	2.27	0.68
3:I:720:ASN:O	3:I:722:ILE:N	2.27	0.68
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.76	0.67
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.76	0.67
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.77	0.67
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.76	0.67
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.29	0.67
3:I:1191:PRO:O	3:I:1193:TRP:N	2.27	0.67
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.29	0.67
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.25	0.67
2:C:54:ARG:CG	2:C:55:SER:HB2	2.25	0.67
2:H:21:VAL:HG13	2:H:22:LEU:H	1.59	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.77	0.67
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:ARG:H	2:H:55:SER:CB	2.05	0.66
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.75	0.66
5:X:240:ARG:HD3	5:X:244:THR:HB	1.75	0.66
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.76	0.66
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.77	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.77	0.66
3:D:245:LEU:O	3:D:250:ARG:NH1	2.29	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
5:X:511:ILE:HG23	5:X:512:GLY:H	1.58	0.66
2:C:529:ARG:CZ	6:C:1401:1RL:H171	2.25	0.66
3:I:139:LEU:HD13	3:I:140:TYR:N	2.11	0.66
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.25	0.66
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.25	0.66
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.61	0.66
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.77	0.66
3:D:610:ARG:HG2	3:D:864:LEU:HD22	1.78	0.66
3:D:711:GLY:O	3:D:712:GLN:HG2	1.95	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.29	0.66
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.11	0.66
3:D:139:LEU:HD13	3:D:140:TYR:N	2.11	0.65
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.77	0.65
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.77	0.65
2:C:54:ARG:N	2:C:55:SER:HB2	2.09	0.65
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.31	0.65
3:D:932:MET:O	3:D:933:ARG:HG3	1.96	0.65
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.78	0.65
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.78	0.65
2:C:402:ARG:NH2	2:C:419:ILE:O	2.30	0.65
3:D:546:ALA:N	3:D:547:ARG:HA	2.11	0.65
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.77	0.65
3:I:643:ASP:O	3:I:720:ASN:ND2	2.21	0.65
2:C:845:LEU:H	2:C:845:LEU:HD13	1.60	0.65
2:H:1239:VAL:O	2:H:1241:ASP:N	2.30	0.65
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.25	0.65
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.77	0.65
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.78	0.65
1:B:12:ARG:H	1:B:30:PRO:HG2	1.60	0.65
1:B:49:SER:HA	1:B:151:GLY:HA2	1.78	0.65
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.97	0.65
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.77	0.65
3:I:546:ALA:N	3:I:547:ARG:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.78	0.65
2:H:127:ILE:HD13	2:H:127:ILE:H	1.62	0.65
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.62	0.65
2:H:131:THR:HG21	2:H:135:THR:HG22	1.76	0.65
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.78	0.65
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.30	0.65
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.79	0.65
3:D:546:ALA:H	3:D:547:ARG:HA	1.61	0.64
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.77	0.64
5:X:476:ARG:H	5:X:476:ARG:HD2	1.62	0.64
2:C:800:MET:HE2	2:C:800:MET:HA	1.78	0.64
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.78	0.64
3:I:546:ALA:H	3:I:547:ARG:HA	1.62	0.64
2:H:845:LEU:H	2:H:845:LEU:HD13	1.62	0.64
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.33	0.64
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.27	0.64
3:I:151:MET:N	3:I:151:MET:SD	2.70	0.64
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.27	0.64
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.78	0.64
3:I:450:HIS:NE2	3:I:625:MET:SD	2.71	0.64
3:I:822:MET:SD	3:I:838:ARG:NH1	2.71	0.64
3:D:720:ASN:O	3:D:722:ILE:N	2.31	0.64
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.80	0.64
2:H:1252:SER:OG	2:H:1255:THR:O	2.15	0.63
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.80	0.63
3:I:711:GLY:O	3:I:712:GLN:HG2	1.99	0.63
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.81	0.63
2:C:660:VAL:HG22	2:C:661:VAL:H	1.62	0.63
3:D:389:GLY:O	3:D:391:ALA:N	2.32	0.63
3:I:1362:GLY:O	3:I:1364:ALA:N	2.31	0.63
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.80	0.63
3:I:709:ARG:O	3:I:711:GLY:N	2.32	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.98	0.63
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.63
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.81	0.63
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.80	0.62
2:C:488:MET:N	2:C:489:PRO:HD3	2.15	0.62
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.81	0.62
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.62
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.25	0.62
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.81	0.62
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.80	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.32	0.62
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.34	0.62
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.32	0.62
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.81	0.62
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.32	0.62
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.62
2:C:54:ARG:H	2:C:55:SER:CB	2.12	0.62
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.62
2:H:459:MET:SD	2:H:511:LEU:HD22	2.40	0.62
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.35	0.62
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.81	0.62
2:H:529:ARG:NE	6:H:1401:1RL:H171	2.15	0.62
2:H:504:GLU:O	2:H:508:SER:HB3	2.00	0.62
5:X:517:SER:O	5:X:518:HIS:ND1	2.32	0.62
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.80	0.62
5:X:457:ILE:O	5:X:461:ASN:ND2	2.33	0.62
3:I:768:ASN:O	3:I:771:GLN:NE2	2.33	0.61
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.35	0.61
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.61
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.82	0.61
4:E:5:THR:HA	4:E:6:VAL:CG1	2.29	0.61
3:I:389:GLY:O	3:I:391:ALA:N	2.33	0.61
2:H:505:PHE:O	2:H:512:SER:OG	2.16	0.61
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.65	0.61
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.30	0.61
1:G:29:GLU:HA	1:G:200:LYS:CB	2.30	0.61
2:H:590:PRO:O	2:H:659:GLN:NE2	2.33	0.61
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.83	0.61
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.83	0.61
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.82	0.61
2:H:99:LYS:H	2:H:99:LYS:HD3	1.65	0.61
3:D:316:ILE:HG23	3:D:317:THR:H	1.66	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.15	0.61
5:X:139:GLU:HA	5:X:142:THR:HG22	1.82	0.61
2:C:768:MET:O	2:C:785:ASP:N	2.33	0.61
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.81	0.61
3:I:145:VAL:HG22	3:I:180:MET:SD	2.40	0.61
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.81	0.61
2:C:189:ASP:OD1	2:C:193:ASN:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.61
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.16	0.61
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.83	0.60
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.84	0.60
2:C:1200:LYS:O	2:C:1202:GLY:N	2.33	0.60
2:C:127:ILE:HD13	2:C:127:ILE:H	1.67	0.60
2:C:119:GLU:CD	2:C:489:PRO:HG2	2.22	0.60
3:D:1149:ARG:H	3:D:1149:ARG:HD3	1.65	0.60
3:D:120:LEU:CB	3:D:121:PRO:CD	2.78	0.60
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.82	0.60
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.84	0.60
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.37	0.60
2:H:163:LYS:HD3	2:H:163:LYS:H	1.66	0.60
3:I:589:TYR:O	3:I:591:ILE:N	2.35	0.60
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.83	0.60
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.84	0.60
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.31	0.60
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.35	0.60
3:D:79:LYS:HE3	5:X:569:THR:N	2.17	0.60
1:G:227:GLN:C	1:G:228:LEU:HD23	2.21	0.60
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.35	0.60
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.84	0.60
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.82	0.60
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.32	0.60
2:H:660:VAL:HG22	2:H:661:VAL:H	1.65	0.60
2:H:768:MET:O	2:H:785:ASP:N	2.35	0.60
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.32	0.59
6:H:1401:1RL:O9	6:H:1401:1RL:O10	2.17	0.59
3:I:405:GLU:O	3:I:407:VAL:N	2.35	0.59
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.32	0.59
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.84	0.59
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.38	0.59
3:D:546:ALA:H	3:D:547:ARG:CA	2.14	0.59
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.36	0.59
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.84	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.33	0.59
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.59
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.35	0.59
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.38	0.59
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.85	0.59
2:C:309:LEU:HD23	2:C:309:LEU:H	1.68	0.59
3:D:56:LEU:O	3:D:250:ARG:NH2	2.36	0.59
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.67	0.59
3:I:88:CYS:O	3:I:90:VAL:N	2.36	0.59
5:X:240:ARG:O	5:X:242:HIS:N	2.35	0.59
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.67	0.59
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.85	0.59
2:C:752:ASN:O	2:C:753:LEU:HG	2.03	0.59
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.85	0.59
2:C:143:ARG:NH1	2:C:512:SER:O	2.36	0.58
2:H:20:GLN:O	2:H:22:LEU:N	2.36	0.58
2:H:309:LEU:HD23	2:H:309:LEU:H	1.68	0.58
3:I:1173:ARG:HB3	3:I:1174:ARG:O	2.02	0.58
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.38	0.58
3:I:514:THR:HG23	3:I:576:ARG:HE	1.68	0.58
3:I:828:GLY:HA2	3:I:832:LYS:N	2.18	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.33	0.58
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.38	0.58
3:D:316:ILE:HG13	3:D:317:THR:N	2.18	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.85	0.58
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.68	0.58
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.03	0.58
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.85	0.58
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.38	0.58
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.28	0.58
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.36	0.58
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.34	0.58
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.33	0.58
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.21	0.58
2:C:660:VAL:O	2:C:661:VAL:HG22	2.03	0.58
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.16	0.58
3:D:932:MET:SD	3:D:932:MET:N	2.74	0.58
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.86	0.58
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.85	0.58
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.58
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.34	0.58
2:C:142:GLU:HG2	2:C:515:MET:SD	2.43	0.58
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.03	0.58
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.86	0.58
5:X:584:ARG:O	5:X:587:ILE:HG22	2.04	0.58
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.37	0.58
3:I:827:GLU:O	3:I:831:VAL:HG12	2.03	0.58
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.39	0.58
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.36	0.58
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.39	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.69	0.58
2:C:106:GLU:N	2:C:107:ARG:HA	2.18	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.23	0.57
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.84	0.57
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.86	0.57
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.39	0.57
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.18	0.57
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.86	0.57
2:C:510:GLN:O	2:C:511:LEU:HB2	2.04	0.57
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.34	0.57
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.04	0.57
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.57
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.69	0.57
2:C:526:HIS:HA	2:C:529:ARG:NH1	2.19	0.57
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.85	0.57
2:H:106:GLU:N	2:H:107:ARG:HA	2.19	0.57
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.70	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.34	0.57
3:D:316:ILE:HG23	3:D:317:THR:N	2.19	0.57
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.38	0.57
2:H:54:ARG:CG	2:H:55:SER:HB2	2.34	0.57
3:I:828:GLY:HA2	3:I:832:LYS:H	1.69	0.57
2:C:1252:SER:OG	2:C:1255:THR:O	2.21	0.57
2:H:38:PHE:O	2:H:39:ILE:HB	2.05	0.57
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.20	0.57
1:A:207:THR:OG1	1:A:208:ASN:N	2.38	0.57
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.86	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.35	0.57
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.40	0.57
2:H:531:SER:OG	6:H:1401:1RL:O2	2.20	0.57
3:I:546:ALA:H	3:I:547:ARG:CA	2.17	0.57
3:I:583:VAL:HG13	3:I:584:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.86	0.57
1:B:227:GLN:O	1:B:228:LEU:HG	2.04	0.57
2:C:740:GLU:HB2	2:C:741:MET:SD	2.44	0.57
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.85	0.57
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.35	0.56
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.34	0.56
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.69	0.56
3:D:573:THR:HG22	3:D:576:ARG:CD	2.34	0.56
3:I:197:GLU:O	3:I:201:LEU:HD23	2.05	0.56
1:B:65:LEU:HD23	1:B:65:LEU:H	1.69	0.56
3:D:546:ALA:HB3	3:D:547:ARG:O	2.05	0.56
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.19	0.56
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.04	0.56
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.38	0.56
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.35	0.56
2:C:741:MET:SD	2:C:741:MET:N	2.78	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.21	0.56
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.87	0.56
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.05	0.56
2:C:1255:THR:O	2:C:1257:GLN:N	2.36	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.28	0.56
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.87	0.56
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.20	0.56
3:D:128:LEU:HA	3:D:192:MET:HE1	1.87	0.56
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.33	0.56
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.37	0.56
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.85	0.56
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.21	0.56
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.36	0.56
3:I:545:HIS:HB2	3:I:546:ALA:HA	1.86	0.56
2:H:488:MET:HE3	2:H:489:PRO:HA	1.88	0.56
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.86	0.56
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.70	0.56
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.88	0.56
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.88	0.56
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.41	0.56
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.06	0.56
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.26	0.56
2:H:170:VAL:HG23	2:H:171:LEU:H	1.70	0.56
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.36	0.56
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.88	0.56
3:I:120:LEU:CB	3:I:121:PRO:CD	2.83	0.56
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.88	0.56
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.88	0.56
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.39	0.56
1:A:42:ALA:O	1:A:46:ILE:HG12	2.06	0.56
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.36	0.56
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.06	0.56
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.87	0.55
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.24	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.87	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.31	0.55
5:X:445:ASP:N	5:X:445:ASP:OD1	2.39	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.39	0.55
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.88	0.55
2:C:1141:LEU:HD13	2:C:1141:LEU:H	1.72	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.89	0.55
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.89	0.55
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.21	0.55
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.88	0.55
3:D:697:MET:SD	3:D:741:ALA:HB3	2.47	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.42	0.55
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.31	0.55
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.88	0.55
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.06	0.55
2:H:540:ARG:NH2	2:H:568:ASN:OD1	2.40	0.55
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.89	0.55
2:H:747:GLY:O	2:H:748:ILE:HG13	2.06	0.55
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.88	0.55
3:I:918:ILE:HD13	3:I:919:ALA:N	2.22	0.55
5:X:363:ARG:O	5:X:367:ILE:HG12	2.07	0.55
5:Y:355:ILE:O	5:Y:355:ILE:HD13	2.07	0.55
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.08	0.54
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.72	0.54
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.89	0.54
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.37	0.54
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.89	0.54
1:F:9:LEU:O	1:G:227:GLN:NE2	2.40	0.54
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.88	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.89	0.54
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.22	0.54
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.40	0.54
2:C:894:GLN:O	2:C:895:LEU:HB2	2.07	0.54
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.37	0.54
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.89	0.54
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.38	0.54
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.38	0.54
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.41	0.54
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.21	0.54
3:I:77:ARG:HG3	3:I:78:LEU:H	1.72	0.54
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.89	0.54
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.90	0.54
1:A:91:ARG:NH2	1:A:209:GLY:O	2.40	0.54
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.89	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.90	0.54
3:I:473:THR:HB	3:I:476:ALA:HB2	1.90	0.54
2:C:681:MET:O	2:C:685:MET:HG2	2.07	0.54
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.73	0.54
3:D:858:VAL:HB	3:D:859:PRO:CD	2.29	0.54
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.90	0.54
2:C:496:LYS:N	2:C:497:PRO:HD2	2.21	0.54
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.54
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.40	0.54
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.89	0.54
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.08	0.54
3:D:316:ILE:HG13	3:D:317:THR:H	1.72	0.54
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.90	0.54
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.90	0.54
2:H:488:MET:HB2	2:H:489:PRO:CA	2.38	0.54
5:X:503:GLU:N	5:X:504:PRO:HA	2.22	0.54
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.89	0.54
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.90	0.54
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.88	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.89	0.54
2:H:143:ARG:NH1	2:H:512:SER:O	2.41	0.54
2:C:562:GLU:HG2	2:C:574:SER:CB	2.38	0.53
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.89	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.88	0.53
2:H:21:VAL:HG13	2:H:22:LEU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
2:H:800:MET:HE2	2:H:800:MET:HA	1.88	0.53
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.37	0.53
3:I:681:LYS:NZ	3:I:681:LYS:HB2	2.22	0.53
2:C:397:LEU:O	2:C:398:SER:OG	2.21	0.53
3:D:88:CYS:O	3:D:90:VAL:N	2.42	0.53
2:H:514:PHE:O	6:H:1401:1RL:H321	2.09	0.53
3:I:152:THR:O	3:I:154:LEU:N	2.40	0.53
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.90	0.53
2:C:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.90	0.53
3:D:422:LEU:HA	3:D:436:ALA:HA	1.89	0.53
3:D:85:CYS:HB3	3:D:88:CYS:O	2.08	0.53
3:I:227:PHE:O	3:I:230:SER:OG	2.18	0.53
3:I:824:PRO:O	3:I:826:ILE:HG13	2.08	0.53
1:B:64:VAL:HG13	1:B:69:SER:OG	2.08	0.53
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.90	0.53
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.42	0.53
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.07	0.53
3:D:545:HIS:HB2	3:D:546:ALA:HA	1.91	0.53
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.89	0.53
3:I:546:ALA:HB3	3:I:547:ARG:O	2.09	0.53
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.42	0.53
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.20	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.42	0.53
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.89	0.53
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.08	0.53
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.91	0.53
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.90	0.53
2:C:55:SER:HB3	2:C:56:VAL:CB	2.38	0.53
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.90	0.53
5:X:580:PHE:O	5:X:582:VAL:N	2.42	0.53
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.41	0.53
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.91	0.53
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.23	0.53
3:D:1173:ARG:HB3	3:D:1174:ARG:O	2.08	0.53
3:D:608:CYS:O	3:D:612:LEU:HB2	2.09	0.53
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.91	0.53
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:ILE:HD11	3:D:1320:ILE:HD11	1.90	0.53
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.24	0.53
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.90	0.53
1:B:151:GLY:O	1:B:177:TYR:HB2	2.09	0.53
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.39	0.53
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.90	0.53
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.41	0.53
5:X:355:ILE:HD13	5:X:355:ILE:O	2.08	0.53
5:X:35:ILE:HG23	5:X:36:VAL:N	2.24	0.53
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.08	0.52
3:D:546:ALA:N	3:D:547:ARG:CA	2.70	0.52
3:D:768:ASN:O	3:D:771:GLN:NE2	2.42	0.52
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.90	0.52
5:X:515:GLU:N	5:X:516:ASP:HA	2.24	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.09	0.52
2:C:975:ILE:HD13	2:C:975:ILE:O	2.08	0.52
2:H:840:SER:OG	2:H:1048:LYS:O	2.27	0.52
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.74	0.52
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.90	0.52
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.45	0.52
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.24	0.52
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.52
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.44	0.52
2:C:660:VAL:HG22	2:C:661:VAL:N	2.25	0.52
2:C:690:VAL:HG11	2:C:830:THR:HG21	1.91	0.52
3:D:77:ARG:HG3	3:D:78:LEU:H	1.74	0.52
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.44	0.52
2:H:9:LYS:HD3	2:H:9:LYS:N	2.24	0.52
3:I:508:LEU:O	3:I:508:LEU:HD23	2.09	0.52
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.91	0.52
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.90	0.52
2:C:728:ASP:OD2	2:C:729:ALA:N	2.42	0.52
3:D:227:PHE:O	3:D:230:SER:OG	2.19	0.52
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.91	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.52
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.90	0.52
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.74	0.52
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.91	0.52
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.90	0.52
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.52
2:C:1251:TYR:O	5:X:525:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD23	1:B:65:LEU:N	2.25	0.52
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.45	0.52
3:D:1290:ARG:NH1	3:D:1296:GLY:O	2.43	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.90	0.52
5:X:600:HIS:H	5:X:601:PRO:CD	2.22	0.52
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.43	0.52
1:B:42:ALA:O	1:B:46:ILE:HG12	2.10	0.52
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.91	0.52
2:C:540:ARG:NH2	2:C:568:ASN:OD1	2.43	0.52
2:C:690:VAL:HG13	2:C:691:PRO:HD2	1.90	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.42	0.52
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.92	0.52
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.90	0.52
5:X:112:THR:HG22	5:X:113:ARG:H	1.74	0.52
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.40	0.52
2:C:590:PRO:O	2:C:659:GLN:NE2	2.41	0.52
2:C:72:SER:O	2:C:98:VAL:HG23	2.10	0.52
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.92	0.52
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.91	0.52
2:H:896:THR:HG23	2:H:897:PRO:HD2	1.91	0.52
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.24	0.52
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.92	0.52
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.92	0.52
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.92	0.52
2:C:528:ARG:NH2	2:C:576:SER:O	2.43	0.52
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.91	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.43	0.52
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	1.92	0.52
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.52
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.45	0.52
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.43	0.52
2:C:539:THR:O	2:C:540:ARG:HG3	2.10	0.52
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.92	0.51
2:H:131:THR:HG22	2:H:135:THR:HG22	1.92	0.51
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.40	0.51
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.91	0.51
5:X:600:HIS:H	5:X:601:PRO:HD2	1.74	0.51
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.92	0.51
1:G:49:SER:HA	1:G:151:GLY:HA2	1.92	0.51
2:H:1268:GLN:O	3:I:346:ARG:HA	2.10	0.51
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.40	0.51
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.51
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.41	0.51
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.41	0.51
3:I:515:ARG:NH2	3:I:718:SER:O	2.44	0.51
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.51
2:C:840:SER:OG	2:C:1048:LYS:O	2.27	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.92	0.51
3:D:514:THR:HG21	3:D:595:ALA:O	2.10	0.51
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.93	0.51
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.43	0.51
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.10	0.51
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.44	0.51
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.34	0.51
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.92	0.51
2:H:519:ASN:ND2	2:H:689:ALA:O	2.44	0.51
2:C:694:ARG:NH2	2:C:768:MET:SD	2.84	0.51
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.25	0.51
3:D:828:GLY:HA2	3:D:832:LYS:H	1.74	0.51
4:E:5:THR:HA	4:E:6:VAL:HG12	1.92	0.51
2:H:403:MET:HG3	2:H:414:ILE:HB	1.93	0.51
1:B:19:VAL:O	1:B:20:SER:HB3	2.10	0.51
2:C:127:ILE:HD13	2:C:127:ILE:N	2.26	0.51
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.93	0.51
1:A:79:LEU:O	1:A:83:LEU:HD13	2.11	0.51
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.40	0.51
3:D:451:PRO:HG2	3:D:625:MET:SD	2.50	0.51
1:G:118:ASP:OD1	1:G:119:GLY:N	2.43	0.51
2:H:528:ARG:NH2	2:H:576:SER:O	2.44	0.51
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.51
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.40	0.51
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.92	0.51
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.41	0.51
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.91	0.51
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.41	0.51
5:X:301:ASN:O	5:X:305:LEU:HD13	2.11	0.51
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.46	0.50
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.41	0.50
2:H:134:GLY:O	2:H:527:LYS:NZ	2.44	0.50
2:H:660:VAL:HG22	2:H:661:VAL:N	2.27	0.50
2:H:800:MET:CE	2:H:800:MET:HA	2.40	0.50
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.40	0.50
3:D:125:GLY:O	3:D:129:ASP:N	2.43	0.50
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.75	0.50
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.50
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.41	0.50
3:I:1290:ARG:NH1	3:I:1296:GLY:O	2.43	0.50
3:I:390:LEU:HD21	3:I:407:VAL:HG11	1.94	0.50
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.50
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.12	0.50
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.50
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.77	0.50
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.50
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.93	0.50
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.45	0.50
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.92	0.50
5:X:525:ASP:OD1	5:X:527:THR:HG22	2.11	0.50
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.92	0.50
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.93	0.50
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.76	0.50
2:H:514:PHE:HB2	6:H:1401:1RL:O8	2.12	0.50
2:H:521:LEU:CD2	2:H:686:GLN:HB3	2.42	0.50
2:H:753:LEU:HD12	2:H:753:LEU:O	2.11	0.50
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.26	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.42	0.50
4:J:3:ARG:O	4:J:4:VAL:HG13	2.11	0.50
2:C:1107:MET:N	2:C:1107:MET:SD	2.85	0.50
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.94	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.93	0.50
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.41	0.50
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.46	0.50
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.94	0.50
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.51	0.50
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.12	0.50
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.94	0.50
3:I:356:THR:O	3:I:448:GLN:HA	2.11	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.92	0.50
2:C:511:LEU:HD12	6:C:1401:1RL:H141	1.93	0.50
2:C:892:GLU:O	2:C:893:THR:OG1	2.24	0.50
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.92	0.50
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.46	0.50
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.45	0.50
2:H:740:GLU:HB2	2:H:741:MET:SD	2.51	0.50
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.93	0.50
3:I:773:PHE:O	3:I:776:THR:HG22	2.12	0.50
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.11	0.50
2:C:21:VAL:HG13	2:C:22:LEU:N	2.27	0.50
2:C:800:MET:HA	2:C:800:MET:CE	2.41	0.50
2:C:876:GLU:N	2:C:876:GLU:OE2	2.45	0.50
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.26	0.50
3:D:590:SER:O	3:D:594:GLN:N	2.44	0.50
3:D:810:THR:OG1	3:D:811:GLU:N	2.44	0.50
4:E:45:LYS:O	4:E:49:ILE:HG12	2.12	0.50
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.27	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
2:H:975:ILE:HD13	2:H:975:ILE:O	2.11	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.94	0.50
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.42	0.50
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.12	0.50
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.42	0.50
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.42	0.50
2:H:1107:MET:N	2:H:1107:MET:SD	2.85	0.50
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.27	0.50
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.44	0.49
3:D:356:THR:O	3:D:448:GLN:HA	2.12	0.49
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.45	0.49
2:H:487:LEU:HB3	2:H:488:MET:CG	2.40	0.49
3:D:546:ALA:H	3:D:547:ARG:C	2.15	0.49
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.47	0.49
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.94	0.49
3:D:213:LYS:O	3:D:217:LEU:HG	2.11	0.49
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.41	0.49
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.73	0.49
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	1.94	0.49
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.77	0.49
1:A:192:VAL:O	1:A:194:GLN:N	2.44	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.95	0.49
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.94	0.49
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.27	0.49
1:F:11:PRO:CG	1:G:228:LEU:H	2.26	0.49
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.25	0.49
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.47	0.49
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.47	0.49
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.76	0.49
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.28	0.49
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.94	0.49
1:A:310:ARG:HA	1:A:310:ARG:HE	1.76	0.49
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.42	0.49
1:G:227:GLN:O	1:G:229:GLU:N	2.45	0.49
3:I:125:GLY:O	3:I:129:ASP:N	2.45	0.49
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.43	0.49
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.94	0.49
2:H:697:LYS:HG3	2:H:698:PRO:HD2	1.94	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.12	0.49
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.94	0.49
3:D:85:CYS:SG	3:D:86:GLU:N	2.85	0.49
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.43	0.49
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.76	0.49
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.27	0.49
2:H:1251:TYR:O	5:Y:525:ASP:N	2.45	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
3:I:316:ILE:N	3:I:316:ILE:HD13	2.28	0.49
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.94	0.49
1:A:134:THR:HG21	2:C:727:VAL:HG23	1.95	0.49
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.49
2:C:897:PRO:HB3	5:X:564:GLY:O	2.13	0.49
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.49
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.12	0.49
3:I:147:ILE:HG23	3:I:156:ARG:C	2.33	0.49
5:Y:240:ARG:O	5:Y:242:HIS:N	2.46	0.49
5:Y:477:GLU:N	5:Y:477:GLU:OE1	2.44	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.46	0.49
1:B:118:ASP:OD1	1:B:119:GLY:N	2.45	0.49
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.95	0.49
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.49
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.43	0.49
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.93	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.13	0.48
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.43	0.48
3:D:545:HIS:HB2	3:D:546:ALA:CA	2.42	0.48
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.95	0.48
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.93	0.48
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.28	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.28	0.48
2:C:1276:TRP:HE3	2:C:1276:TRP:HA	1.79	0.48
2:C:572:ILE:HD13	6:C:1401:1RL:O1	2.12	0.48
2:C:403:MET:HG3	2:C:414:ILE:HB	1.95	0.48
3:D:807:LEU:O	3:D:807:LEU:HD12	2.12	0.48
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.95	0.48
3:I:919:ALA:O	3:I:923:ILE:HG12	2.14	0.48
2:C:1276:TRP:CE3	2:C:1276:TRP:HA	2.49	0.48
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.28	0.48
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.45	0.48
2:H:548:ARG:NH2	2:H:567:PRO:O	2.46	0.48
2:H:876:GLU:N	2:H:876:GLU:OE2	2.46	0.48
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.95	0.48
3:I:239:LEU:HD12	3:I:239:LEU:O	2.13	0.48
5:X:561:MET:SD	5:X:576:VAL:HG22	2.53	0.48
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.95	0.48
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.48
2:C:57:PHE:CE1	2:C:475:VAL:HG11	2.48	0.48
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.79	0.48
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.95	0.48
3:D:50:LYS:NZ	3:D:50:LYS:HB3	2.28	0.48
2:H:127:ILE:HD13	2:H:127:ILE:N	2.27	0.48
2:H:514:PHE:HB2	6:H:1401:1RL:C35	2.44	0.48
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.95	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.29	0.48
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
3:D:147:ILE:HG13	3:D:148:GLU:N	2.28	0.48
1:F:118:ASP:OD1	1:F:119:GLY:N	2.46	0.48
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.95	0.48
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.14	0.48
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.48
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.43	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.14	0.48
3:D:500:ILE:H	3:D:500:ILE:HD13	1.79	0.48
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.95	0.48
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.49	0.48
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.96	0.48
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.14	0.48
2:C:490:GLN:O	5:X:472:GLN:HG3	2.13	0.48
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.94	0.48
3:D:473:THR:HB	3:D:476:ALA:HB2	1.96	0.48
3:D:786:THR:O	3:D:790:THR:HG23	2.12	0.48
2:H:484:LEU:H	2:H:484:LEU:HD22	1.78	0.48
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.95	0.48
3:I:128:LEU:HD12	3:I:192:MET:CE	2.44	0.48
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.49	0.48
3:I:85:CYS:HB3	3:I:88:CYS:O	2.14	0.48
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.13	0.48
2:C:989:LEU:HG	2:C:990:ASP:H	1.79	0.48
3:D:412:LEU:O	3:D:416:ILE:HD12	2.14	0.48
3:D:647:PRO:HG3	3:D:697:MET:HA	1.96	0.48
3:D:8:LEU:N	3:D:8:LEU:HD23	2.29	0.48
1:G:47:LEU:CD2	1:G:220:ALA:HB2	2.44	0.48
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.44	0.48
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.96	0.48
3:I:213:LYS:O	3:I:217:LEU:HG	2.13	0.48
1:A:102:LEU:HD12	1:A:115:ILE:HG12	1.95	0.48
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.37	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:753:LEU:O	2:C:753:LEU:HD12	2.13	0.48
3:D:704:GLU:O	3:D:705:THR:OG1	2.25	0.48
1:F:45:ARG:NE	1:G:38:THR:OG1	2.45	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:741:MET:N	2:H:741:MET:SD	2.86	0.48
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.96	0.48
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.95	0.48
3:I:858:VAL:HB	3:I:859:PRO:CD	2.29	0.48
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.14	0.48
2:C:690:VAL:HG11	2:C:830:THR:CG2	2.44	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.47	0.47
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:521:LEU:HD23	2:H:686:GLN:HB3	1.96	0.47
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.96	0.47
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.28	0.47
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.26	0.47
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.44	0.47
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.96	0.47
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.96	0.47
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.96	0.47
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.13	0.47
3:I:24:LEU:HD11	3:I:116:PHE:CZ	2.50	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.29	0.47
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.14	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
2:C:149:LEU:HD12	2:C:452:ARG:O	2.14	0.47
2:C:119:GLU:OE1	2:C:490:GLN:HB3	2.15	0.47
2:C:660:VAL:C	2:C:661:VAL:HG13	2.34	0.47
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.29	0.47
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.96	0.47
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.97	0.47
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.96	0.47
2:H:159:SER:OG	2:H:442:VAL:HG11	2.15	0.47
3:I:385:LEU:HD21	3:I:411:ILE:HG13	1.97	0.47
3:I:786:THR:O	3:I:790:THR:HG23	2.14	0.47
3:I:810:THR:OG1	3:I:811:GLU:N	2.45	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.47	0.47
3:D:611:ILE:HG13	3:D:612:LEU:CD2	2.45	0.47
3:D:901:ARG:HB3	3:D:908:ILE:HA	1.95	0.47
3:D:914:ALA:O	3:D:918:ILE:HG22	2.14	0.47
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.44	0.47
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.96	0.47
2:H:971:LEU:HD12	2:H:1018:TYR:HD1	1.78	0.47
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.49	0.47
5:X:113:ARG:O	5:X:117:ILE:HD13	2.14	0.47
2:C:748:ILE:O	2:C:748:ILE:HD12	2.14	0.47
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.45	0.47
3:D:828:GLY:HA2	3:D:832:LYS:N	2.29	0.47
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.47	0.47
2:H:119:GLU:HG2	2:H:120:GLN:N	2.29	0.47
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.97	0.47
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.96	0.47
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:704:GLU:O	3:I:705:THR:OG1	2.26	0.47
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.96	0.47
5:X:262:VAL:HG12	5:X:264:LYS:H	1.78	0.47
5:X:503:GLU:HB3	5:X:504:PRO:O	2.13	0.47
5:X:532:LEU:O	5:X:536:THR:HG23	2.15	0.47
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.80	0.47
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.80	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.95	0.47
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.47
3:I:1171:GLY:N	3:I:1172:LYS:O	2.47	0.47
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.15	0.47
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.79	0.47
5:X:264:LYS:HD2	5:X:264:LYS:N	2.29	0.47
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.47	0.47
1:A:303:ILE:O	1:A:307:LEU:HD13	2.14	0.47
1:B:19:VAL:HG12	1:B:19:VAL:O	2.15	0.47
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.96	0.47
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.29	0.47
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.79	0.47
3:D:139:LEU:HD22	3:D:139:LEU:O	2.15	0.47
3:D:166:LEU:HD12	3:D:167:ASP:N	2.30	0.47
3:D:355:ILE:HG12	3:D:464:ASP:O	2.14	0.47
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.95	0.47
4:E:5:THR:HB	4:E:7:GLN:HB2	1.97	0.47
2:H:127:ILE:O	2:H:127:ILE:HG12	2.14	0.47
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.96	0.47
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.44	0.47
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.30	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.97	0.47
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.96	0.47
5:X:551:LEU:HD22	5:X:597:LYS:HD2	1.97	0.47
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.96	0.47
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.50	0.47
3:D:294:ASN:ND2	3:D:298:MET:SD	2.87	0.47
1:G:42:ALA:O	1:G:46:ILE:HG12	2.15	0.47
2:H:73:TYR:O	2:H:74:ARG:HB2	2.14	0.47
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.30	0.47
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.95	0.47
2:C:533:LEU:HG	6:C:1401:1RL:H142	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.45	0.47
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.47
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.49	0.47
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.95	0.47
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.97	0.47
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.14	0.47
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.13	0.47
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.50	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
3:D:141:PHE:O	3:D:297:ARG:HD3	2.15	0.47
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.80	0.47
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.45	0.47
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.95	0.47
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.96	0.47
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.26	0.47
2:C:519:ASN:ND2	2:C:689:ALA:O	2.47	0.47
2:C:71:VAL:O	2:C:72:SER:OG	2.30	0.47
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.45	0.47
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.45	0.47
3:D:145:VAL:HG22	3:D:180:MET:SD	2.55	0.47
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.45	0.47
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.80	0.47
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.29	0.47
2:H:989:LEU:HG	2:H:990:ASP:H	1.80	0.47
3:I:147:ILE:HG13	3:I:148:GLU:N	2.29	0.47
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.97	0.47
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.50	0.46
2:C:542:ARG:O	2:C:544:GLY:N	2.41	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.14	0.46
3:D:543:SER:O	3:D:574:VAL:HB	2.14	0.46
3:D:573:THR:HG22	3:D:576:ARG:CG	2.44	0.46
1:F:11:PRO:HG2	1:G:228:LEU:H	1.80	0.46
2:H:494:ASN:OD1	2:H:495:ALA:N	2.47	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.50	0.46
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.96	0.46
3:I:678:ARG:O	3:I:681:LYS:HG3	2.15	0.46
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.50	0.46
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.49	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.97	0.46
5:Y:355:ILE:O	5:Y:358:VAL:HG22	2.14	0.46
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.46	0.46
1:A:318:LEU:HD13	1:A:318:LEU:N	2.30	0.46
1:A:134:THR:HG21	2:C:727:VAL:O	2.16	0.46
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.50	0.46
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.40	0.46
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.49	0.46
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.51	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.98	0.46
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.46
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.30	0.46
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.98	0.46
2:C:1239:VAL:HG12	2:C:1240:ASP:N	2.27	0.46
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.50	0.46
1:G:227:GLN:C	1:G:229:GLU:H	2.19	0.46
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.30	0.46
3:I:161:THR:HG22	3:I:162:GLU:N	2.30	0.46
1:A:69:SER:OG	1:A:70:THR:N	2.48	0.46
2:C:1006:GLU:HG2	2:C:1006:GLU:O	2.16	0.46
2:C:106:GLU:HG2	2:C:109:ALA:H	1.80	0.46
2:C:163:LYS:H	2:C:163:LYS:CD	2.12	0.46
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.31	0.46
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.46
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.15	0.46
3:I:403:ARG:O	3:I:405:GLU:N	2.49	0.46
2:C:850:ILE:HG23	2:C:885:GLY:O	2.16	0.46
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.81	0.46
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.79	0.46
3:D:22:ILE:HG12	3:D:1336:ALA:HA	1.98	0.46
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.50	0.46
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.98	0.46
3:D:235:GLU:N	3:D:235:GLU:OE1	2.48	0.46
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.98	0.46
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.97	0.46
2:H:453:ILE:HG23	2:H:453:ILE:O	2.16	0.46
3:I:366:CYS:SG	3:I:437:PHE:HB2	2.56	0.46
3:I:582:ILE:HG23	3:I:623:GLN:HB3	1.98	0.46
1:B:14:VAL:HG13	1:B:28:LEU:CD2	2.46	0.46
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.51	0.46
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.51	0.46
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.98	0.46
3:D:535:ARG:HB3	3:D:541:LEU:HD11	1.98	0.46
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.46
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.50	0.46
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.97	0.46
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.45	0.46
2:H:748:ILE:HD12	2:H:748:ILE:O	2.16	0.46
2:H:72:SER:O	2:H:98:VAL:HG23	2.16	0.46
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.16	0.46
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.98	0.46
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.98	0.46
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.31	0.46
2:C:202:ARG:NE	2:C:369:MET:HG2	2.31	0.46
3:D:1241:TYR:CD1	3:D:1248:ILE:HG21	2.51	0.46
3:D:161:THR:HG22	3:D:162:GLU:N	2.31	0.46
1:F:79:LEU:O	1:F:83:LEU:HD13	2.16	0.46
2:H:55:SER:CB	2:H:56:VAL:HG13	2.43	0.46
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.15	0.46
3:I:608:CYS:O	3:I:612:LEU:HB2	2.16	0.46
4:J:5:THR:HA	4:J:6:VAL:HG12	1.98	0.46
5:X:115:GLY:O	5:X:119:ILE:HG12	2.16	0.46
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.98	0.45
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.98	0.45
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.99	0.45
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.31	0.45
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.51	0.45
3:D:909:ILE:O	3:D:909:ILE:HD12	2.17	0.45
2:H:1006:GLU:O	2:H:1006:GLU:HG2	2.16	0.45
2:H:189:ASP:HB2	2:H:190:PRO:CD	2.47	0.45
5:Y:471:LEU:HD12	5:Y:472:GLN:N	2.31	0.45
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.42	0.45
2:H:1005:GLU:O	2:H:1007:LYS:N	2.49	0.45
6:H:1401:1RL:O2	6:H:1401:1RL:O1	2.35	0.45
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.17	0.45
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.98	0.45
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.46	0.45
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.31	0.45
1:B:22:THR:HG22	1:B:208:ASN:O	2.16	0.45
2:C:963:GLU:O	2:C:966:ILE:HG22	2.16	0.45
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:546:ALA:H	3:I:547:ARG:C	2.20	0.45
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.98	0.45
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.51	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.16	0.45
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.99	0.45
2:C:901:LEU:O	2:C:905:ILE:HG13	2.17	0.45
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.32	0.45
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.45	0.45
3:D:515:ARG:NH2	3:D:718:SER:O	2.50	0.45
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.82	0.45
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.98	0.45
1:F:86:LYS:HE2	1:F:173:VAL:HG23	1.98	0.45
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.81	0.45
2:H:488:MET:H	2:H:489:PRO:HA	1.81	0.45
3:I:1306:LEU:HD13	3:I:1307:LEU:N	2.31	0.45
3:I:265:LEU:HD11	3:I:330:MET:SD	2.57	0.45
3:I:647:PRO:HG3	3:I:697:MET:HA	1.98	0.45
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.98	0.45
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.16	0.45
2:C:166:SER:O	2:C:167:SER:OG	2.30	0.45
3:D:162:GLU:HG2	3:D:163:GLU:N	2.31	0.45
3:D:316:ILE:O	3:D:317:THR:OG1	2.19	0.45
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.99	0.45
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.47	0.45
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.99	0.45
1:F:41:ASN:HD21	2:H:1218:GLY:CA	2.29	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:CG2	2.47	0.45
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.82	0.45
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.99	0.45
3:I:382:TYR:HB3	3:I:394:ILE:CD1	2.46	0.45
3:I:513:MET:O	3:I:575:GLY:HA3	2.16	0.45
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.46	0.45
3:I:58:CYS:SG	3:I:60:ARG:N	2.89	0.45
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.99	0.45
3:I:733:SER:O	3:I:737:ILE:HG12	2.17	0.45
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.82	0.45
1:A:178:SER:HA	1:A:179:PRO:HD3	1.77	0.45
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.45
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.99	0.45
3:D:918:ILE:HD13	3:D:919:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:500:ALA:O	2:H:504:GLU:HB2	2.17	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.32	0.45
3:I:138:VAL:O	3:I:143:SER:HB3	2.17	0.45
3:I:179:LYS:HD3	3:I:179:LYS:N	2.32	0.45
3:I:422:LEU:HA	3:I:436:ALA:HA	1.99	0.45
5:X:459:THR:O	5:X:463:LEU:HD13	2.15	0.45
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.46	0.45
2:C:44:GLU:HG3	2:C:45:GLY:N	2.32	0.45
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.49	0.45
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.99	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
2:H:106:GLU:HG2	2:H:109:ALA:H	1.82	0.45
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.52	0.45
3:I:579:LEU:HD13	3:I:579:LEU:O	2.16	0.45
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.97	0.45
5:X:379:MET:HE2	5:X:379:MET:HA	1.99	0.45
3:D:395:LYS:NZ	5:X:607:LEU:O	2.36	0.45
2:C:893:THR:O	2:C:894:GLN:HB2	2.17	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
2:H:31:GLN:HG3	2:H:130:MET:HE1	1.99	0.45
2:H:660:VAL:C	2:H:661:VAL:HG13	2.37	0.45
3:I:1247:LYS:CD	3:I:1247:LYS:H	2.26	0.45
3:I:1256:ILE:O	3:I:1260:MET:HB2	2.17	0.45
3:I:390:LEU:N	3:I:390:LEU:HD12	2.31	0.45
3:I:886:VAL:HG23	3:I:1254:GLU:HB3	1.99	0.45
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.45
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.99	0.45
2:C:533:LEU:HD23	2:C:533:LEU:N	2.32	0.45
2:C:80:PHE:O	2:C:84:GLU:HB3	2.16	0.45
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.17	0.45
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.46	0.45
2:H:941:LYS:HD2	2:H:941:LYS:O	2.16	0.45
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.45
5:X:379:MET:CE	5:X:379:MET:HA	2.47	0.45
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.98	0.45
2:C:1290:MET:SD	2:C:1294:LYS:HD3	2.57	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.52	0.45
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.99	0.45
3:D:841:GLY:CA	3:D:901:ARG:HD3	2.46	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.52	0.45
5:X:519:LEU:HD13	5:X:519:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.17	0.45
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.52	0.44
2:C:551:HIS:CD2	2:C:552:PRO:HD2	2.52	0.44
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.25	0.44
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.99	0.44
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.52	0.44
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.50	0.44
1:A:321:TRP:HA	1:A:322:PRO:HA	1.71	0.44
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.53	0.44
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.16	0.44
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.99	0.44
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.00	0.44
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.99	0.44
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.98	0.44
2:H:843:THR:HB	2:H:845:LEU:CD2	2.47	0.44
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.98	0.44
3:I:482:ALA:C	3:I:483:LEU:HD12	2.38	0.44
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.98	0.44
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.97	0.44
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.58	0.44
2:C:542:ARG:HG2	2:C:543:ALA:N	2.32	0.44
3:D:124:ILE:HA	3:D:237:MET:HE2	1.99	0.44
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.18	0.44
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.44
3:I:1168:GLU:O	3:I:1169:THR:OG1	2.35	0.44
3:I:1190:ILE:N	3:I:1190:ILE:HD12	2.32	0.44
5:X:288:MET:HA	5:X:302:PHE:CZ	2.52	0.44
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.47	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.99	0.44
3:D:1306:LEU:HD13	3:D:1307:LEU:N	2.33	0.44
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.52	0.44
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.44
3:D:610:ARG:CG	3:D:864:LEU:HD22	2.45	0.44
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.44
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.49	0.44
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	1.99	0.44
3:I:252:LEU:HD23	3:I:252:LEU:H	1.81	0.44
3:I:363:LEU:O	3:I:486:SER:OG	2.29	0.44
3:I:886:VAL:HG13	3:I:1230:THR:HG21	2.00	0.44
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.82	0.44
1:A:317:ARG:C	1:A:318:LEU:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.43	0.44
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.99	0.44
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.47	0.44
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.83	0.44
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.53	0.44
2:H:699:LEU:HD11	2:H:1179:GLY:CA	2.44	0.44
3:I:288:PRO:HB2	3:I:291:ILE:HG12	2.00	0.44
1:A:221:ALA:HB1	1:B:228:LEU:HD13	2.00	0.44
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.98	0.44
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.18	0.44
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.17	0.44
2:C:1158:LYS:O	2:C:1158:LYS:HD2	2.18	0.44
3:D:205:LEU:HB3	3:D:217:LEU:HD22	1.99	0.44
3:D:233:LYS:HG3	3:D:234:PRO:HD2	2.00	0.44
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.53	0.44
2:H:1277:ALA:HB3	3:I:434:ILE:HD13	2.00	0.44
2:H:653:MET:HG2	2:H:654:ASP:N	2.33	0.44
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.48	0.44
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.44
1:A:29:GLU:O	1:A:31:LEU:N	2.50	0.44
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.53	0.44
2:C:42:ASP:O	2:C:44:GLU:HG2	2.17	0.44
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.18	0.44
3:D:841:GLY:HA3	3:D:901:ARG:HD3	1.99	0.44
2:H:122:VAL:HG13	2:H:124:MET:HG3	2.00	0.44
2:H:1298:VAL:HG13	2:H:1321:GLU:HG3	1.99	0.44
2:H:488:MET:HB2	2:H:489:PRO:HA	1.99	0.44
2:H:551:HIS:CD2	2:H:552:PRO:HD2	2.52	0.44
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.33	0.44
3:I:242:LEU:HD12	3:I:243:PRO:HD2	2.00	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.17	0.44
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.32	0.44
3:I:610:ARG:CG	3:I:864:LEU:HD22	2.48	0.44
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.51	0.44
5:Y:139:GLU:HG3	5:Y:351:THR:HA	2.00	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.48	0.44
2:C:841:ARG:HA	2:C:1046:VAL:HG13	2.00	0.44
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.17	0.44
3:D:144:TYR:HB3	3:D:159:ILE:CG2	2.48	0.44
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.99	0.44
3:D:709:ARG:HD2	3:D:714:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.47	0.44
4:E:82:ALA:O	4:E:86:ILE:HG13	2.17	0.44
1:F:234:LEU:HD12	1:F:234:LEU:N	2.33	0.44
2:H:218:GLU:HG2	2:H:299:LYS:HA	2.00	0.44
2:H:549:ASP:OD1	2:H:550:VAL:N	2.50	0.44
2:H:747:GLY:C	2:H:748:ILE:HG13	2.38	0.44
2:H:843:THR:HB	2:H:845:LEU:HD22	1.99	0.44
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.48	0.44
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.33	0.44
3:I:1258:ARG:HG3	3:I:1259:GLN:N	2.33	0.44
5:Y:96:ASP:CG	5:Y:97:PRO:HD2	2.37	0.44
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.98	0.43
3:D:482:ALA:C	3:D:483:LEU:HD12	2.39	0.43
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.90	0.43
3:I:162:GLU:HG2	3:I:163:GLU:N	2.33	0.43
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.47	0.43
3:I:545:HIS:CB	3:I:546:ALA:HA	2.41	0.43
5:Y:395:THR:HA	5:Y:404:LEU:CD2	2.48	0.43
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.43
3:D:1190:ILE:HD12	3:D:1190:ILE:N	2.32	0.43
3:D:139:LEU:HD22	3:D:139:LEU:C	2.39	0.43
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.43
3:D:390:LEU:HD12	3:D:390:LEU:N	2.33	0.43
3:D:579:LEU:O	3:D:579:LEU:HD13	2.17	0.43
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.43
2:H:1017:GLN:O	2:H:1020:GLU:HB3	2.18	0.43
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.33	0.43
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.48	0.43
3:I:534:GLU:O	3:I:538:ARG:HB2	2.18	0.43
3:I:582:ILE:HG23	3:I:623:GLN:CB	2.48	0.43
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.18	0.43
5:X:47:MET:O	5:X:55:VAL:HG11	2.18	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
2:C:122:VAL:HG22	2:C:123:TYR:N	2.33	0.43
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.53	0.43
2:C:994:ARG:N	2:C:994:ARG:HD3	2.33	0.43
3:D:202:ARG:O	3:D:206:ASN:ND2	2.51	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43
3:D:648:GLU:N	3:D:648:GLU:OE2	2.51	0.43
2:H:465:ARG:O	2:H:469:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1258:PRO:HG2	3:I:346:ARG:HB3	1.99	0.43
3:I:856:ILE:HG13	3:I:857:LEU:O	2.19	0.43
3:I:901:ARG:CB	3:I:908:ILE:HA	2.49	0.43
5:X:17:LYS:HB3	5:X:17:LYS:NZ	2.32	0.43
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	2.00	0.43
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.49	0.43
2:C:993:PRO:HB2	2:C:994:ARG:H	1.60	0.43
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.80	0.43
3:D:63:GLY:O	3:D:98:ARG:NH2	2.50	0.43
2:H:37:LYS:HA	2:H:37:LYS:HE3	2.00	0.43
2:H:397:LEU:O	2:H:398:SER:OG	2.23	0.43
2:H:705:GLU:HB2	2:H:794:LEU:HB3	2.01	0.43
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.99	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.51	0.43
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.18	0.43
1:A:234:LEU:HD12	1:A:234:LEU:N	2.34	0.43
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.50	0.43
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.38	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.34	0.43
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.18	0.43
3:I:590:SER:O	3:I:594:GLN:N	2.51	0.43
3:I:909:ILE:O	3:I:909:ILE:HD12	2.18	0.43
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.43
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.99	0.43
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.00	0.43
2:C:106:GLU:H	2:C:107:ARG:HA	1.83	0.43
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.47	0.43
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.43
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.19	0.43
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.54	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:H:529:ARG:CD	6:H:1401:1RL:H171	2.48	0.43
2:H:892:GLU:O	2:H:893:THR:OG1	2.22	0.43
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.53	0.43
3:I:572:THR:HB	3:I:576:ARG:HD2	2.01	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.83	0.43
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.99	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
2:C:189:ASP:HB2	2:C:190:PRO:CD	2.49	0.43
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.19	0.43
3:D:240:THR:HG23	3:D:241:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:252:LEU:HD23	3:D:252:LEU:H	1.82	0.43
3:D:519:ASN:OD1	3:D:520:ALA:N	2.51	0.43
3:I:305:ALA:O	3:I:309:ASN:ND2	2.51	0.43
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.84	0.43
2:C:135:THR:OG1	2:C:143:ARG:O	2.35	0.43
2:C:747:GLY:C	2:C:748:ILE:HG13	2.39	0.43
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.33	0.43
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.99	0.43
3:D:27:PRO:O	3:D:31:ARG:HD3	2.19	0.43
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.49	0.43
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.19	0.43
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.99	0.43
3:I:799:ARG:NH1	3:I:1146:GLU:OE1	2.51	0.43
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.43
3:I:834:PRO:C	3:I:835:LEU:HD12	2.39	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.00	0.43
2:C:73:TYR:O	2:C:74:ARG:HB2	2.18	0.43
2:C:82:VAL:HG13	2:C:83:GLN:N	2.34	0.43
3:D:690:ASN:ND2	3:D:745:GLY:HA3	2.34	0.43
3:D:824:PRO:O	3:D:826:ILE:HG13	2.19	0.43
3:D:919:ALA:O	3:D:923:ILE:HG12	2.18	0.43
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.54	0.43
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.43
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.52	0.43
2:H:73:TYR:CD2	2:H:73:TYR:N	2.85	0.43
2:H:888:THR:O	2:H:914:LYS:N	2.51	0.43
2:H:868:SER:OG	2:H:942:ASP:OD1	2.36	0.43
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.43	0.43
3:I:367:GLY:HA3	3:I:448:GLN:HB2	2.00	0.43
3:I:848:VAL:HG11	3:I:880:VAL:HA	2.00	0.43
5:X:264:LYS:HD2	5:X:264:LYS:H	1.83	0.43
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.99	0.43
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.48	0.43
2:C:736:VAL:HG11	2:C:740:GLU:CA	2.48	0.43
3:D:1226:VAL:HG11	3:I:1292:LEU:HA	2.01	0.43
3:D:124:ILE:CG1	3:D:189:LEU:HD11	2.49	0.43
3:D:403:ARG:O	3:D:405:GLU:N	2.52	0.43
3:D:58:CYS:SG	3:D:60:ARG:N	2.92	0.43
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.48	0.43
3:D:834:PRO:C	3:D:835:LEU:HD12	2.39	0.43
2:H:818:VAL:HG22	2:H:819:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.19	0.43
3:I:648:GLU:N	3:I:648:GLU:OE2	2.52	0.43
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
4:J:10:VAL:HG21	4:J:16:ARG:HG2	2.01	0.43
5:Y:108:VAL:HB	5:Y:110:LEU:HG	2.01	0.43
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.84	0.43
5:Y:600:HIS:N	5:Y:601:PRO:CD	2.82	0.43
1:A:300:LEU:HD13	1:A:300:LEU:O	2.19	0.42
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	2.01	0.42
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.84	0.42
2:C:52:ALA:O	2:C:53:PHE:HB2	2.19	0.42
3:D:107:LEU:HD23	3:D:299:LEU:HD21	2.00	0.42
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.81	0.42
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.48	0.42
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.54	0.42
3:D:579:LEU:HD23	3:D:627:THR:HG21	2.00	0.42
2:H:205:PRO:O	2:H:208:ILE:HG22	2.19	0.42
3:I:361:LEU:HD23	3:I:366:CYS:HA	2.00	0.42
3:I:519:ASN:OD1	3:I:520:ALA:N	2.52	0.42
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.49	0.42
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.34	0.42
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.33	0.42
2:C:494:ASN:OD1	2:C:495:ALA:N	2.52	0.42
2:C:759:SER:OG	2:C:760:ASN:N	2.52	0.42
2:C:10:ARG:NH1	2:C:775:GLU:OE2	2.52	0.42
3:D:423:LEU:HB3	3:D:466:MET:HE2	2.01	0.42
2:H:1294:LYS:HE2	3:I:348:ASP:O	2.19	0.42
2:H:185:ASP:N	2:H:185:ASP:OD1	2.51	0.42
2:H:773:LEU:HD22	2:H:773:LEU:C	2.39	0.42
2:H:845:LEU:HD13	2:H:845:LEU:N	2.30	0.42
2:H:998:LEU:O	2:H:998:LEU:HD13	2.19	0.42
3:I:139:LEU:HD22	3:I:139:LEU:O	2.19	0.42
3:I:686:TRP:HB3	3:I:758:PRO:HG2	2.00	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.19	0.42
2:C:41:GLN:CD	2:C:42:ASP:H	2.23	0.42
2:C:622:ASN:OD1	2:C:623:LEU:N	2.52	0.42
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.42
2:C:748:ILE:C	2:C:748:ILE:HD12	2.40	0.42
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.19	0.42
2:H:337:PHE:O	2:H:338:THR:OG1	2.32	0.42
2:H:59:ILE:HD13	2:H:479:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:THR:HG22	2:H:601:ASP:H	1.84	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.48	0.42
2:C:557:ARG:NH2	2:C:606:LEU:O	2.52	0.42
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.42
3:D:124:ILE:HD11	3:D:189:LEU:HD11	2.01	0.42
3:D:154:LEU:HD21	3:D:160:LEU:HD21	2.01	0.42
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.54	0.42
2:H:691:PRO:HA	2:H:788:SER:OG	2.19	0.42
3:I:139:LEU:HD22	3:I:139:LEU:C	2.39	0.42
3:I:368:LEU:HD12	3:I:369:PRO:HD2	2.01	0.42
3:I:482:ALA:O	3:I:488:ASN:ND2	2.52	0.42
3:I:611:ILE:HG13	3:I:612:LEU:HD23	2.01	0.42
5:X:565:ILE:HG12	5:X:566:ASP:N	2.34	0.42
5:X:582:VAL:HG11	5:X:586:ARG:HG2	2.01	0.42
5:Y:143:TYR:CD1	5:Y:269:LEU:HD21	2.54	0.42
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.32	0.42
2:C:948:ILE:HG13	2:C:949:GLU:N	2.34	0.42
3:D:369:PRO:HG3	3:D:446:ALA:O	2.19	0.42
4:E:5:THR:CA	4:E:6:VAL:CB	2.80	0.42
1:F:51:MET:HB2	1:F:179:PRO:HD2	2.01	0.42
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	2.01	0.42
2:H:759:SER:OG	2:H:760:ASN:N	2.53	0.42
2:H:10:ARG:NH1	2:H:775:GLU:OE2	2.51	0.42
2:H:948:ILE:HG13	2:H:949:GLU:N	2.34	0.42
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	2.01	0.42
5:X:442:SER:OG	5:X:446:GLN:NE2	2.52	0.42
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.42
5:X:461:ASN:HB3	5:X:465:ARG:CZ	2.49	0.42
2:C:177:ILE:HD12	2:C:177:ILE:N	2.34	0.42
3:D:242:LEU:HD12	3:D:243:PRO:HD2	2.01	0.42
3:D:313:GLY:O	3:D:314:ARG:HB2	2.20	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.54	0.42
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.53	0.42
3:D:886:VAL:HG23	3:D:1254:GLU:HB3	2.00	0.42
2:H:106:GLU:CB	2:H:107:ARG:CA	2.97	0.42
3:I:413:ASP:HA	3:I:416:ILE:HD12	2.01	0.42
3:I:526:VAL:HG12	3:I:549:LYS:HB2	2.00	0.42
3:I:901:ARG:HB3	3:I:908:ILE:HA	2.02	0.42
5:X:143:TYR:O	5:X:147:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NE	1:B:38:THR:OG1	2.49	0.42
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	2.02	0.42
2:C:127:ILE:HG12	2:C:127:ILE:O	2.19	0.42
2:C:603:ILE:HD12	2:C:603:ILE:O	2.19	0.42
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.50	0.42
1:B:83:LEU:CD1	3:D:527:LEU:HA	2.50	0.42
3:D:596:LEU:N	3:D:596:LEU:HD23	2.34	0.42
3:D:605:LEU:O	3:D:605:LEU:HD13	2.20	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.49	0.42
1:F:42:ALA:O	1:F:46:ILE:HG12	2.20	0.42
2:H:177:ILE:N	2:H:177:ILE:HD12	2.35	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.85	0.42
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.55	0.42
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	2.01	0.42
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.79	0.42
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.92	0.42
3:I:596:LEU:HD23	3:I:596:LEU:N	2.34	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
3:I:932:MET:O	3:I:933:ARG:HG3	2.19	0.42
5:X:108:VAL:HG23	5:X:109:GLU:N	2.30	0.42
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.19	0.42
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	2.01	0.42
1:A:44:ARG:HG3	1:A:183:ILE:HG22	2.02	0.42
3:D:1270:GLY:CA	3:D:1299:GLY:HA2	2.49	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.19	0.42
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.35	0.42
2:H:894:GLN:O	2:H:895:LEU:HB2	2.20	0.42
3:I:1297:LYS:HE2	3:I:1297:LYS:HA	2.00	0.42
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.84	0.42
3:I:72:CYS:SG	3:I:73:GLY:N	2.93	0.42
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.42
3:I:298:MET:HE3	5:Y:402:LEU:HB3	2.02	0.42
1:A:323:PRO:CA	1:A:324:ALA:HB2	2.50	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:685:MET:HE2	2:C:1067:ALA:CB	2.49	0.42
2:C:73:TYR:CG	2:C:74:ARG:N	2.86	0.42
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
3:D:292:VAL:HG13	3:D:293:ARG:N	2.34	0.42
3:D:517:CYS:N	3:D:544:LEU:O	2.47	0.42
1:G:207:THR:OG1	1:G:208:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:LYS:NZ	3:I:526:VAL:O	2.52	0.42
2:H:135:THR:OG1	2:H:143:ARG:O	2.30	0.42
2:H:634:VAL:HG22	2:H:645:PHE:HE2	1.85	0.42
3:I:189:LEU:HB3	3:I:234:PRO:HB2	2.02	0.42
3:I:369:PRO:HG3	3:I:446:ALA:O	2.20	0.42
3:I:771:GLN:HE21	3:I:772:TYR:N	2.18	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
5:X:12:LEU:HD21	5:X:27:VAL:HG21	1.98	0.42
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.49	0.42
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.42
1:A:42:ALA:HA	1:B:38:THR:HG23	2.02	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.01	0.42
2:C:639:LYS:HA	2:C:639:LYS:HE2	2.02	0.42
2:C:818:VAL:HG22	2:C:819:SER:N	2.35	0.42
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.49	0.42
3:D:320:ASN:HB3	3:D:322:ARG:HG2	2.01	0.42
3:D:392:THR:HG22	5:X:603:ARG:HG2	2.00	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
2:H:163:LYS:O	2:H:163:LYS:HG2	2.20	0.42
2:H:166:SER:O	2:H:167:SER:OG	2.32	0.42
2:H:484:LEU:HB3	2:H:486:THR:HG22	2.01	0.42
2:H:59:ILE:HD11	2:H:63:SER:HB3	2.02	0.42
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.35	0.42
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.48	0.42
3:I:292:VAL:HG13	3:I:293:ARG:N	2.35	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.50	0.42
3:I:644:MET:O	3:I:764:ARG:NH1	2.53	0.42
1:B:190:ALA:HB2	1:B:200:LYS:HB3	2.01	0.41
1:B:9:LEU:H	1:B:9:LEU:HD23	1.85	0.41
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.55	0.41
2:C:91:THR:HG22	2:C:138:ILE:HA	2.02	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.53	0.41
2:H:384:LEU:O	2:H:388:LEU:HG	2.20	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.35	0.41
2:H:639:LYS:HE2	2:H:639:LYS:HA	2.00	0.41
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.50	0.41
2:H:893:THR:O	2:H:894:GLN:HB2	2.20	0.41
2:H:971:LEU:HD12	2:H:1018:TYR:CD1	2.54	0.41
3:I:1173:ARG:NH1	3:I:1176:VAL:HG21	2.34	0.41
3:I:240:THR:HG23	3:I:241:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:252:LEU:HG	3:I:252:LEU:O	2.20	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.52	0.41
2:C:152:SER:HA	2:C:153:PRO:HD3	1.89	0.41
2:C:166:SER:O	2:C:168:GLY:N	2.45	0.41
2:C:773:LEU:HD22	2:C:773:LEU:C	2.40	0.41
2:C:896:THR:HG23	2:C:897:PRO:HD2	2.02	0.41
2:C:873:ILE:HD11	2:C:931:VAL:HG22	2.02	0.41
4:E:3:ARG:O	4:E:4:VAL:HG13	2.20	0.41
1:F:54:CYS:SG	1:F:148:ARG:NH1	2.93	0.41
2:H:727:VAL:HG22	2:H:773:LEU:HB3	2.00	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
3:I:233:LYS:HG3	3:I:234:PRO:HD2	2.01	0.41
3:I:550:VAL:HG23	3:I:552:ILE:HD11	2.02	0.41
3:I:508:LEU:HD12	3:I:725:MET:HG2	2.03	0.41
3:I:863:LEU:HB2	3:I:866:GLU:HB2	2.03	0.41
5:X:511:ILE:HG23	5:X:512:GLY:N	2.32	0.41
3:D:395:LYS:HG3	5:X:536:THR:HG21	2.02	0.41
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.20	0.41
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.41
2:C:510:GLN:C	2:C:512:SER:H	2.24	0.41
2:C:516:ASP:O	2:C:522:SER:OG	2.29	0.41
2:C:519:ASN:CB	2:C:520:PRO:HD2	2.47	0.41
3:D:412:LEU:O	3:D:416:ILE:HG23	2.19	0.41
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.35	0.41
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.34	0.41
3:I:451:PRO:HG2	3:I:625:MET:SD	2.60	0.41
3:I:63:GLY:O	3:I:98:ARG:NH2	2.52	0.41
3:D:394:ILE:HG21	5:X:536:THR:HA	2.03	0.41
5:X:52:GLY:O	5:X:53:ILE:HB	2.19	0.41
2:C:201:ARG:HD2	2:C:370:MET:SD	2.60	0.41
2:C:538:LEU:HD12	2:C:538:LEU:N	2.35	0.41
3:D:310:GLY:O	3:D:314:ARG:HG2	2.19	0.41
3:D:514:THR:HG23	3:D:576:ARG:HE	1.86	0.41
3:D:706:VAL:C	3:D:707:ILE:HG13	2.41	0.41
3:D:911:LYS:HG3	4:E:15:ASN:ND2	2.36	0.41
3:I:1226:VAL:O	3:I:1230:THR:HG23	2.20	0.41
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.40	0.41
3:I:503:SER:O	3:I:507:VAL:HG23	2.20	0.41
3:I:573:THR:HG22	3:I:576:ARG:CD	2.50	0.41
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.20	0.41
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:LEU:HD23	2:C:533:LEU:H	1.85	0.41
2:C:546:GLU:O	2:C:547:VAL:HB	2.20	0.41
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.02	0.41
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.41
3:D:474:LEU:HD13	3:D:478:LEU:HD13	2.01	0.41
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.41
1:B:182:ARG:NH1	3:D:581:MET:SD	2.93	0.41
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.50	0.41
3:D:909:ILE:HG13	3:D:909:ILE:H	1.62	0.41
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.35	0.41
2:H:54:ARG:CA	2:H:55:SER:HB2	2.51	0.41
2:H:870:ILE:HG22	2:H:944:ARG:NH1	2.35	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.50	0.41
3:I:221:ILE:HG13	3:I:222:LYS:N	2.36	0.41
3:I:527:LEU:HD13	3:I:531:LYS:HB3	2.02	0.41
3:I:583:VAL:HG13	3:I:587:LEU:HD22	2.01	0.41
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.03	0.41
1:A:104:LYS:HD3	1:A:105:SER:N	2.35	0.41
1:A:104:LYS:HD2	1:A:110:VAL:HG22	2.02	0.41
2:C:106:GLU:CB	2:C:107:ARG:HA	2.46	0.41
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.55	0.41
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.50	0.41
2:H:748:ILE:HD12	2:H:748:ILE:C	2.40	0.41
3:I:1138:LEU:N	3:I:1139:PRO:CD	2.84	0.41
3:I:139:LEU:HD21	3:I:185:ILE:HD13	2.02	0.41
2:H:1332:SER:O	3:I:243:PRO:HG2	2.21	0.41
3:I:886:VAL:HG22	3:I:1257:VAL:CG1	2.51	0.41
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.20	0.41
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.34	0.41
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.21	0.41
2:C:487:LEU:H	2:C:487:LEU:HD12	1.86	0.41
2:C:898:GLU:N	2:C:898:GLU:OE1	2.51	0.41
2:C:908:GLU:CG	2:C:909:LYS:H	2.33	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB3	2.02	0.41
3:D:1256:ILE:HA	3:D:1259:GLN:HE21	1.85	0.41
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.36	0.41
3:D:269:TYR:HA	3:D:272:VAL:HG12	2.02	0.41
3:D:545:HIS:HB2	3:D:546:ALA:HB2	2.03	0.41
2:H:1156:ARG:O	2:H:1157:GLN:HB2	2.21	0.41
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.35	0.41
2:H:603:ILE:HD12	2:H:603:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:112:THR:HG22	5:X:113:ARG:N	2.36	0.41
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.32	0.41
6:C:1401:1RL:O9	6:C:1401:1RL:O10	2.18	0.41
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.50	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:106:GLU:H	2:H:107:ARG:HA	1.86	0.41
2:H:496:LYS:N	2:H:497:PRO:CD	2.84	0.41
3:I:1210:ILE:O	3:I:1210:ILE:HG13	2.21	0.41
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.36	0.41
3:I:313:GLY:O	3:I:314:ARG:HB2	2.21	0.41
3:I:660:GLU:O	3:I:664:ILE:HG12	2.20	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.89	0.41
2:C:667:LEU:O	2:C:1069:ARG:NH2	2.54	0.41
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	2.03	0.41
2:C:988:LYS:O	2:C:991:LYS:HE3	2.20	0.41
3:D:1210:ILE:O	3:D:1210:ILE:HG13	2.21	0.41
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.21	0.41
3:D:221:ILE:HG13	3:D:222:LYS:N	2.35	0.41
4:E:30:MET:O	4:E:35:LYS:HG2	2.20	0.41
1:F:10:LYS:HE3	1:G:226:GLU:HB3	2.03	0.41
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.36	0.41
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.55	0.41
2:H:378:ARG:NE	2:H:382:GLU:OE2	2.54	0.41
3:I:884:SER:OG	3:I:1254:GLU:OE1	2.31	0.41
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.36	0.41
3:I:501:VAL:HA	3:I:502:PRO:HD3	1.97	0.41
5:X:54:GLN:CA	5:X:54:GLN:HE21	2.34	0.41
5:Y:333:VAL:HG22	5:Y:336:GLU:HB2	2.03	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
3:D:147:ILE:HG23	3:D:156:ARG:C	2.41	0.41
3:D:803:VAL:HB	3:D:1313:SER:HB3	2.03	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.61	0.41
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.61	0.41
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.56	0.41
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.55	0.41
2:H:82:VAL:HG13	2:H:83:GLN:N	2.35	0.41
3:I:316:ILE:HD13	3:I:316:ILE:H	1.86	0.41
2:H:637:ARG:NE	3:I:770:LEU:HD23	2.36	0.41
3:I:822:MET:HG2	3:I:839:VAL:HG22	2.02	0.41
5:X:244:THR:O	5:X:247:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:494:ILE:O	5:X:498:LEU:HD23	2.21	0.41
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.21	0.41
1:B:227:GLN:C	1:B:229:GLU:H	2.24	0.41
1:B:14:VAL:HG13	1:B:28:LEU:HD23	2.03	0.41
3:D:147:ILE:HA	3:D:178:ALA:CB	2.51	0.41
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.41
1:G:181:GLU:HB2	1:G:206:GLU:O	2.21	0.41
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.86	0.41
2:H:146:VAL:HG13	2:H:513:GLN:HG3	2.03	0.41
2:H:524:ILE:HD12	2:H:708:VAL:HG13	2.03	0.41
2:H:681:MET:O	2:H:685:MET:HG2	2.21	0.41
3:I:1169:THR:HA	3:I:1173:ARG:HB3	2.02	0.41
1:A:143:ARG:HD2	1:A:143:ARG:N	2.36	0.40
1:A:246:LYS:N	1:A:246:LYS:HD3	2.35	0.40
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.54	0.40
1:B:176:CYS:C	1:B:178:SER:H	2.25	0.40
1:B:232:VAL:HG12	1:B:233:ASP:O	2.21	0.40
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.40
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.54	0.40
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.51	0.40
3:D:238:ILE:HG13	3:D:238:ILE:O	2.20	0.40
3:D:503:SER:O	3:D:507:VAL:HG23	2.21	0.40
3:D:573:THR:HG23	3:D:576:ARG:H	1.85	0.40
3:D:733:SER:O	3:D:737:ILE:HG12	2.22	0.40
1:F:102:LEU:HG	1:F:115:ILE:HG12	2.03	0.40
1:G:185:TYR:HA	1:G:202:VAL:O	2.21	0.40
2:H:1339:LEU:HD12	2:H:1339:LEU:H	1.86	0.40
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.40
3:I:532:GLU:O	3:I:535:ARG:HB2	2.21	0.40
5:X:361:ILE:HG13	5:X:362:ASN:N	2.36	0.40
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	2.02	0.40
5:Y:361:ILE:HG13	5:Y:362:ASN:N	2.36	0.40
5:Y:540:LEU:HD13	5:Y:607:LEU:HD22	2.04	0.40
1:B:234:LEU:O	1:B:235:ARG:HB2	2.21	0.40
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.57	0.40
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.40
2:C:106:GLU:CB	2:C:107:ARG:CA	2.98	0.40
2:C:98:VAL:HG11	2:C:124:MET:SD	2.60	0.40
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	2.02	0.40
2:C:185:ASP:N	2:C:185:ASP:OD1	2.55	0.40
2:C:342:ASP:O	2:C:437:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.36	0.40
3:D:179:LYS:H	3:D:179:LYS:HD3	1.87	0.40
3:D:265:LEU:HD21	3:D:327:LEU:HD23	2.02	0.40
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.40
1:G:219:ARG:O	1:G:222:THR:HG22	2.21	0.40
2:H:442:VAL:HG12	2:H:443:ASP:N	2.37	0.40
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.21	0.40
2:H:876:GLU:HG3	2:H:927:THR:HG22	2.03	0.40
3:I:128:LEU:HD12	3:I:192:MET:HE3	2.02	0.40
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.56	0.40
3:I:598:LYS:HG3	3:I:599:LYS:N	2.36	0.40
4:J:5:THR:HB	4:J:7:GLN:HB2	2.03	0.40
5:X:224:LEU:HB2	5:X:259:PHE:CZ	2.56	0.40
5:X:455:HIS:O	5:X:459:THR:HG23	2.21	0.40
2:C:1017:GLN:O	2:C:1020:GLU:HB3	2.20	0.40
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	2.02	0.40
2:C:56:VAL:HB	2:C:57:PHE:H	1.60	0.40
2:C:600:THR:HG22	2:C:601:ASP:H	1.87	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.21	0.40
3:D:558:ASP:OD1	3:D:559:ALA:N	2.54	0.40
3:D:610:ARG:N	3:D:610:ARG:HD2	2.36	0.40
1:F:117:HIS:ND1	1:F:117:HIS:O	2.50	0.40
1:F:51:MET:HA	1:F:52:PRO:HD3	1.87	0.40
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.22	0.40
3:I:165:TYR:CE1	3:I:169:LEU:HD23	2.56	0.40
3:I:238:ILE:HG13	3:I:238:ILE:O	2.20	0.40
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.40
3:I:85:CYS:SG	3:I:86:GLU:N	2.93	0.40
5:X:493:LYS:O	5:X:497:VAL:HG23	2.21	0.40
5:X:559:LEU:HD12	5:X:594:ALA:HB1	2.03	0.40
5:Y:288:MET:HA	5:Y:302:PHE:CZ	2.57	0.40
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.21	0.40
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.57	0.40
3:D:213:LYS:O	3:D:215:LYS:N	2.54	0.40
3:D:233:LYS:CG	3:D:234:PRO:HD2	2.51	0.40
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.57	0.40
2:H:898:GLU:CB	5:Y:540:LEU:HD21	2.52	0.40
3:I:483:LEU:N	3:I:483:LEU:HD12	2.36	0.40
1:B:183:ILE:HD11	1:B:205:MET:HG3	2.04	0.40
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:ILE:HD13	2:C:487:LEU:HB3	2.04	0.40
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	2.03	0.40
3:D:1258:ARG:HG3	3:D:1259:GLN:N	2.37	0.40
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.21	0.40
3:D:1369:ARG:HH11	3:D:1369:ARG:HB3	1.86	0.40
3:D:43:THR:OG1	3:D:44:ILE:N	2.55	0.40
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.21	0.40
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.52	0.40
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.03	0.40
2:H:1296:ASP:OD2	2:H:1320:PRO:HB2	2.21	0.40
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.57	0.40
3:I:40:LYS:HA	3:I:41:PRO:HD3	1.80	0.40
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	263 (82%)	42 (13%)	16 (5%)	2	22
1	B	217/329 (66%)	187 (86%)	25 (12%)	5 (2%)	6	37
1	F	227/329 (69%)	195 (86%)	27 (12%)	5 (2%)	6	37
1	G	213/329 (65%)	188 (88%)	22 (10%)	3 (1%)	11	45
2	C	1333/1342 (99%)	1087 (82%)	204 (15%)	42 (3%)	4	31
2	H	1333/1342 (99%)	1091 (82%)	197 (15%)	45 (3%)	3	30
3	D	1154/1407 (82%)	933 (81%)	180 (16%)	41 (4%)	3	28
3	I	1154/1407 (82%)	934 (81%)	180 (16%)	40 (4%)	3	29
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	1	19
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	X	511/613 (83%)	453 (89%)	44 (9%)	14 (3%)	5	34
5	Y	454/613 (74%)	414 (91%)	30 (7%)	10 (2%)	6	37
All	All	7079/8222 (86%)	5886 (83%)	962 (14%)	231 (3%)	4	30

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	319	GLU
1	B	20	SER
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	53	PHE
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	686	GLN
2	C	748	ILE
2	C	753	LEU
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1363	TYR
4	E	6	VAL
5	X	241	SER
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL

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Mol	Chain	Res	Type
2	H	39	ILE
2	H	53	PHE
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	542	ALA
3	I	710	ASP
3	I	847	ASP
3	I	851	PRO
4	J	4	VAL
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER
1	A	193	GLU
1	A	201	LEU
1	A	232	VAL
1	B	19	VAL
1	B	52	PRO
2	C	437	ASN
2	C	812	PHE
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	214	ARG
3	D	417	ARG
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	728	SER
3	D	851	PRO
3	D	901	ARG
3	D	914	ALA
3	D	1192	LYS

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Mol	Chain	Res	Type
4	E	35	LYS
5	X	20	GLY
5	X	23	THR
5	X	108	VAL
5	X	490	PRO
5	X	514	ASP
5	X	581	ASP
1	G	188	GLU
1	G	228	LEU
2	H	170	VAL
2	H	437	ASN
2	H	669	PRO
2	H	753	LEU
2	H	812	PHE
2	H	1006	GLU
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
3	I	89	GLY
3	I	214	ARG
3	I	345	LYS
3	I	417	ARG
3	I	595	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	901	ARG
3	I	914	ALA
3	I	1192	LYS
3	I	1195	GLN
3	I	1268	ASN
3	I	1363	TYR
5	Y	308	GLY
5	Y	490	PRO
1	A	93	GLN
1	A	196	THR
1	B	188	GLU
2	C	143	ARG
2	C	1240	ASP
3	D	53	ARG
3	D	210	SER
3	D	316	ILE

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Mol	Chain	Res	Type
3	D	559	ALA
3	D	590	SER
3	D	672	LEU
3	D	703	THR
3	D	707	ILE
3	D	913	GLU
3	D	1195	GLN
4	E	4	VAL
5	X	308	GLY
5	X	491	GLU
1	F	33	ARG
1	F	188	GLU
2	H	44	GLU
2	H	487	LEU
2	H	543	ALA
2	H	1046	VAL
2	H	1137	GLU
2	H	1240	ASP
2	H	1256	GLN
3	I	53	ARG
3	I	153	ASN
3	I	210	SER
3	I	559	ALA
3	I	590	SER
3	I	728	SER
3	I	913	GLU
5	Y	108	VAL
5	Y	491	GLU
5	Y	514	ASP
1	A	166	ARG
1	A	188	GLU
1	B	235	ARG
2	C	44	GLU
2	C	487	LEU
2	C	1006	GLU
2	C	1080	ASN
2	C	1137	GLU
2	C	1139	ALA
3	D	153	ASN
3	D	832	LYS
3	D	888	CYS
4	E	5	THR

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Mol	Chain	Res	Type
5	X	600	HIS
1	F	153	VAL
1	F	166	ARG
2	H	143	ARG
2	H	488	MET
2	H	535	PRO
2	H	895	LEU
2	H	1045	GLY
2	H	1080	ASN
2	H	1139	ALA
3	I	672	LEU
3	I	703	THR
3	I	832	LYS
3	I	888	CYS
3	I	1194	ARG
5	Y	107	THR
5	Y	581	ASP
1	A	14	VAL
1	A	322	PRO
1	A	324	ALA
2	C	699	LEU
2	C	746	ALA
2	C	1203	ASP
2	C	1315	MET
3	D	816	THR
5	X	50	ASP
5	X	107	THR
2	H	1093	PRO
2	H	1315	MET
3	I	1290	ARG
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	A	194	GLN
2	C	69	GLN
2	C	895	LEU
2	C	1045	GLY
2	C	1046	VAL
2	C	1093	PRO
2	C	1201	LEU
3	D	255	LEU
3	D	902	ASP

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Mol	Chain	Res	Type
3	D	1173	ARG
3	D	1194	ARG
4	E	59	ILE
2	H	56	VAL
2	H	739	ASP
2	H	746	ALA
2	H	1238	LEU
3	I	596	LEU
3	I	712	GLN
3	I	731	ARG
3	I	816	THR
5	X	97	PRO
4	J	59	ILE
1	A	153	VAL
2	C	56	VAL
2	C	373	GLY
5	X	35	ILE
2	C	59	ILE
2	H	59	ILE
2	H	373	GLY
3	I	850	LYS
5	Y	97	PRO
1	A	30	PRO
3	D	850	LYS
3	D	1185	PRO
2	H	78	PRO
2	H	134	GLY
2	H	43	PRO
2	H	489	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	281/286 (98%)	272 (97%)	9 (3%)	39 62
1	B	189/286 (66%)	183 (97%)	6 (3%)	39 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	197/286 (69%)	193 (98%)	4 (2%)	55	73
1	G	185/286 (65%)	184 (100%)	1 (0%)	88	93
2	C	1150/1157 (99%)	1090 (95%)	60 (5%)	23	51
2	H	1150/1157 (99%)	1090 (95%)	60 (5%)	23	51
3	D	971/1168 (83%)	916 (94%)	55 (6%)	20	49
3	I	971/1168 (83%)	916 (94%)	55 (6%)	20	49
4	E	74/75 (99%)	72 (97%)	2 (3%)	44	66
4	J	65/75 (87%)	64 (98%)	1 (2%)	65	79
5	X	460/540 (85%)	443 (96%)	17 (4%)	34	59
5	Y	407/540 (75%)	392 (96%)	15 (4%)	34	59
All	All	6100/7024 (87%)	5815 (95%)	285 (5%)	26	53

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	79	LEU
1	A	88	LEU
1	A	117	HIS
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	65	LEU
1	B	182	ARG
1	B	196	THR
1	B	228	LEU
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL

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Mol	Chain	Res	Type
2	C	70	TYR
2	C	80	PHE
2	C	88	ARG
2	C	127	ILE
2	C	133	ASN
2	C	150	HIS
2	C	163	LYS
2	C	185	ASP
2	C	479	LEU
2	C	487	LEU
2	C	645	PHE
2	C	661	VAL
2	C	693	LEU
2	C	704	MET
2	C	711	ASP
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	843	THR
2	C	845	LEU
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1011	LEU
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1106	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG

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Mol	Chain	Res	Type
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
3	D	13	LYS
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	175	GLU
3	D	179	LYS
3	D	207	GLU
3	D	239	LEU
3	D	248	ASP
3	D	250	ARG
3	D	416	ILE
3	D	430	HIS
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	590	SER
3	D	605	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS

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Mol	Chain	Res	Type
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1227	HIS
3	D	1247	LYS
3	D	1306	LEU
3	D	1341	ARG
3	D	1366	HIS
4	E	4	VAL
4	E	6	VAL
5	X	21	TYR
5	X	28	ASN
5	X	54	GLN
5	X	99	ARG
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	400	GLN
5	X	452	ILE
5	X	457	ILE
5	X	471	LEU
5	X	476	ARG
5	X	545	HIS
5	X	562	ARG
5	X	565	ILE
5	X	607	LEU

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Mol	Chain	Res	Type
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	F	181	GLU
1	G	37	HIS
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	185	ASP
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	645	PHE
2	H	661	VAL
2	H	704	MET
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	953	LEU
2	H	955	GLN
2	H	964	LEU
2	H	971	LEU

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Mol	Chain	Res	Type
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1011	LEU
2	H	1017	GLN
2	H	1032	LYS
2	H	1042	LEU
2	H	1106	ARG
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1264	GLN
2	H	1276	TRP
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	175	GLU
3	I	179	LYS
3	I	207	GLU
3	I	235	GLU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	316	ILE
3	I	325	LYS

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Mol	Chain	Res	Type
3	I	416	ILE
3	I	430	HIS
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	605	LEU
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	816	THR
3	I	832	LYS
3	I	847	ASP
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1341	ARG
3	I	1366	HIS
4	J	4	VAL
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET

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Mol	Chain	Res	Type
5	Y	384	LEU
5	Y	400	GLN
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
2	C	513	GLN
2	C	673	HIS
2	C	684	ASN
2	C	955	GLN
2	C	1010	GLN
2	C	1017	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1264	GLN
2	C	1313	HIS
3	D	164	GLN
3	D	209	ASN
3	D	504	GLN
3	D	875	ASN
3	D	921	GLN
3	D	1197	ASN
3	D	1268	ASN
3	D	1326	GLN
4	E	31	GLN
5	X	8	GLN
5	X	40	GLN
5	X	54	GLN
5	X	406	GLN
5	X	446	GLN
1	F	66	HIS
2	H	46	GLN
2	H	510	GLN

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Mol	Chain	Res	Type
2	H	513	GLN
2	H	526	HIS
2	H	649	GLN
2	H	684	ASN
2	H	1010	GLN
2	H	1108	ASN
2	H	1111	GLN
2	H	1116	HIS
2	H	1134	GLN
2	H	1220	GLN
2	H	1264	GLN
3	I	164	GLN
3	I	274	ASN
3	I	309	ASN
3	I	504	GLN
3	I	1227	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1RL	H	1401	-	65,70,70	3.07	18 (27%)	90,104,104	2.24	26 (28%)
6	1RL	C	1401	-	65,70,70	3.07	18 (27%)	90,104,104	2.14	22 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1RL	H	1401	-	-	29/65/84/84	0/5/6/6
6	1RL	C	1401	-	-	31/65/84/84	0/5/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	1RL	O3-C6	12.06	1.60	1.37
6	H	1401	1RL	O3-C6	12.06	1.60	1.37
6	C	1401	1RL	C6-C7	10.96	1.58	1.39
6	H	1401	1RL	C6-C7	10.86	1.58	1.39
6	H	1401	1RL	C17-C16	7.13	1.55	1.34
6	C	1401	1RL	C17-C16	6.83	1.54	1.34
6	C	1401	1RL	C4-C10	6.40	1.53	1.43
6	H	1401	1RL	C4-C10	6.22	1.52	1.43
6	C	1401	1RL	C4-N3	5.58	1.38	1.32
6	H	1401	1RL	C15-N1	5.52	1.47	1.35
6	C	1401	1RL	C15-N1	5.42	1.47	1.35
6	H	1401	1RL	C4-N3	5.32	1.38	1.32
6	H	1401	1RL	C12-C11	-5.26	1.33	1.54
6	C	1401	1RL	C12-C11	-5.25	1.33	1.54
6	C	1401	1RL	C18-C19	5.11	1.53	1.33
6	H	1401	1RL	C18-C19	5.05	1.53	1.33
6	H	1401	1RL	C5-C10	4.43	1.52	1.43
6	C	1401	1RL	C5-C10	4.39	1.52	1.43
6	C	1401	1RL	O7-C35	3.61	1.43	1.35
6	H	1401	1RL	O7-C35	3.43	1.42	1.35
6	C	1401	1RL	C3-C4	-3.34	1.41	1.47
6	H	1401	1RL	C18-C17	3.33	1.53	1.43
6	H	1401	1RL	C3-C4	-3.30	1.41	1.47
6	C	1401	1RL	C18-C17	3.25	1.53	1.43
6	H	1401	1RL	C5-C11	-3.04	1.27	1.41
6	C	1401	1RL	C5-C11	-2.99	1.27	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	1RL	C5-C6	-2.89	1.29	1.41
6	H	1401	1RL	C5-C6	-2.88	1.29	1.41
6	H	1401	1RL	O01-C01	2.87	1.41	1.36
6	C	1401	1RL	O01-C01	2.86	1.41	1.36
6	H	1401	1RL	C34-C26	-2.83	1.47	1.53
6	C	1401	1RL	O-C06	2.80	1.45	1.36
6	H	1401	1RL	O-C06	2.78	1.45	1.36
6	C	1401	1RL	C34-C26	-2.73	1.47	1.53
6	C	1401	1RL	O2-C8	2.16	1.42	1.35
6	H	1401	1RL	O7-C25	-2.14	1.41	1.44

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	1RL	C20-C19-C18	-8.21	108.88	126.16
6	H	1401	1RL	C12-O3-C6	-7.62	94.83	107.68
6	C	1401	1RL	C12-O3-C6	-7.42	95.17	107.68
6	C	1401	1RL	C20-C19-C18	-6.74	111.97	126.16
6	C	1401	1RL	C12-C11-C5	6.40	119.83	107.30
6	H	1401	1RL	C12-C11-C5	6.36	119.75	107.30
6	C	1401	1RL	C06-C02-N3	6.30	124.49	118.97
6	H	1401	1RL	C06-C02-N3	6.01	124.25	118.97
6	H	1401	1RL	O4-C11-C5	-5.11	122.06	131.81
6	C	1401	1RL	O4-C11-C5	-5.06	122.16	131.81
6	C	1401	1RL	C10-C4-N3	4.77	124.40	119.27
6	H	1401	1RL	C10-C4-N3	4.59	124.20	119.27
6	C	1401	1RL	O7-C35-C36	4.25	118.91	111.09
6	H	1401	1RL	C34-C26-C25	-3.85	104.50	111.40
6	H	1401	1RL	C17-C18-C19	-3.78	115.36	124.53
6	H	1401	1RL	O7-C35-C36	3.56	117.65	111.09
6	H	1401	1RL	C8-C7-C6	-3.20	106.66	116.35
6	H	1401	1RL	C18-C17-C16	-3.13	117.41	126.61
6	C	1401	1RL	C17-C18-C19	-3.12	116.97	124.53
6	C	1401	1RL	C8-C7-C6	-3.02	107.20	116.35
6	H	1401	1RL	C5-C10-C9	-2.92	114.33	119.66
6	C	1401	1RL	C5-C10-C9	-2.90	114.38	119.66
6	H	1401	1RL	O11-C15-N1	-2.87	117.80	123.92
6	H	1401	1RL	C2-N1-C15	-2.84	116.44	123.41
6	C	1401	1RL	C18-C17-C16	-2.79	118.42	126.61
6	C	1401	1RL	O-C06-C02	2.75	118.54	115.16
6	C	1401	1RL	O11-C15-N1	-2.73	118.09	123.92
6	C	1401	1RL	C2-N1-C15	-2.72	116.74	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	1RL	O-C06-C02	2.65	118.42	115.16
6	C	1401	1RL	C34-C26-C25	-2.63	106.68	111.40
6	H	1401	1RL	C7-C8-C9	2.59	127.07	121.82
6	C	1401	1RL	C06-C02-C01	-2.49	116.11	118.22
6	H	1401	1RL	C06-C02-C01	-2.32	116.25	118.22
6	C	1401	1RL	C26-C25-C24	-2.22	110.14	114.68
6	C	1401	1RL	O3-C12-C13	2.22	115.75	109.55
6	C	1401	1RL	C13-C12-C11	2.22	119.39	113.90
6	H	1401	1RL	C13-C12-C11	2.17	119.28	113.90
6	H	1401	1RL	O3-C12-C13	2.16	115.57	109.55
6	H	1401	1RL	C31-C20-C21	2.16	115.82	111.31
6	H	1401	1RL	C26-C25-C24	-2.15	110.29	114.68
6	H	1401	1RL	C23-C22-C21	-2.12	108.28	112.54
6	C	1401	1RL	C7-C8-C9	2.11	126.10	121.82
6	C	1401	1RL	C1-C9-C8	-2.09	116.66	119.17
6	C	1401	1RL	C8-C9-C10	2.06	123.64	119.41
6	H	1401	1RL	C31-C20-C19	-2.06	105.00	109.99
6	H	1401	1RL	C1-C9-C8	-2.06	116.70	119.17
6	H	1401	1RL	O7-C25-C24	2.03	112.22	107.50
6	H	1401	1RL	C14-C7-C6	2.01	124.38	121.30

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	1RL	C11-C12-O5-C29
6	C	1401	1RL	C13-C12-O5-C29
6	C	1401	1RL	C16-C17-C18-C19
6	C	1401	1RL	C19-C20-C21-O10
6	C	1401	1RL	C31-C20-C21-C22
6	C	1401	1RL	C21-C22-C23-C24
6	C	1401	1RL	C32-C22-C23-C24
6	C	1401	1RL	C26-C27-C28-C29
6	H	1401	1RL	C11-C12-O5-C29
6	H	1401	1RL	C13-C12-O5-C29
6	H	1401	1RL	C30-C16-C17-C18
6	H	1401	1RL	C19-C20-C21-O10
6	H	1401	1RL	C31-C20-C21-C22
6	H	1401	1RL	C21-C22-C23-C24
6	H	1401	1RL	C32-C22-C23-C24
6	H	1401	1RL	C26-C27-C28-C29
6	H	1401	1RL	O8-C35-O7-C25

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RL	O8-C35-O7-C25
6	C	1401	1RL	C32-C22-C23-O9
6	H	1401	1RL	C32-C22-C23-O9
6	C	1401	1RL	C21-C22-C23-O9
6	H	1401	1RL	C21-C22-C23-O9
6	C	1401	1RL	C17-C18-C19-C20
6	H	1401	1RL	C17-C18-C19-C20
6	C	1401	1RL	C33-C24-C25-C26
6	H	1401	1RL	C33-C24-C25-C26
6	C	1401	1RL	C36-C35-O7-C25
6	C	1401	1RL	C23-C24-C25-C26
6	H	1401	1RL	C36-C35-O7-C25
6	C	1401	1RL	C31-C20-C21-O10
6	H	1401	1RL	C31-C20-C21-O10
6	C	1401	1RL	C30-C16-C17-C18
6	C	1401	1RL	C19-C20-C21-C22
6	H	1401	1RL	C19-C20-C21-C22
6	C	1401	1RL	C33-C24-C25-O7
6	C	1401	1RL	C23-C24-C25-O7
6	H	1401	1RL	C23-C24-C25-O7
6	H	1401	1RL	C23-C24-C25-C26
6	H	1401	1RL	C33-C24-C25-O7
6	C	1401	1RL	C-C39-N-C08
6	H	1401	1RL	C-C39-N-C08
6	H	1401	1RL	C-C39-N-C09
6	C	1401	1RL	C15-C16-C17-C18
6	H	1401	1RL	C15-C16-C17-C18
6	C	1401	1RL	C-C39-N-C09
6	C	1401	1RL	O3-C12-O5-C29
6	H	1401	1RL	O3-C12-O5-C29
6	H	1401	1RL	C16-C17-C18-C19
6	C	1401	1RL	C28-C29-O5-C12
6	H	1401	1RL	C28-C29-O5-C12
6	C	1401	1RL	N1-C15-C16-C17
6	H	1401	1RL	N1-C15-C16-C17
6	H	1401	1RL	O11-C15-C16-C17
6	C	1401	1RL	O7-C25-C26-C34
6	H	1401	1RL	O7-C25-C26-C34
6	C	1401	1RL	O7-C25-C26-C27
6	C	1401	1RL	O11-C15-C16-C17
6	C	1401	1RL	O6-C27-C28-C29
6	H	1401	1RL	O6-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RL	O11-C15-C16-C30

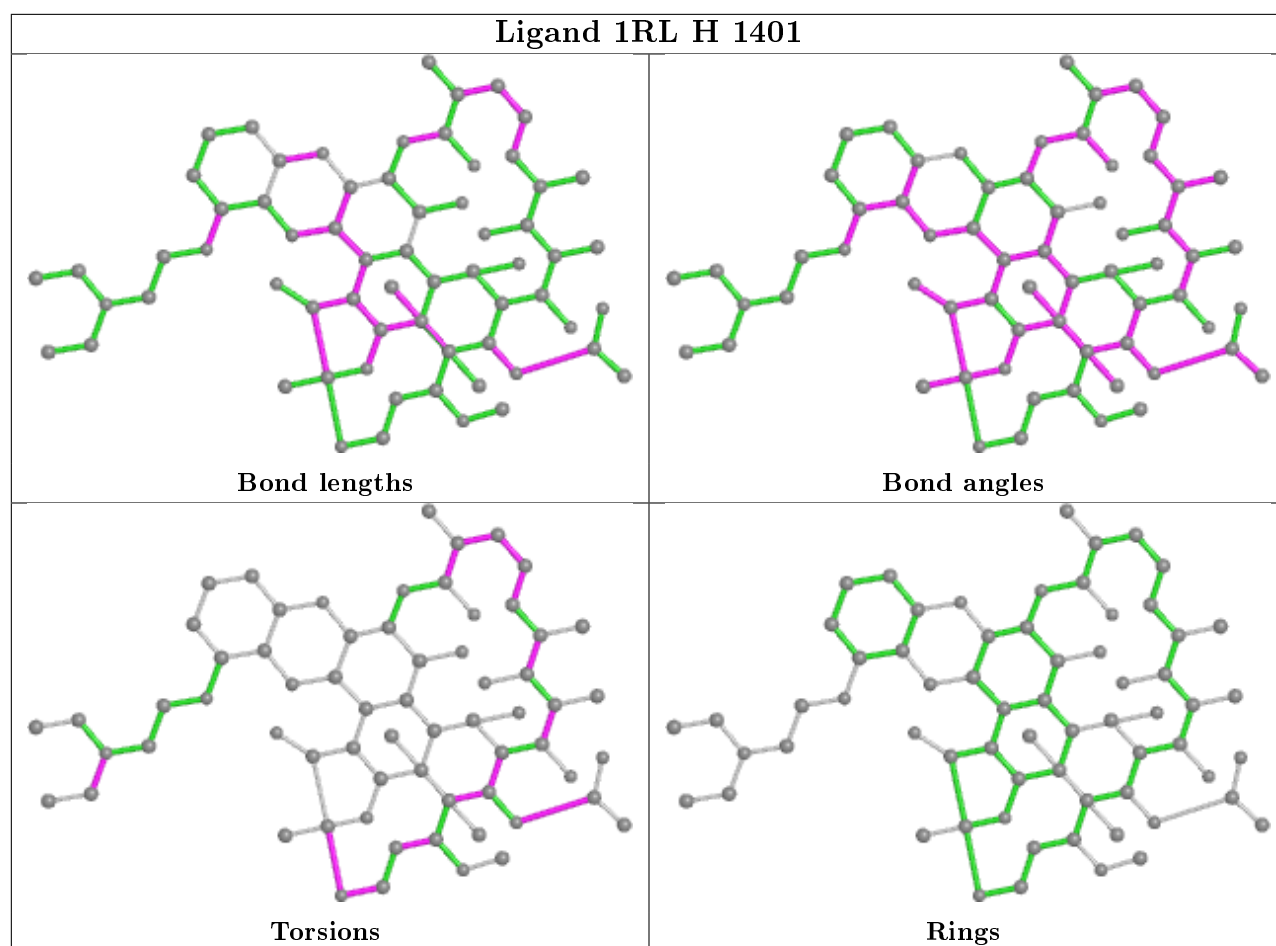
There are no ring outliers.

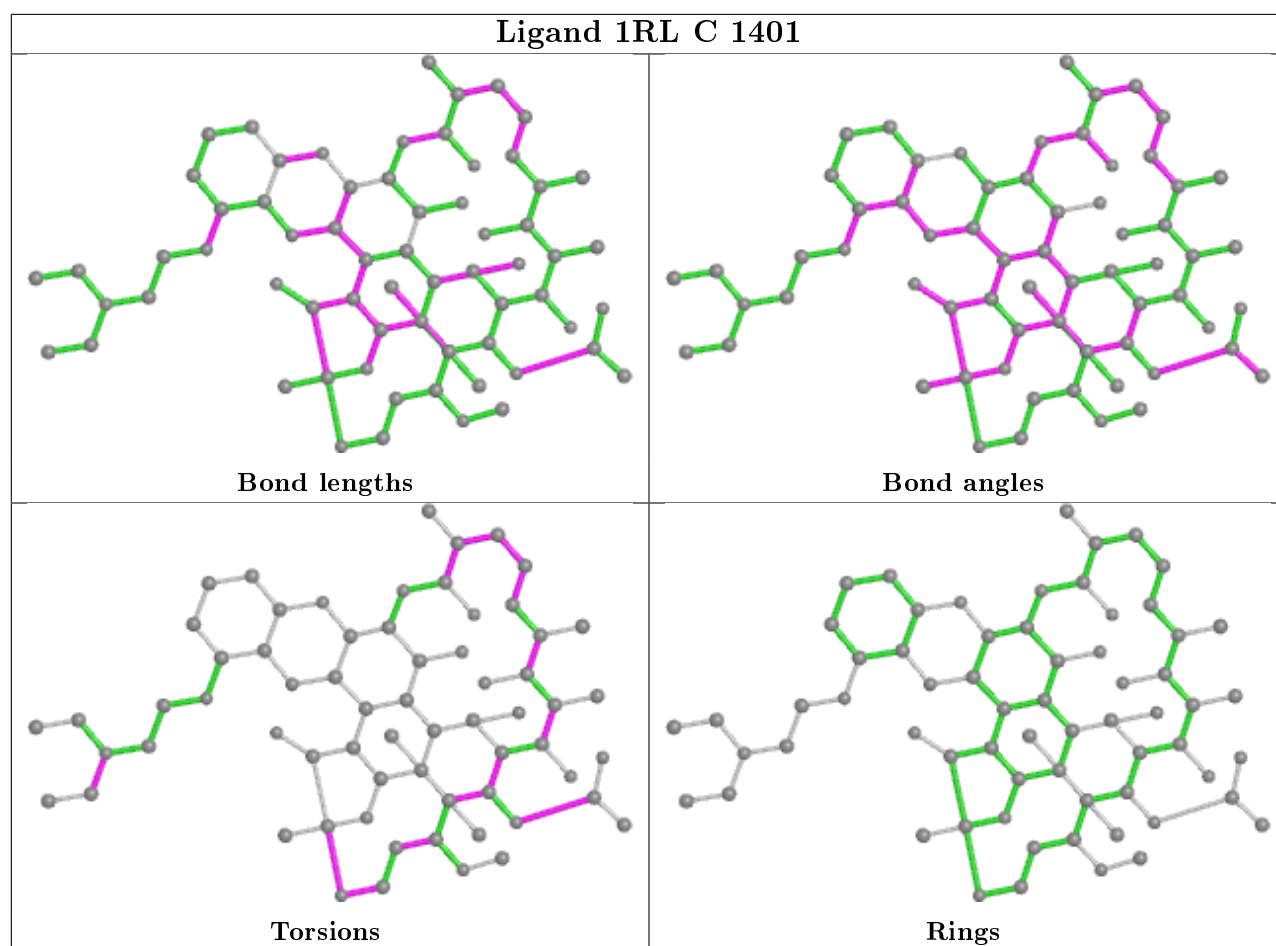
2 monomers are involved in 16 short contacts:

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

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/329 (98%)	0.01	10 (3%) 49 38	0, 68, 172, 270	0
1	B	221/329 (67%)	0.33	15 (6%) 17 14	6, 90, 201, 277	0
1	F	229/329 (69%)	0.41	22 (9%) 8 7	9, 123, 209, 249	0
1	G	217/329 (65%)	0.40	21 (9%) 7 7	34, 112, 176, 230	0
2	C	1335/1342 (99%)	-0.06	47 (3%) 44 35	0, 43, 165, 367	0
2	H	1335/1342 (99%)	0.10	81 (6%) 21 17	0, 81, 205, 388	0
3	D	1160/1407 (82%)	-0.03	38 (3%) 46 37	0, 34, 158, 313	0
3	I	1160/1407 (82%)	0.11	72 (6%) 20 16	0, 50, 190, 338	0
4	E	90/91 (98%)	-0.35	1 (1%) 80 72	0, 34, 108, 170	0
4	J	76/91 (83%)	0.16	4 (5%) 26 23	3, 75, 160, 201	0
5	X	517/613 (84%)	0.26	44 (8%) 10 9	1, 99, 236, 425	0
5	Y	458/613 (74%)	0.19	37 (8%) 12 10	1, 102, 234, 374	0
All	All	7121/8222 (86%)	0.09	392 (5%) 25 22	0, 66, 199, 425	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	X	319	ALA	12.8
5	X	36	VAL	11.2
5	Y	239	GLY	9.5
5	X	35	ILE	9.2
3	I	11	GLN	8.8
3	I	10	ALA	8.5
5	X	24	TYR	8.1
2	C	251	ALA	7.5
2	H	1002	LEU	7.5
2	C	231	GLU	7.4
5	X	56	MET	7.2

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Mol	Chain	Res	Type	RSRZ
5	X	53	ILE	7.0
1	B	169	GLY	6.9
2	H	334	GLU	6.8
2	C	232	ILE	6.7
3	I	212	THR	6.6
5	X	318	ALA	6.5
5	Y	337	VAL	6.2
3	I	208	THR	6.2
5	Y	317	ASN	6.0
3	D	1199	PHE	5.7
3	D	1171	GLY	5.7
1	F	194	GLN	5.7
1	G	171	LEU	5.6
3	I	1161	GLY	5.6
3	I	13	LYS	5.5
5	Y	320	ILE	5.5
2	C	116	ASP	5.5
1	F	162	GLU	5.5
2	H	1000	LEU	5.5
1	F	148	ARG	5.5
3	I	12	THR	5.4
2	H	1001	GLY	5.4
3	D	1203	ARG	5.4
3	I	1203	ARG	5.3
2	C	332	ARG	5.2
1	A	193	GLU	5.2
5	X	315	TRP	5.1
1	B	172	LEU	5.0
1	F	161	SER	5.0
2	H	998	LEU	4.9
1	B	171	LEU	4.8
1	G	172	LEU	4.8
2	C	238	GLN	4.8
2	H	981	ALA	4.7
2	C	305	SER	4.7
5	Y	241	SER	4.7
3	I	521	LYS	4.7
3	I	732	GLY	4.7
2	H	1004	ASP	4.6
2	H	1003	THR	4.6
3	I	830	ASP	4.6
2	H	258	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	193	GLU	4.6
3	I	1375	ALA	4.6
2	C	233	ARG	4.5
2	H	299	LYS	4.5
3	I	9	LYS	4.5
3	I	217	LEU	4.4
2	H	996	ARG	4.4
2	H	1007	LYS	4.4
5	X	6	GLN	4.4
5	X	54	GLN	4.3
2	H	990	ASP	4.3
2	C	165	HIS	4.3
2	H	332	ARG	4.2
3	D	210	SER	4.2
5	X	239	GLY	4.2
3	D	80	HIS	4.2
3	I	213	LYS	4.2
5	X	241	SER	4.1
3	D	1133	ASP	4.1
2	C	331	LYS	4.1
5	Y	212	ILE	4.0
5	Y	318	ALA	4.0
3	I	205	LEU	4.0
1	G	122	GLU	4.0
2	H	264	GLU	4.0
5	Y	321	ALA	4.0
3	I	333	GLY	3.9
2	H	483	ASP	3.9
3	I	1162	ILE	3.9
1	A	3	GLY	3.9
1	A	41	ASN	3.9
5	Y	305	LEU	3.9
1	F	164	ASP	3.8
2	C	266	GLY	3.8
5	Y	421	TYR	3.8
5	Y	489	MET	3.8
2	C	118	LYS	3.8
2	H	972	PHE	3.8
5	X	52	GLY	3.8
2	H	999	GLU	3.8
5	Y	293	GLU	3.7
3	D	830	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	41	ASN	3.7
5	X	307	THR	3.7
5	X	44	ILE	3.7
2	H	305	SER	3.7
2	H	265	LYS	3.6
3	I	712	GLN	3.6
2	H	1008	GLN	3.6
5	Y	240	ARG	3.6
5	X	340	ALA	3.6
3	I	477	GLN	3.6
2	H	251	ALA	3.6
2	H	1006	GLU	3.6
3	I	876	SER	3.6
3	I	564	VAL	3.6
3	I	563	LEU	3.6
5	X	57	GLU	3.6
2	H	983	GLY	3.5
5	Y	574	GLU	3.5
2	C	311	CYS	3.5
2	H	744	GLY	3.5
1	G	18	GLN	3.5
3	D	211	GLU	3.5
1	G	96	ASP	3.5
1	G	13	LEU	3.4
5	Y	311	THR	3.4
2	H	165	HIS	3.4
2	H	970	GLY	3.4
3	D	212	THR	3.4
3	I	1376	GLY	3.4
2	C	172	TYR	3.4
3	D	1172	LYS	3.4
1	B	147	GLN	3.4
2	C	1000	LEU	3.4
1	B	73	GLY	3.4
2	H	1152	GLY	3.4
2	H	982	GLY	3.3
5	Y	340	ALA	3.3
3	D	878	ASP	3.3
5	X	237	ALA	3.3
5	X	43	ASP	3.3
5	Y	319	ALA	3.3
3	D	932	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	4	SER	3.2
5	X	306	PHE	3.2
2	C	267	ARG	3.2
3	D	1179	PRO	3.2
2	C	334	GLU	3.2
2	C	250	THR	3.2
3	I	204	GLU	3.2
3	D	477	GLN	3.2
1	B	121	VAL	3.2
3	I	831	VAL	3.2
1	F	110	VAL	3.2
2	H	742	TYR	3.2
2	H	969	ALA	3.2
2	C	77	GLU	3.2
2	H	252	SER	3.2
5	X	485	GLU	3.1
1	F	95	LYS	3.1
2	H	1010	GLN	3.1
3	D	314	ARG	3.1
2	H	374	GLU	3.1
3	D	528	THR	3.1
1	G	191	ARG	3.1
3	D	1198	VAL	3.1
2	H	912	ASP	3.0
3	I	708	ASN	3.0
5	X	240	ARG	3.0
5	Y	316	PHE	3.0
3	I	540	GLY	3.0
1	B	170	ARG	3.0
2	C	304	GLU	3.0
3	I	80	HIS	3.0
1	F	192	VAL	2.9
2	H	1072	ASN	2.9
2	C	483	ASP	2.9
2	C	999	GLU	2.9
2	H	60	GLN	2.9
3	I	676	GLY	2.9
1	G	127	GLN	2.9
3	D	831	VAL	2.9
5	X	314	THR	2.9
3	I	559	ALA	2.9
2	H	725	GLN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	I	174	ASP	2.9
5	Y	315	TRP	2.9
2	C	258	ASN	2.9
1	G	182	ARG	2.8
5	X	322	MET	2.8
3	I	1172	LYS	2.8
5	X	478	PRO	2.8
2	C	76	GLY	2.8
2	C	237	LEU	2.8
3	D	333	GLY	2.8
3	D	1170	LYS	2.8
5	Y	478	PRO	2.8
1	F	147	GLN	2.8
2	C	252	SER	2.8
1	G	51	MET	2.8
3	I	1374	ALA	2.8
5	X	305	LEU	2.8
2	H	995	ASP	2.8
2	H	298	ALA	2.8
3	I	675	ALA	2.8
1	F	163	GLU	2.8
2	H	975	ILE	2.8
5	Y	322	MET	2.7
3	I	1250	ASP	2.7
2	H	1005	GLU	2.7
1	G	75	GLN	2.7
1	A	245	GLU	2.7
5	Y	309	ASN	2.7
2	C	265	LYS	2.7
3	I	837	ASP	2.7
2	H	333	ILE	2.7
2	H	107	ARG	2.7
1	G	23	HIS	2.7
2	H	986	ALA	2.7
1	G	204	GLU	2.7
3	D	829	GLY	2.7
3	I	1168	GLU	2.7
3	D	931	THR	2.7
5	X	327	SER	2.6
2	C	236	LYS	2.6
2	H	172	TYR	2.6
2	H	974	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	832	LYS	2.6
3	I	209	ASN	2.6
1	F	94	GLY	2.6
2	H	269	ILE	2.6
3	D	547	ARG	2.6
2	C	1001	GLY	2.6
5	X	260	ARG	2.6
5	Y	336	GLU	2.6
1	F	234	LEU	2.6
1	G	107	ILE	2.6
2	H	662	SER	2.6
2	H	1070	HIS	2.6
2	H	301	TYR	2.6
5	Y	310	GLU	2.6
2	H	111	GLU	2.6
3	I	218	THR	2.6
2	H	987	GLU	2.6
2	H	108	GLU	2.5
2	H	984	VAL	2.5
3	I	1273	ASP	2.5
2	H	1009	ASN	2.5
2	H	263	VAL	2.5
3	D	1200	GLU	2.5
5	Y	273	MET	2.5
5	X	328	GLU	2.5
1	B	168	ILE	2.5
2	H	727	VAL	2.5
3	I	674	THR	2.5
1	B	122	GLU	2.5
2	H	908	GLU	2.5
5	X	8	GLN	2.5
5	Y	312	SER	2.5
5	Y	341	LEU	2.5
1	G	24	ALA	2.5
2	H	169	LYS	2.5
1	B	57	THR	2.5
1	F	96	ASP	2.4
2	H	234	ASP	2.4
5	X	583	THR	2.4
3	D	344	GLY	2.4
3	D	445	LYS	2.4
3	I	709	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
5	X	34	ASP	2.4
2	C	230	PHE	2.4
3	I	1198	VAL	2.4
3	I	746	LEU	2.4
2	H	997	TRP	2.4
2	C	257	ALA	2.4
1	A	5	VAL	2.4
2	C	319	LEU	2.4
2	H	720	ARG	2.4
5	X	293	GLU	2.4
5	X	515	GLU	2.4
2	H	1071	GLY	2.4
5	Y	237	ALA	2.4
3	D	471	PRO	2.4
5	X	422	ARG	2.4
1	G	157	THR	2.4
3	I	210	SER	2.4
1	A	241	GLU	2.3
1	G	123	ILE	2.3
5	X	289	LYS	2.3
2	H	106	GLU	2.3
2	H	979	LEU	2.3
1	G	86	LYS	2.3
3	I	1204	VAL	2.3
3	D	875	ASN	2.3
3	I	847	ASP	2.3
1	F	131	CYS	2.3
3	I	392	THR	2.3
1	A	162	GLU	2.3
3	D	1185	PRO	2.3
3	D	69	GLU	2.3
2	C	482	GLY	2.3
4	J	2	ALA	2.3
2	C	978	VAL	2.3
2	H	980	VAL	2.3
5	Y	238	LYS	2.3
3	I	747	MET	2.3
3	I	565	ALA	2.3
2	C	996	ARG	2.3
5	Y	578	LYS	2.3
1	B	70	THR	2.3
3	I	586	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	473	THR	2.3
3	I	1167	LYS	2.3
3	I	587	LEU	2.2
3	I	8	LEU	2.2
5	X	310	GLU	2.2
5	X	311	THR	2.2
1	B	59	VAL	2.2
2	H	232	ILE	2.2
3	I	207	GLU	2.2
3	I	1295	ASN	2.2
3	I	154	LEU	2.2
2	C	1016	GLU	2.2
5	Y	490	PRO	2.2
1	G	173	VAL	2.2
3	I	1171	GLY	2.2
5	Y	333	VAL	2.2
3	D	1168	GLU	2.2
2	H	254	ASP	2.2
2	H	268	ARG	2.2
3	I	713	GLU	2.2
2	H	1153	ALA	2.2
3	I	716	GLN	2.2
1	G	87	GLY	2.1
3	I	473	THR	2.1
2	C	310	ILE	2.1
1	F	73	GLY	2.1
4	E	91	ARG	2.1
3	D	82	GLY	2.1
3	I	811	GLU	2.1
1	F	211	ILE	2.1
2	H	1134	GLN	2.1
3	I	1373	ARG	2.1
3	I	211	GLU	2.1
2	C	1002	LEU	2.1
2	H	1020	GLU	2.1
2	H	61	SER	2.1
3	D	670	SER	2.1
2	C	282	VAL	2.1
1	F	97	GLU	2.1
3	I	1213	GLY	2.1
1	A	133	LEU	2.1
2	C	1040	ASP	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	I	267	ASP	2.1
5	X	482	GLU	2.1
1	B	146	VAL	2.1
1	A	243	LYS	2.1
1	F	196	THR	2.1
1	B	178	SER	2.1
2	H	1018	TYR	2.1
1	F	24	ALA	2.1
2	C	57	PHE	2.1
2	C	1023	HIS	2.1
3	D	1204	VAL	2.1
3	I	1202	GLU	2.1
4	J	36	ASP	2.1
4	J	37	PRO	2.1
2	H	1264	GLN	2.1
5	Y	420	GLU	2.1
3	I	1249	ASN	2.1
2	C	268	ARG	2.0
1	F	41	ASN	2.0
2	H	953	LEU	2.0
5	Y	483	LEU	2.0
2	C	375	PRO	2.0
3	I	19	ALA	2.0
5	X	514	ASP	2.0
1	G	181	GLU	2.0
3	I	520	ALA	2.0
2	H	601	ASP	2.0
5	Y	261	LEU	2.0
3	I	875	ASN	2.0
3	D	638	SER	2.0
5	Y	330	LEU	2.0
2	C	374	GLU	2.0
2	H	718	ALA	2.0
1	F	128	HIS	2.0
2	C	574	SER	2.0
5	X	9	LEU	2.0
5	X	32	PRO	2.0
2	H	988	LYS	2.0
5	Y	488	LEU	2.0
3	D	207	GLU	2.0
5	X	423	ARG	2.0
2	C	982	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	413	GLU	2.0
4	J	77	ALA	2.0
5	X	325	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

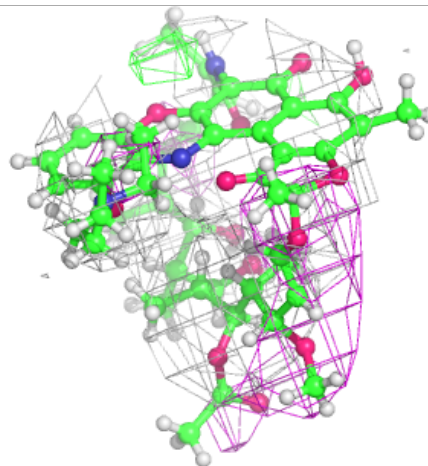
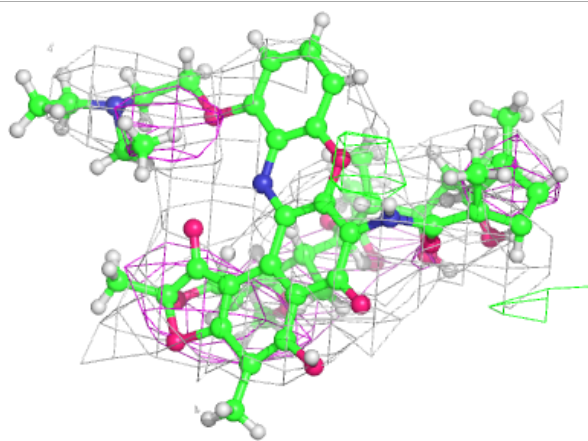
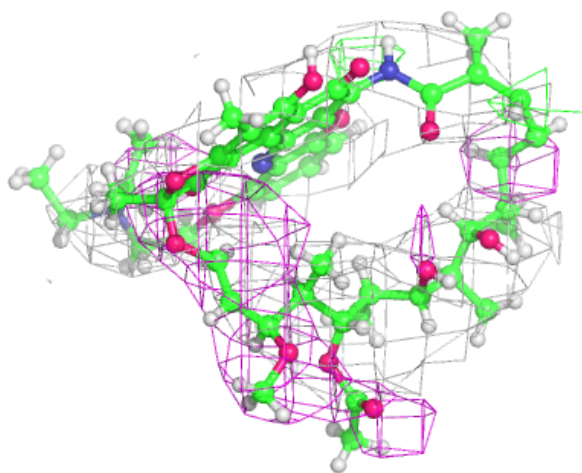
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	1RL	H	1401	65/65	0.79	0.42	20,20,20,20	0
6	1RL	C	1401	65/65	0.82	0.36	20,20,20,20	0
8	MG	I	1503	1/1	0.92	0.66	20,20,20,20	0
7	ZN	D	1501	1/1	0.94	0.05	54,54,54,54	0
7	ZN	I	1501	1/1	0.95	0.03	60,60,60,60	0
7	ZN	D	1502	1/1	0.96	0.19	8,8,8,8	0
8	MG	D	1503	1/1	0.96	0.32	24,24,24,24	0
7	ZN	I	1502	1/1	0.98	0.11	49,49,49,49	0

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

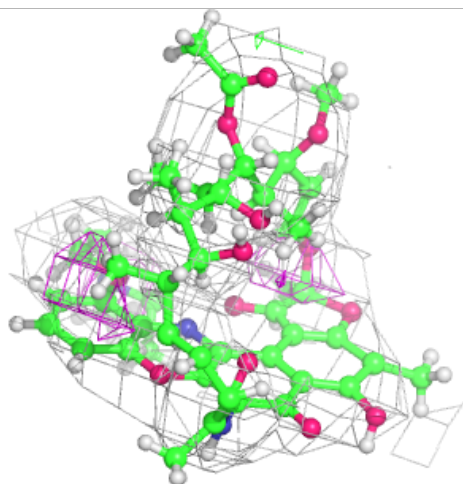
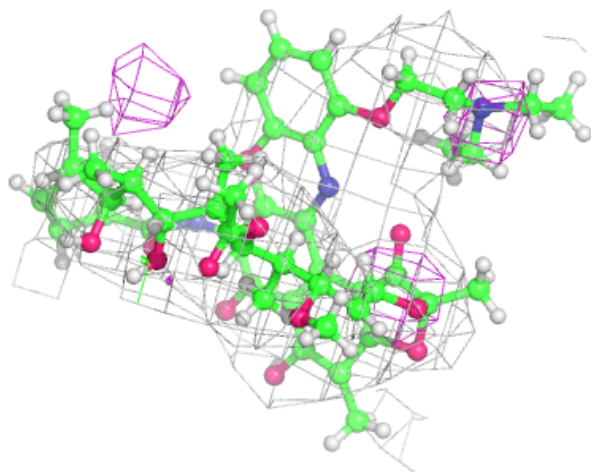
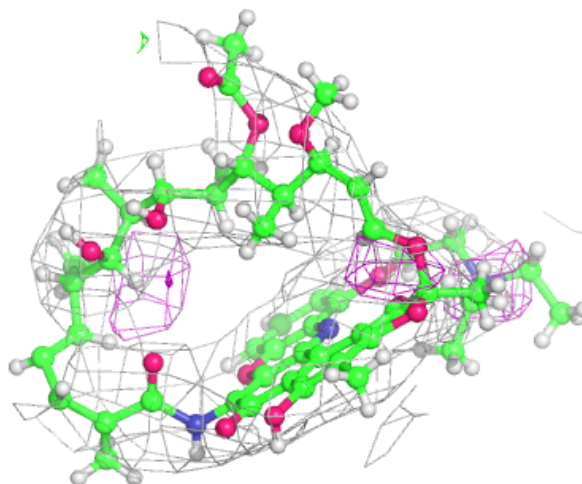
**Electron density around 1RL H 1401:**

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



**Electron density around 1RL C 1401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.