



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:19 pm BST

PDB ID : 3UUS  
Title : Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reductase complex  
Authors : Zimanyi, C.M.; Drennan, C.L.  
Deposited on : 2011-11-28  
Resolution : 5.65 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

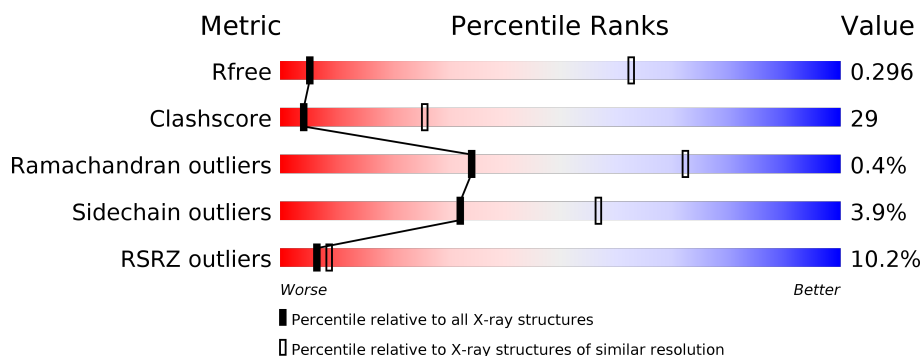
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.65 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	1006 (7.40-3.84)
Clashscore	141614	1018 (7.40-3.90)
Ramachandran outliers	138981	1001 (7.40-3.84)
Sidechain outliers	138945	1203 (7.50-3.80)
RSRZ outliers	127900	1000 (7.54-3.78)

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	761	<div> <div>7%</div> <div>48%</div> <div>45%</div> <div>• •</div> </div>
1	B	761	<div> <div>7%</div> <div>48%</div> <div>46%</div> <div>• •</div> </div>
1	C	761	<div> <div>21%</div> <div>50%</div> <div>44%</div> <div>• •</div> </div>
1	D	761	<div> <div>22%</div> <div>51%</div> <div>43%</div> <div>• •</div> </div>
2	E	375	<div> <div>%</div> <div>49%</div> <div>43%</div> <div>• 7%</div> </div>
2	F	375	<div> <div>%</div> <div>50%</div> <div>42%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	375	
2	H	375	

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
3	DTP	A	800	-	-	X	X
3	DTP	B	800	-	-	-	X
3	DTP	B	900	-	-	-	X
3	DTP	C	800	-	-	X	X
3	DTP	C	900	-	-	-	X
3	DTP	D	800	-	-	X	X
3	DTP	D	900	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35029 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

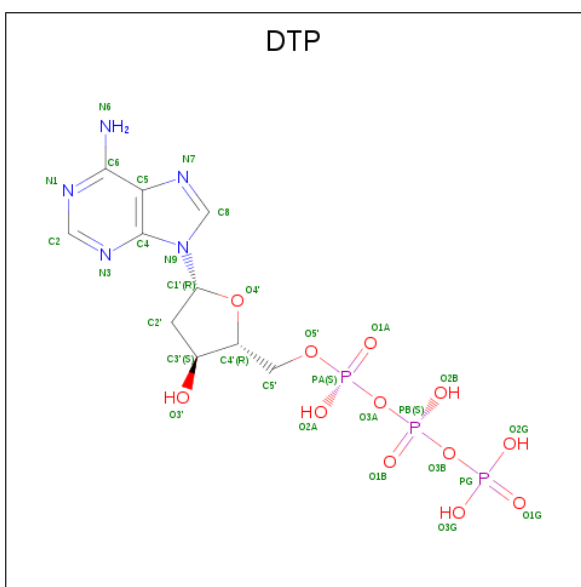
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5829	3702	1001	1102	24			
1	B	732	Total	C	N	O	S	0	0	0
			5829	3702	1001	1102	24			
1	C	732	Total	C	N	O	S	0	0	0
			5829	3702	1001	1102	24			
1	D	732	Total	C	N	O	S	0	0	0
			5829	3702	1001	1102	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	348	Total	C	N	O	S	0	0	0
			2855	1824	474	544	13			
2	F	348	Total	C	N	O	S	0	0	0
			2855	1824	474	544	13			
2	G	352	Total	C	N	O	S	0	0	0
			2885	1841	478	553	13			
2	H	350	Total	C	N	O	S	0	0	0
			2870	1833	476	548	13			

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

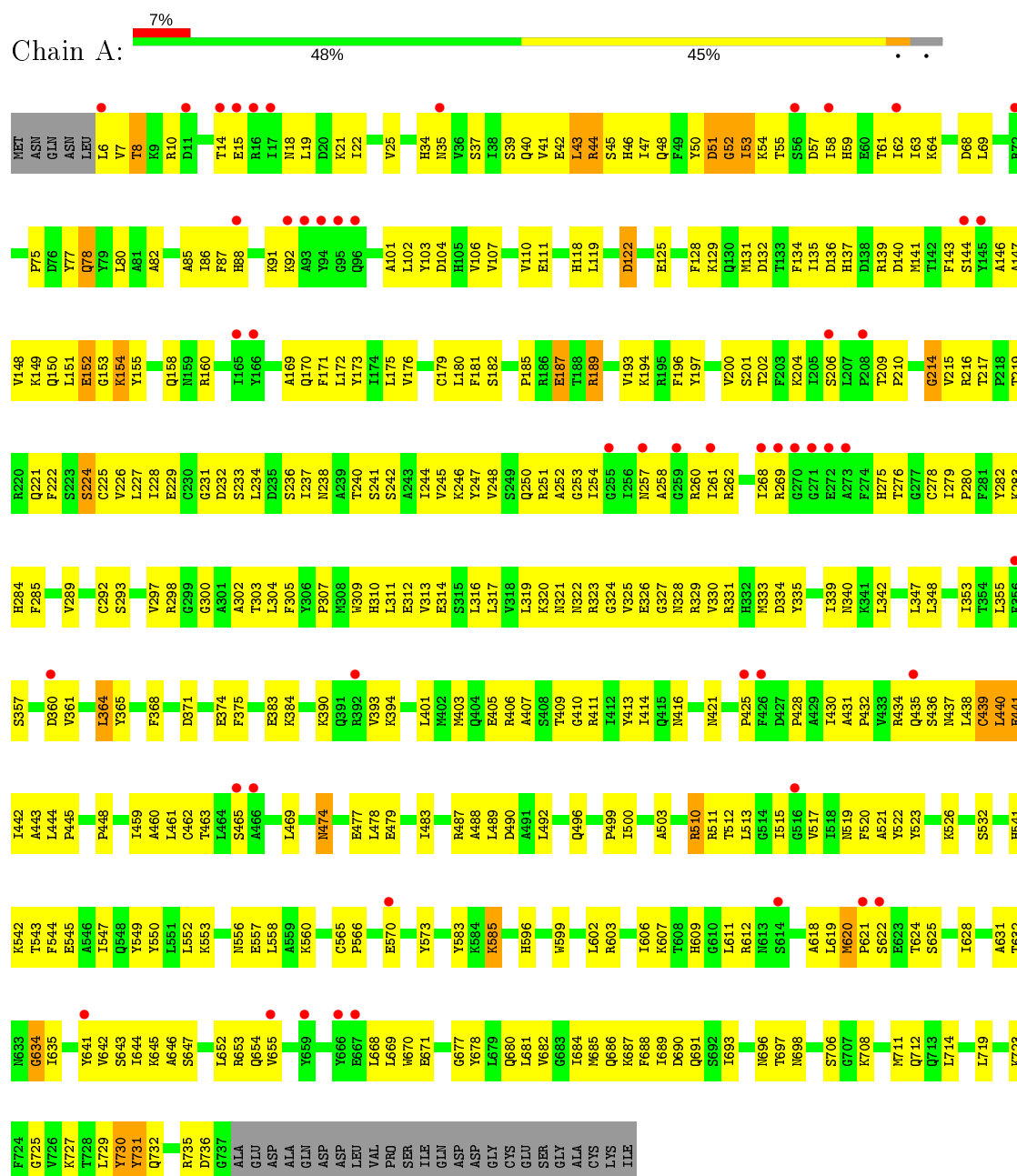
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	Fe	0	0
			2	2		
4	G	2	Total	Fe	0	0
			2	2		
4	F	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

### 3 Residue-property plots

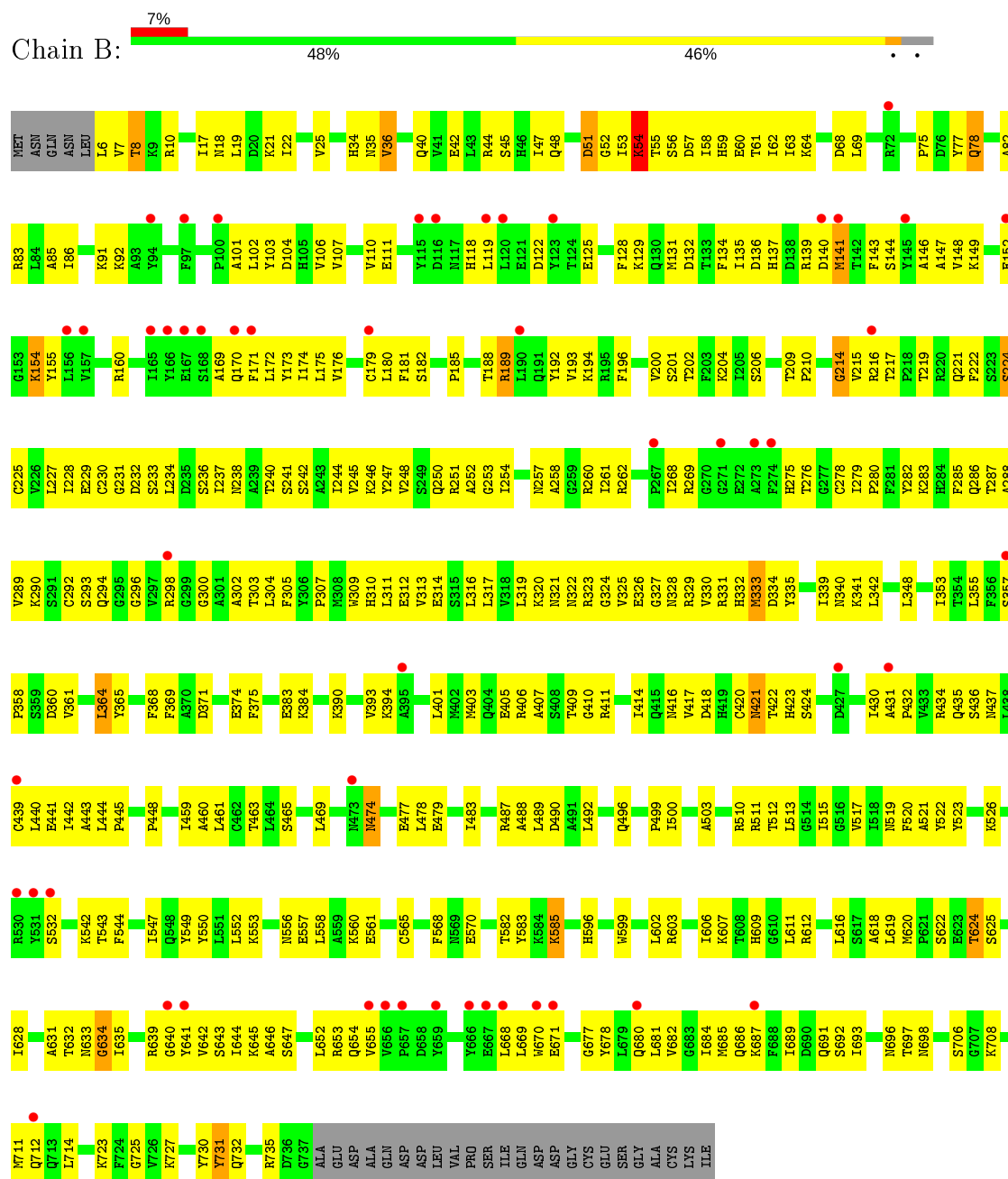
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ribonucleoside-diphosphate reductase 1 subunit alpha



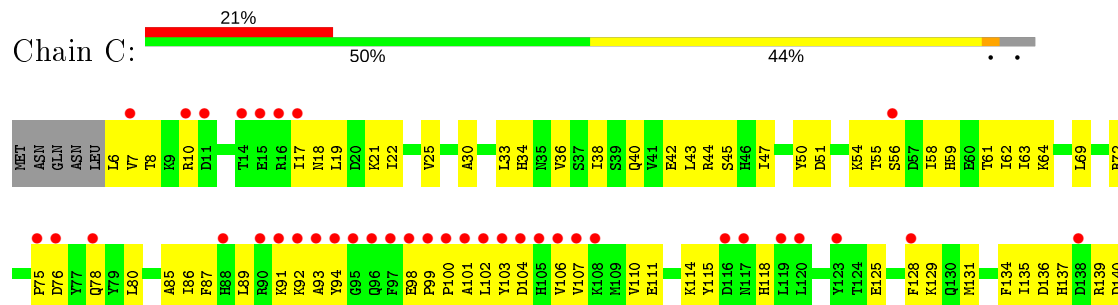
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

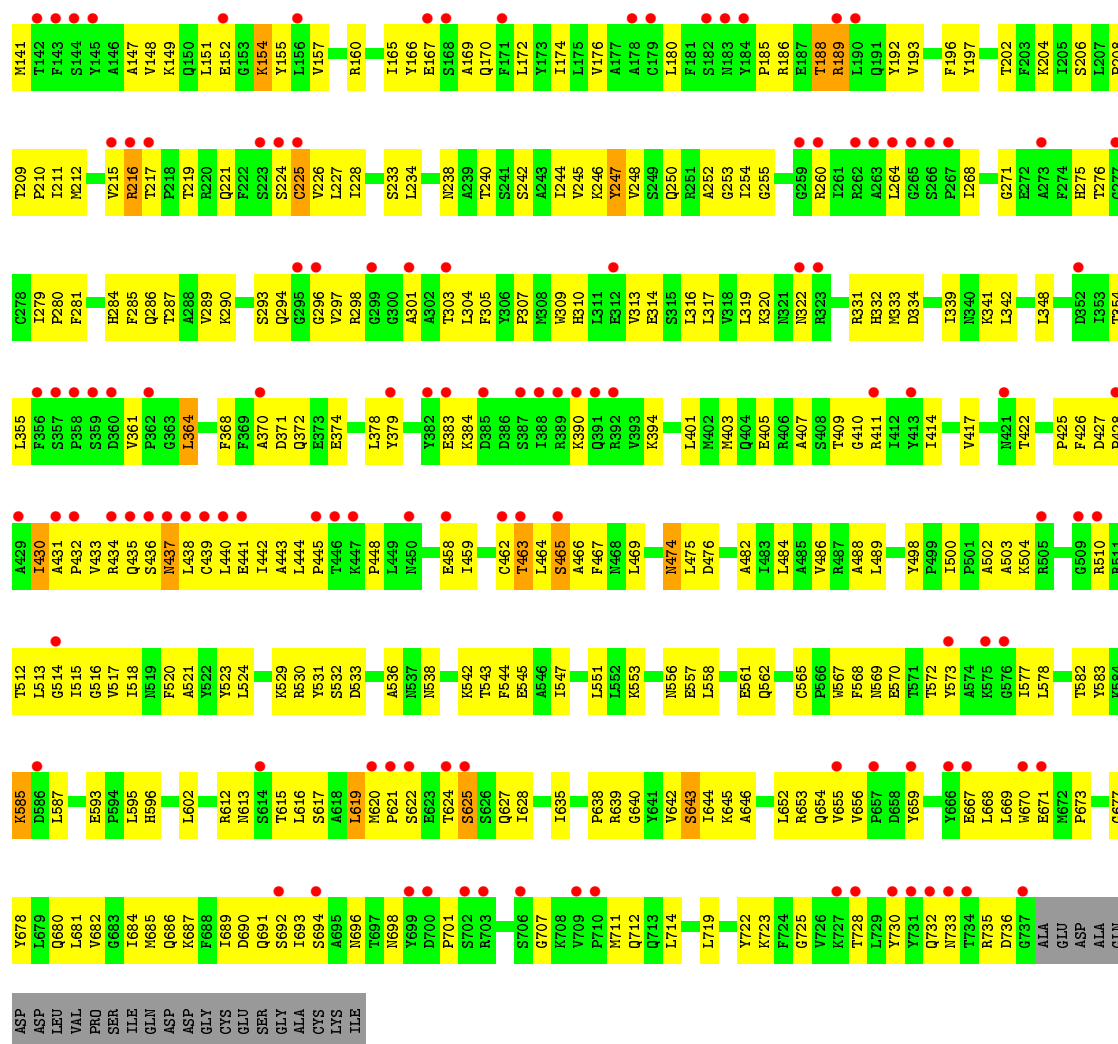
Chain B:



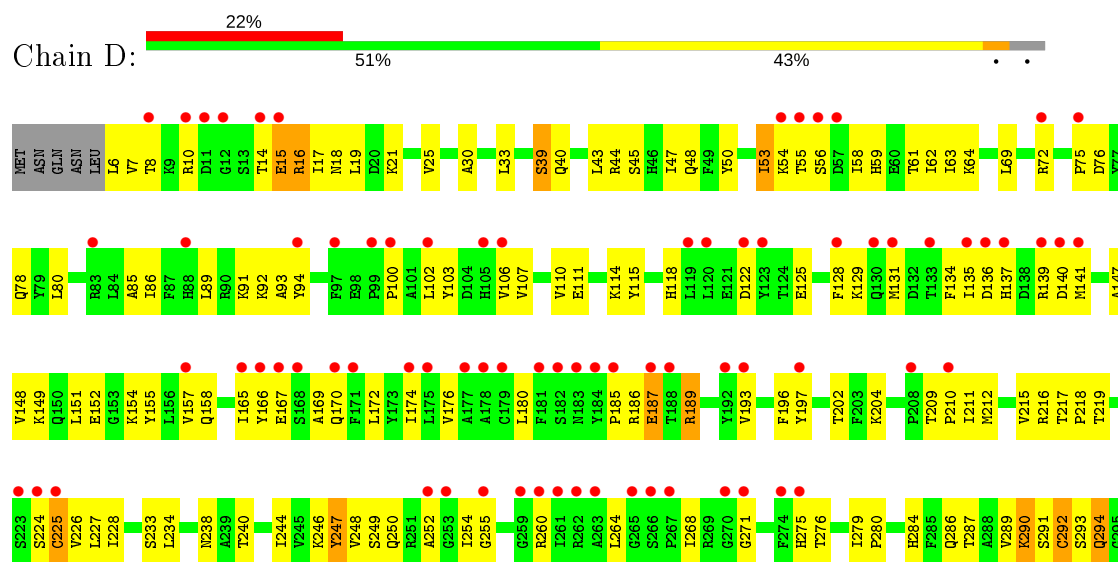
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

Chain C:

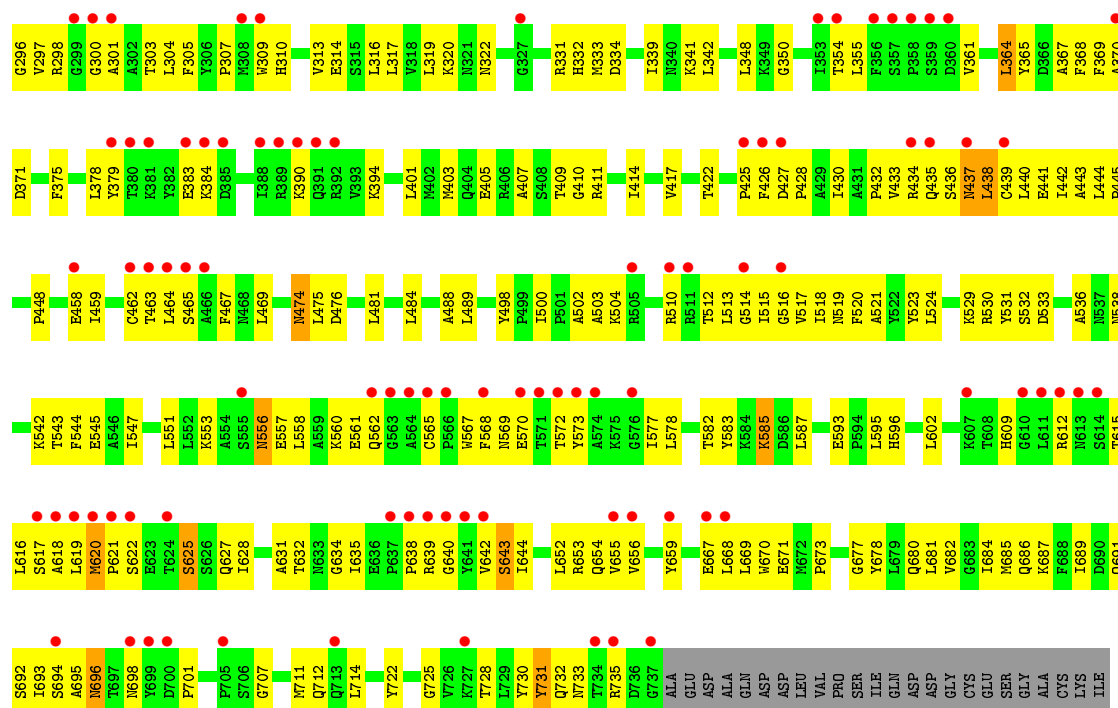




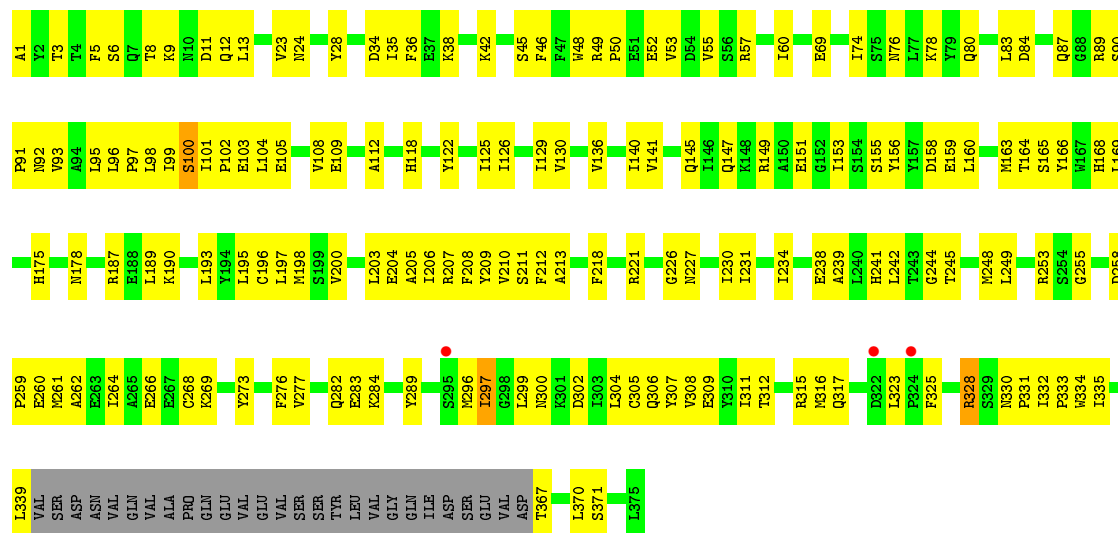
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



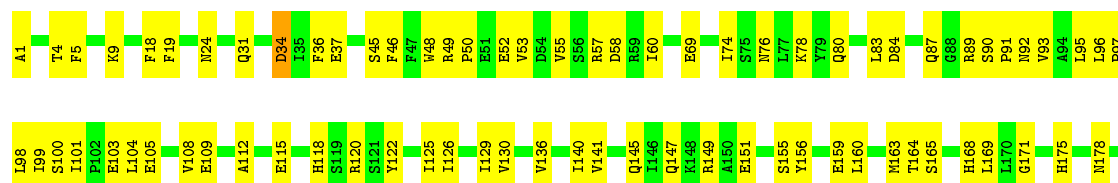


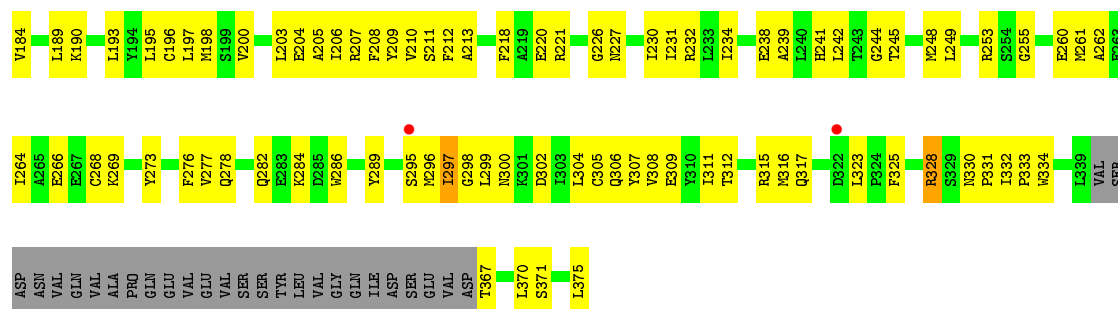


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

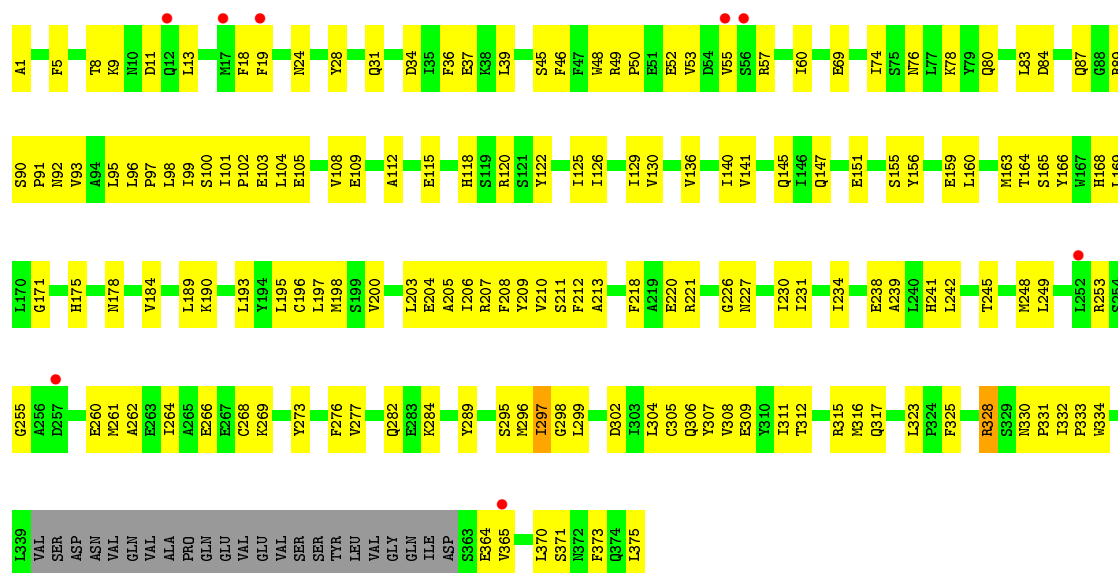


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

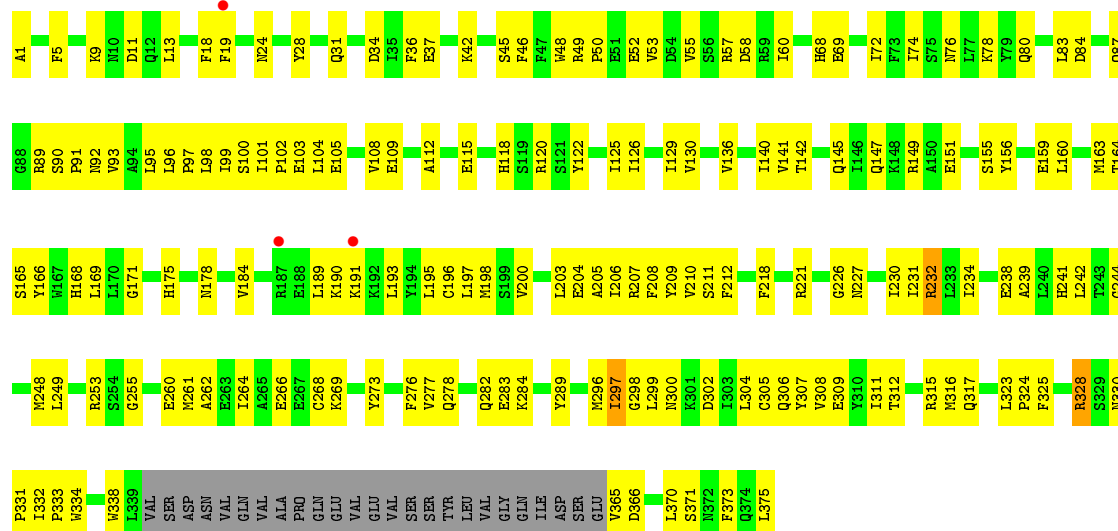




• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	287.36 Å   153.46 Å   169.42 Å 90.00°   119.91°   90.00°	Depositor
Resolution (Å)	50.00 – 5.65 48.95 – 5.64	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-5.65) 90.9 (48.95-5.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 5.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.257   ,   0.303 0.247   ,   0.296	Depositor DCC
$R_{free}$ test set	967 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	194.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 178.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	35029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	242.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: DTP, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/5957	0.47	1/8068 (0.0%)
1	B	0.25	0/5957	0.47	1/8068 (0.0%)
1	C	0.24	0/5957	0.46	0/8068
1	D	0.25	0/5957	0.47	1/8068 (0.0%)
2	E	0.25	0/2919	0.44	0/3957
2	F	0.25	0/2919	0.43	0/3957
2	G	0.25	0/2949	0.43	0/3998
2	H	0.25	0/2934	0.43	0/3978
All	All	0.25	0/35549	0.46	3/48162 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	GLN	O-C-N	5.91	132.15	122.70
1	B	48	GLN	O-C-N	5.87	132.09	122.70
1	A	48	GLN	O-C-N	5.84	132.05	122.70

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	5829	0	5753	400	0
1	B	5829	0	5751	358	0
1	C	5829	0	5751	414	0
1	D	5829	0	5751	405	0
2	E	2855	0	2789	150	0
2	F	2855	0	2789	140	0
2	G	2885	0	2813	139	0
2	H	2870	0	2802	140	0
3	A	60	0	22	19	0
3	B	60	0	22	12	0
3	C	60	0	22	20	0
3	D	60	0	22	19	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
All	All	35029	0	34287	2042	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 29.

All (2042) 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)
1:C:206:SER:HB2	1:C:466:ALA:CB	1.42	1.48
2:E:5:PHE:CD1	2:E:24:ASN:HB2	1.61	1.34
1:C:432:PRO:CG	1:C:434:ARG:HD2	1.62	1.30
1:C:206:SER:CB	1:C:466:ALA:HB3	1.63	1.28
1:A:544:PHE:CE2	1:A:685:MET:HG2	1.69	1.25
1:B:303:THR:HA	1:B:334:ASP:O	1.39	1.22
1:C:441:GLU:HB2	1:C:619:LEU:O	1.38	1.22
1:D:7:VAL:CG2	1:D:17:ILE:HG12	1.70	1.20
1:C:208:PRO:CB	1:C:464:LEU:HD11	1.76	1.15
1:A:227:LEU:HB3	1:A:435:GLN:NE2	1.59	1.15
1:A:55:THR:OG1	3:A:800:DTP:H8	1.44	1.15
1:C:6:LEU:CD2	1:C:51:ASP:HB2	1.80	1.12
1:C:432:PRO:CB	1:C:434:ARG:HD2	1.78	1.12
1:C:430:ILE:HG21	1:C:570:GLU:HB3	1.21	1.11
1:B:244:ILE:HG23	1:B:254:ILE:HG13	1.33	1.11
1:A:7:VAL:HB	1:A:15:GLU:O	1.51	1.10
1:B:185:PRO:HG2	1:B:188:THR:OG1	1.50	1.10
1:C:6:LEU:HD22	1:C:51:ASP:CB	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:HB	1:A:54:LYS:HA	1.30	1.10
1:D:560:LYS:HD3	1:D:609:HIS:CE1	1.86	1.10
1:A:6:LEU:HD13	1:A:51:ASP:OD1	1.49	1.08
1:A:437:ASN:HD21	1:A:439:CYS:HB2	1.15	1.08
1:D:427:ASP:OD1	1:D:428:PRO:HD2	1.52	1.08
1:C:208:PRO:HB3	1:C:464:LEU:CD1	1.83	1.07
1:A:244:ILE:HG23	1:A:254:ILE:HG13	1.32	1.07
1:C:208:PRO:HB3	1:C:464:LEU:HD11	1.14	1.07
2:E:5:PHE:CE1	2:E:24:ASN:HB2	1.90	1.05
1:D:249:SER:HA	1:D:292:CYS:SG	1.96	1.04
1:A:463:THR:CG2	1:A:492:LEU:HD23	1.88	1.02
1:A:293:SER:HB3	1:A:298:ARG:O	1.57	1.02
1:C:432:PRO:HG2	1:C:434:ARG:HD2	1.35	1.02
1:D:40:GLN:OE1	2:E:334:TRP:HB3	1.60	1.01
1:C:227:LEU:HB3	1:C:435:GLN:NE2	1.76	1.01
1:D:186:ARG:HH21	1:D:189:ARG:HH22	1.06	1.01
1:D:514:GLY:CA	1:D:618:ALA:HB3	1.91	1.00
1:C:532:SER:HA	1:C:677:GLY:HA3	1.42	1.00
1:B:155:TYR:CE1	1:B:209:THR:HG23	1.97	0.99
1:B:6:LEU:HB2	1:B:52:GLY:H	1.26	0.99
1:D:532:SER:HA	1:D:677:GLY:HA3	1.43	0.98
1:C:431:ALA:HB1	1:C:445:PRO:HB3	1.45	0.98
1:C:432:PRO:HB2	1:C:434:ARG:HD2	1.42	0.98
1:D:514:GLY:HA2	1:D:618:ALA:HB3	1.45	0.98
1:C:322:ASN:HA	1:C:331:ARG:HE	1.28	0.97
1:B:36:VAL:HG12	1:B:77:TYR:CZ	2.01	0.96
1:D:322:ASN:HA	1:D:331:ARG:HE	1.29	0.95
1:C:6:LEU:HD22	1:C:51:ASP:HB2	0.95	0.95
1:D:7:VAL:HG21	1:D:17:ILE:HG12	1.47	0.95
1:B:40:GLN:O	1:B:44:ARG:HG2	1.68	0.94
1:D:215:VAL:O	1:D:216:ARG:HG2	1.66	0.94
1:A:53:ILE:HD11	1:A:58:ILE:CD1	1.98	0.94
1:A:439:CYS:HG	1:A:621:PRO:HD2	1.32	0.94
1:B:320:LYS:HB3	1:B:409:THR:HG21	1.47	0.94
1:A:297:VAL:HG12	1:A:298:ARG:CG	1.98	0.94
1:A:670:TRP:CZ2	1:A:735:ARG:HB2	2.03	0.93
1:C:619:LEU:HD13	1:C:693:ILE:HG23	1.50	0.93
1:D:55:THR:OG1	3:D:800:DTP:H8	1.69	0.93
1:D:189:ARG:O	1:D:193:VAL:HG23	1.67	0.93
1:D:290:LYS:HG2	1:D:296:GLY:O	1.69	0.93
1:A:50:TYR:O	1:A:53:ILE:HG22	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG22	1:D:17:ILE:HG12	1.48	0.93
1:A:439:CYS:HB3	1:A:441:GLU:OE1	1.68	0.92
1:C:185:PRO:HG2	1:C:188:THR:OG1	1.68	0.92
1:D:301:ALA:O	1:D:438:LEU:HD13	1.68	0.92
1:A:618:ALA:HB2	1:A:691:GLN:HB2	1.49	0.92
1:C:427:ASP:HB3	1:C:430:ILE:HD12	1.51	0.92
1:C:155:TYR:OH	1:C:624:THR:HG22	1.69	0.92
1:C:206:SER:CB	1:C:466:ALA:CB	2.36	0.91
1:A:297:VAL:HG12	1:A:298:ARG:HG3	1.49	0.91
1:C:430:ILE:HG21	1:C:570:GLU:CB	2.00	0.91
1:C:619:LEU:HD13	1:C:693:ILE:CG2	2.01	0.91
1:A:439:CYS:SG	1:A:441:GLU:OE1	2.29	0.90
1:D:276:THR:HG22	3:D:900:DTP:H2	1.54	0.89
1:C:42:GLU:OE1	2:G:298:GLY:HA2	1.71	0.89
1:D:7:VAL:CG2	1:D:17:ILE:CG1	2.49	0.89
1:D:290:LYS:CG	1:D:296:GLY:O	2.20	0.89
1:B:618:ALA:HB2	1:B:691:GLN:HB2	1.52	0.89
1:D:696:ASN:ND2	1:D:730:TYR:HB3	1.87	0.89
1:A:44:ARG:HH11	1:A:69:LEU:CD2	1.86	0.89
2:H:92:ASN:HA	2:H:96:LEU:HD23	1.56	0.88
1:B:441:GLU:HG2	1:B:442:ILE:HG12	1.55	0.88
1:C:465:SER:CB	1:C:515:ILE:HG12	2.04	0.88
1:D:514:GLY:HA2	1:D:618:ALA:CB	2.04	0.88
1:D:40:GLN:OE1	2:E:334:TRP:CD1	2.27	0.88
1:B:303:THR:CA	1:B:334:ASP:O	2.21	0.88
1:A:439:CYS:CB	1:A:441:GLU:OE1	2.22	0.87
1:A:437:ASN:O	1:A:440:LEU:HD22	1.73	0.87
1:A:463:THR:HG23	1:A:492:LEU:HD23	1.53	0.87
1:A:439:CYS:SG	1:A:621:PRO:HD2	2.13	0.87
1:C:432:PRO:HG2	1:C:434:ARG:CD	2.04	0.87
1:D:560:LYS:HG2	1:D:609:HIS:CD2	2.09	0.87
1:C:621:PRO:HD3	1:C:694:SER:OG	1.73	0.87
1:C:432:PRO:CG	1:C:434:ARG:CD	2.52	0.87
1:D:50:TYR:O	1:D:53:ILE:CG2	2.22	0.87
1:A:689:ILE:HG22	1:A:691:GLN:O	1.75	0.87
1:A:53:ILE:CD1	1:A:58:ILE:CD1	2.53	0.86
2:F:92:ASN:HA	2:F:96:LEU:HD23	1.57	0.86
1:C:441:GLU:CB	1:C:619:LEU:O	2.23	0.86
1:A:437:ASN:ND2	1:A:439:CYS:HB2	1.89	0.86
1:C:18:ASN:O	3:C:800:DTP:H2	1.75	0.86
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLY:HA3	1:C:438:LEU:HD22	1.58	0.85
1:B:215:VAL:O	1:B:216:ARG:HG2	1.77	0.85
1:B:618:ALA:HB2	1:B:691:GLN:CB	2.06	0.85
1:D:249:SER:CA	1:D:292:CYS:SG	2.64	0.85
1:A:22:ILE:HG13	3:A:800:DTP:H2'1	1.57	0.85
1:D:430:ILE:HG21	1:D:570:GLU:HG2	1.59	0.85
1:A:7:VAL:CB	1:A:15:GLU:O	2.24	0.85
1:B:154:LYS:HA	1:B:160:ARG:HH22	1.39	0.85
1:C:217:THR:OG1	1:C:219:THR:HG22	1.77	0.84
1:B:320:LYS:HE3	1:B:411:ARG:CB	2.07	0.84
1:C:206:SER:HB2	1:C:466:ALA:HB1	1.53	0.84
1:A:438:LEU:O	1:A:440:LEU:HD23	1.78	0.84
2:G:92:ASN:HA	2:G:96:LEU:HD23	1.58	0.84
1:A:712:GLN:HE22	2:F:370:LEU:HG	1.41	0.84
1:B:293:SER:HB3	1:B:298:ARG:O	1.77	0.84
1:C:22:ILE:HG12	3:C:800:DTP:H2'1	1.60	0.84
1:C:427:ASP:CB	1:C:430:ILE:HD12	2.09	0.83
1:A:227:LEU:CB	1:A:435:GLN:NE2	2.42	0.83
1:D:558:LEU:HD23	1:D:612:ARG:HG2	1.61	0.83
2:E:1:ALA:HB3	2:E:168:HIS:HA	1.59	0.83
1:B:320:LYS:HE3	1:B:411:ARG:HB2	1.58	0.83
1:C:430:ILE:CG2	1:C:570:GLU:HB3	2.09	0.82
1:B:6:LEU:HD12	1:B:51:ASP:HB2	1.62	0.82
1:A:320:LYS:HE2	1:A:333:MET:O	1.80	0.82
1:B:420:CYS:O	1:B:424:SER:HB3	1.80	0.82
1:C:208:PRO:HB3	1:C:464:LEU:CG	2.10	0.82
1:D:585:LYS:HD3	1:D:585:LYS:H	1.45	0.82
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.62	0.82
1:B:154:LYS:HD2	1:B:155:TYR:HE1	1.43	0.81
1:C:427:ASP:OD1	1:C:428:PRO:HD2	1.80	0.81
1:A:441:GLU:OE1	1:A:620:MET:HB2	1.80	0.81
1:C:689:ILE:HG21	1:C:691:GLN:O	1.81	0.81
1:A:189:ARG:O	1:A:193:VAL:HG23	1.79	0.81
1:C:155:TYR:OH	1:C:624:THR:CG2	2.28	0.81
1:D:186:ARG:HH21	1:D:189:ARG:NH2	1.78	0.81
1:D:276:THR:CG2	3:D:900:DTP:H2	2.10	0.81
1:D:40:GLN:OE1	2:E:334:TRP:CB	2.28	0.81
1:A:432:PRO:HG2	1:A:434:ARG:HD2	1.62	0.81
1:C:585:LYS:H	1:C:585:LYS:HD3	1.44	0.81
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.63	0.81
1:D:215:VAL:O	1:D:216:ARG:CG	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HA	1:A:58:ILE:CG1	2.11	0.80
1:C:280:PRO:HB3	1:D:291:SER:O	1.80	0.80
1:B:642:VAL:HG22	1:B:655:VAL:HG22	1.63	0.80
1:D:730:TYR:O	1:D:731:TYR:O	2.00	0.80
1:B:188:THR:O	1:B:192:TYR:HD2	1.65	0.80
1:C:432:PRO:HB2	1:C:434:ARG:CD	2.11	0.80
1:A:730:TYR:O	1:A:731:TYR:O	1.99	0.80
1:C:206:SER:HB2	1:C:466:ALA:HB3	0.80	0.80
1:B:418:ASP:O	1:B:422:THR:HG23	1.82	0.79
1:D:293:SER:CB	1:D:298:ARG:O	2.30	0.79
1:D:551:LEU:O	1:D:616:LEU:CD1	2.30	0.79
2:F:1:ALA:HB3	2:F:168:HIS:HA	1.64	0.79
1:A:618:ALA:CB	1:A:691:GLN:HB2	2.12	0.79
1:D:689:ILE:HG21	1:D:691:GLN:O	1.81	0.79
1:A:50:TYR:O	1:A:53:ILE:CG2	2.31	0.79
1:C:465:SER:HB2	1:C:514:GLY:O	1.82	0.79
1:D:6:LEU:CD2	1:D:14:THR:HG21	2.12	0.79
2:E:92:ASN:HA	2:E:96:LEU:HD23	1.63	0.79
1:A:325:VAL:HG22	1:A:327:GLY:H	1.48	0.79
1:D:560:LYS:CD	1:D:609:HIS:NE2	2.46	0.79
1:A:53:ILE:HD11	1:A:58:ILE:HD12	1.62	0.79
1:A:544:PHE:HE2	1:A:685:MET:HG2	1.42	0.79
1:B:432:PRO:HG2	1:B:434:ARG:HD2	1.65	0.79
1:D:155:TYR:CE1	1:D:209:THR:HG23	2.18	0.79
1:D:551:LEU:O	1:D:616:LEU:HD13	1.82	0.79
2:G:1:ALA:HB3	2:G:168:HIS:HA	1.64	0.79
1:C:513:LEU:HD12	1:C:616:LEU:HD23	1.63	0.78
1:C:208:PRO:HD3	1:C:464:LEU:HD12	1.63	0.78
1:D:560:LYS:HD3	1:D:609:HIS:NE2	1.97	0.78
2:E:255:GLY:HA2	2:E:258:ASP:O	1.83	0.78
1:D:211:ILE:O	1:D:215:VAL:HG23	1.83	0.78
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.66	0.78
1:D:301:ALA:HB1	1:D:438:LEU:HD11	1.66	0.78
1:D:50:TYR:O	1:D:53:ILE:HG22	1.82	0.78
2:H:1:ALA:HB3	2:H:168:HIS:HA	1.64	0.78
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.66	0.78
1:A:642:VAL:HG22	1:A:655:VAL:HG22	1.65	0.78
1:C:7:VAL:CG2	1:C:17:ILE:HG12	2.13	0.77
1:A:55:THR:OG1	3:A:800:DTP:C8	2.30	0.77
1:A:227:LEU:HB3	1:A:435:GLN:HE21	1.49	0.77
2:G:195:LEU:HD21	2:G:268:CYS:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:THR:OG1	3:C:800:DTP:H8	1.82	0.77
1:A:436:SER:OG	1:A:440:LEU:HA	1.84	0.77
1:A:696:ASN:ND2	1:A:730:TYR:HB3	1.99	0.77
2:F:195:LEU:HD21	2:F:268:CYS:HB3	1.66	0.77
1:B:155:TYR:CZ	1:B:209:THR:HG23	2.20	0.77
1:D:619:LEU:HD12	1:D:693:ILE:HG12	1.66	0.77
2:H:5:PHE:CE1	2:H:24:ASN:O	2.37	0.77
1:C:276:THR:HB	3:C:900:DTP:H2	1.65	0.77
1:B:325:VAL:HG22	1:B:327:GLY:H	1.48	0.77
1:B:36:VAL:HG12	1:B:77:TYR:CE2	2.20	0.77
1:A:439:CYS:O	1:A:440:LEU:HB2	1.84	0.77
1:B:442:ILE:HG23	1:B:691:GLN:OE1	1.84	0.77
1:D:432:PRO:HG2	1:D:434:ARG:HD2	1.67	0.77
2:F:5:PHE:CE1	2:F:24:ASN:O	2.37	0.77
1:A:544:PHE:CE2	1:A:685:MET:CG	2.62	0.76
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.67	0.76
1:C:208:PRO:CA	1:C:464:LEU:HD11	2.15	0.76
1:D:45:SER:OG	1:D:61:THR:HG22	1.84	0.76
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.66	0.76
1:C:21:LYS:HD2	3:C:800:DTP:N1	1.99	0.76
1:C:432:PRO:HG2	1:C:434:ARG:HH11	1.51	0.76
2:E:195:LEU:HD21	2:E:268:CYS:HB3	1.67	0.76
2:H:195:LEU:HD21	2:H:268:CYS:HB3	1.68	0.76
1:C:287:THR:HB	1:D:284:HIS:HA	1.67	0.76
1:A:34:HIS:O	1:A:35:ASN:HB2	1.86	0.76
1:A:44:ARG:NH1	1:A:69:LEU:HD23	2.00	0.76
1:C:51:ASP:OD1	1:C:51:ASP:O	2.04	0.76
2:E:5:PHE:CE1	2:E:24:ASN:CB	2.69	0.76
1:D:622:SER:HB2	1:D:625:SER:HB2	1.69	0.75
1:C:689:ILE:CG2	1:C:691:GLN:O	2.34	0.75
1:A:233:SER:O	1:A:237:ILE:HG13	1.85	0.75
2:E:165:SER:O	2:E:169:LEU:HG	1.87	0.75
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.69	0.75
1:A:53:ILE:CD1	1:A:58:ILE:HD11	2.15	0.75
1:D:276:THR:HG23	1:D:280:PRO:HG2	1.66	0.75
1:D:463:THR:HG22	1:D:489:LEU:HD22	1.68	0.75
1:D:53:ILE:HG13	1:D:58:ILE:HD11	1.69	0.75
2:E:5:PHE:CD1	2:E:24:ASN:CB	2.57	0.75
1:A:293:SER:CB	1:A:298:ARG:O	2.34	0.75
1:D:249:SER:CB	1:D:292:CYS:SG	2.75	0.75
1:B:234:LEU:N	3:B:900:DTP:H3'	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:CG1	1:D:58:ILE:HD11	2.17	0.74
2:F:18:PHE:CZ	2:F:104:LEU:HD21	2.22	0.74
1:A:10:ARG:HE	1:A:91:LYS:NZ	1.85	0.74
1:D:689:ILE:CG2	1:D:691:GLN:O	2.35	0.74
1:A:55:THR:C	1:A:58:ILE:HG12	2.07	0.74
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.69	0.74
3:A:800:DTP:H8	3:A:800:DTP:H5'2	1.69	0.74
1:A:18:ASN:H	3:A:800:DTP:H2	1.50	0.74
1:D:441:GLU:HB2	1:D:619:LEU:O	1.88	0.74
2:G:5:PHE:CE1	2:G:24:ASN:O	2.41	0.74
1:B:185:PRO:HG2	1:B:188:THR:HG1	1.50	0.74
1:B:233:SER:O	1:B:237:ILE:HG13	1.88	0.74
1:D:7:VAL:HG22	1:D:17:ILE:CG1	2.17	0.74
1:A:125:GLU:HG2	1:A:129:LYS:HE2	1.69	0.73
1:A:499:PRO:HG2	1:A:500:ILE:HD12	1.68	0.73
1:B:125:GLU:HG2	1:B:129:LYS:HE2	1.68	0.73
1:C:465:SER:HB2	1:C:515:ILE:HG12	1.69	0.73
1:A:719:LEU:HD22	2:F:375:LEU:HD21	1.70	0.73
1:C:225:CYS:H	1:C:462:CYS:HB2	1.53	0.73
1:B:499:PRO:HG2	1:B:500:ILE:HD12	1.69	0.73
1:D:364:LEU:HD23	1:D:378:LEU:HB2	1.71	0.73
1:B:188:THR:O	1:B:192:TYR:CD2	2.41	0.73
1:C:513:LEU:HD11	1:C:613:ASN:ND2	2.04	0.73
1:D:19:LEU:HD13	2:E:297:ILE:HG22	1.69	0.73
1:D:6:LEU:HD22	1:D:14:THR:HG21	1.70	0.73
1:B:21:LYS:HB2	3:B:800:DTP:C2	2.19	0.73
1:C:465:SER:N	1:C:514:GLY:O	2.22	0.73
1:C:622:SER:HB2	1:C:625:SER:HB2	1.69	0.73
1:A:44:ARG:HH11	1:A:69:LEU:HD23	1.50	0.72
1:D:6:LEU:HA	1:D:14:THR:HG22	1.70	0.72
1:D:689:ILE:HG22	1:D:691:GLN:H	1.54	0.72
1:D:556:ASN:HD21	1:D:609:HIS:HB2	1.54	0.72
1:B:543:THR:O	1:B:547:ILE:HG13	1.90	0.72
1:C:45:SER:OG	1:C:61:THR:HG22	1.89	0.72
1:D:430:ILE:HG21	1:D:570:GLU:CG	2.19	0.72
1:D:430:ILE:HD12	1:D:570:GLU:HA	1.71	0.72
1:A:442:ILE:HG23	1:A:691:GLN:OE1	1.89	0.72
1:C:234:LEU:HB3	1:D:246:LYS:HZ3	1.55	0.72
1:D:678:TYR:OH	1:D:695:ALA:HB1	1.90	0.72
1:D:40:GLN:OE1	2:E:334:TRP:HD1	1.69	0.72
2:G:18:PHE:CZ	2:G:104:LEU:HD21	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:SER:HB2	1:C:296:GLY:HA2	1.72	0.72
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.71	0.72
1:A:8:THR:CB	1:A:54:LYS:HA	2.14	0.72
1:A:19:LEU:HA	1:A:22:ILE:HD12	1.70	0.72
1:C:364:LEU:HD23	1:C:378:LEU:HB2	1.71	0.72
1:C:44:ARG:HA	1:C:44:ARG:HE	1.54	0.72
1:D:348:LEU:O	2:E:371:SER:HB3	1.89	0.72
1:C:276:THR:HG23	1:C:280:PRO:HG2	1.72	0.71
1:A:233:SER:OG	1:A:236:SER:CB	2.39	0.71
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.72	0.71
1:B:685:MET:O	1:B:689:ILE:HG12	1.90	0.71
1:D:157:VAL:HG23	1:D:167:GLU:OE2	1.90	0.71
1:D:268:ILE:HD11	1:D:275:HIS:HA	1.71	0.71
2:E:69:GLU:HG2	2:E:296:MET:HG3	1.72	0.71
1:A:18:ASN:H	3:A:800:DTP:C2	2.03	0.71
1:D:225:CYS:H	1:D:462:CYS:HB2	1.54	0.71
2:F:69:GLU:HG2	2:F:296:MET:HG3	1.73	0.71
1:A:55:THR:HA	1:A:58:ILE:HG12	1.72	0.71
1:D:430:ILE:CG2	1:D:570:GLU:HG2	2.20	0.71
1:D:560:LYS:CD	1:D:609:HIS:CE1	2.72	0.71
2:E:90:SER:HB2	2:E:91:PRO:HD3	1.73	0.71
1:C:465:SER:HB3	1:C:515:ILE:HG23	1.72	0.71
2:E:311:ILE:HG23	2:E:312:THR:H	1.55	0.71
1:C:227:LEU:HD23	1:C:435:GLN:HG3	1.73	0.70
1:B:215:VAL:O	1:B:216:ARG:CG	2.39	0.70
1:C:215:VAL:O	1:C:216:ARG:CG	2.40	0.70
1:D:670:TRP:CH2	1:D:735:ARG:HB2	2.27	0.70
1:C:689:ILE:HG22	1:C:691:GLN:H	1.56	0.70
1:C:297:VAL:HG12	1:C:297:VAL:O	1.92	0.70
1:D:464:LEU:HA	1:D:514:GLY:O	1.91	0.70
1:D:514:GLY:CA	1:D:618:ALA:CB	2.66	0.70
1:D:441:GLU:HG3	1:D:620:MET:HB3	1.72	0.70
1:C:44:ARG:NH2	2:G:220:GLU:OE1	2.22	0.70
1:B:6:LEU:HB2	1:B:52:GLY:N	2.04	0.70
1:A:185:PRO:HB2	1:A:187:GLU:HG2	1.74	0.70
1:B:439:CYS:HB2	1:B:441:GLU:OE1	1.92	0.70
1:B:276:THR:HB	3:B:900:DTP:H2	1.74	0.70
1:C:293:SER:HB3	1:C:298:ARG:O	1.92	0.70
1:C:431:ALA:HB1	1:C:445:PRO:CB	2.20	0.70
1:D:233:SER:HA	3:D:900:DTP:H5'1	1.74	0.70
2:H:18:PHE:CZ	2:H:104:LEU:HD21	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:HG22	1:C:17:ILE:HG12	1.72	0.70
1:D:510:ARG:HG2	1:D:567:TRP:HE3	1.56	0.70
1:A:407:ALA:HA	1:A:732:GLN:OE1	1.91	0.69
3:A:800:DTP:C8	3:A:800:DTP:H5'2	2.22	0.69
1:D:551:LEU:C	1:D:616:LEU:HD13	2.12	0.69
1:B:442:ILE:HD12	1:B:691:GLN:OE1	1.91	0.69
2:F:90:SER:HB2	2:F:91:PRO:HD3	1.74	0.69
1:A:45:SER:OG	1:A:61:THR:HG22	1.92	0.69
1:C:196:PHE:HD1	1:C:484:LEU:HB3	1.57	0.69
1:D:287:THR:O	1:D:291:SER:HB3	1.93	0.69
1:A:317:LEU:HD23	1:A:401:LEU:HD23	1.73	0.69
1:D:430:ILE:HG21	1:D:570:GLU:CB	2.23	0.69
1:C:186:ARG:HH21	1:C:189:ARG:HH22	1.41	0.69
2:G:90:SER:HB2	2:G:91:PRO:HD3	1.74	0.69
2:H:218:PHE:CZ	2:H:296:MET:SD	2.85	0.69
2:H:90:SER:HB2	2:H:91:PRO:HD3	1.74	0.69
2:E:307:TYR:HA	2:E:331:PRO:HG3	1.74	0.69
1:B:320:LYS:CE	1:B:411:ARG:HB2	2.23	0.69
2:G:69:GLU:HG2	2:G:296:MET:HG3	1.72	0.69
2:H:311:ILE:HG23	2:H:312:THR:H	1.56	0.69
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.75	0.69
1:C:370:ALA:HA	1:C:428:PRO:HB2	1.74	0.69
1:A:41:VAL:HG22	1:A:69:LEU:HD12	1.74	0.69
1:B:407:ALA:HA	1:B:732:GLN:OE1	1.93	0.69
1:C:520:PHE:O	1:C:523:TYR:N	2.25	0.69
1:A:7:VAL:HG11	3:A:800:DTP:C6	2.24	0.68
1:D:618:ALA:O	1:D:620:MET:CE	2.41	0.68
2:G:307:TYR:HA	2:G:331:PRO:HG3	1.75	0.68
2:H:221:ARG:HH12	2:H:296:MET:HG2	1.58	0.68
1:B:19:LEU:HA	1:B:22:ILE:HD12	1.76	0.68
1:D:40:GLN:O	1:D:44:ARG:HG2	1.92	0.68
1:B:521:ALA:HB3	1:B:632:THR:HG21	1.75	0.68
2:G:9:LYS:HA	2:H:141:VAL:HG11	1.74	0.68
1:C:10:ARG:HD2	1:C:91:LYS:HE2	1.75	0.68
1:D:320:LYS:HB3	1:D:409:THR:HG21	1.76	0.68
2:H:5:PHE:HE1	2:H:24:ASN:O	1.76	0.68
1:A:40:GLN:O	1:A:44:ARG:N	2.25	0.68
1:A:55:THR:CA	1:A:58:ILE:HG12	2.24	0.68
1:C:42:GLU:OE1	2:G:298:GLY:CA	2.41	0.68
1:A:297:VAL:HG12	1:A:298:ARG:HG2	1.73	0.68
2:F:311:ILE:HG23	2:F:312:THR:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLU:CD	1:A:620:MET:HB2	2.15	0.68
1:C:55:THR:CB	3:C:800:DTP:H8	2.23	0.68
1:C:510:ARG:HG2	1:C:567:TRP:HE3	1.59	0.68
1:D:301:ALA:O	1:D:438:LEU:CD1	2.42	0.68
1:A:292:CYS:HA	1:B:276:THR:HG21	1.74	0.68
1:A:55:THR:O	1:A:58:ILE:HG12	1.92	0.68
1:D:185:PRO:HB2	1:D:187:GLU:HG2	1.76	0.68
1:B:229:GLU:HG3	1:B:257:ASN:HD22	1.59	0.67
1:B:459:ILE:HB	1:B:503:ALA:HA	1.76	0.67
2:G:311:ILE:HG23	2:G:312:THR:H	1.57	0.67
1:A:40:GLN:O	1:A:44:ARG:HB2	1.93	0.67
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.77	0.67
1:C:290:LYS:HE2	1:C:332:HIS:HB3	1.76	0.67
1:A:521:ALA:HB3	1:A:632:THR:HG21	1.75	0.67
1:C:234:LEU:HB3	1:D:246:LYS:NZ	2.08	0.67
2:F:5:PHE:HE1	2:F:24:ASN:O	1.77	0.67
1:C:712:GLN:HE22	2:G:370:LEU:HG	1.59	0.67
1:A:53:ILE:O	1:A:53:ILE:HG13	1.91	0.67
1:B:44:ARG:HA	1:B:44:ARG:HE	1.58	0.67
1:C:513:LEU:CD1	1:C:613:ASN:ND2	2.57	0.67
2:F:307:TYR:HA	2:F:331:PRO:HG3	1.76	0.67
1:B:332:HIS:O	1:B:333:MET:HG2	1.95	0.67
1:D:627:GLN:HA	1:D:654:GLN:HE22	1.58	0.67
2:E:203:LEU:HG	2:E:207:ARG:HD2	1.78	0.67
1:B:307:PRO:HG2	1:B:310:HIS:HB2	1.77	0.66
2:E:83:LEU:HD22	2:E:203:LEU:HD21	1.78	0.66
2:H:76:ASN:HD21	2:H:211:SER:HA	1.60	0.66
1:D:560:LYS:CD	1:D:609:HIS:CD2	2.77	0.66
1:D:33:LEU:HD13	1:D:80:LEU:HB2	1.77	0.66
1:B:585:LYS:HD3	1:B:585:LYS:H	1.60	0.66
1:B:58:ILE:HG21	3:B:800:DTP:H1'	1.77	0.66
1:C:689:ILE:HG22	1:C:691:GLN:N	2.10	0.66
1:D:618:ALA:O	1:D:620:MET:HE1	1.95	0.66
1:D:689:ILE:HG22	1:D:691:GLN:N	2.09	0.66
1:C:475:LEU:HD21	1:C:543:THR:HG23	1.76	0.66
1:A:44:ARG:HH11	1:A:69:LEU:HD21	1.59	0.66
1:B:294:GLN:O	1:B:296:GLY:N	2.25	0.66
2:H:307:TYR:HA	2:H:331:PRO:HG3	1.76	0.66
1:B:321:ASN:ND2	1:B:323:ARG:O	2.28	0.66
1:B:442:ILE:CD1	1:B:691:GLN:OE1	2.43	0.66
1:D:560:LYS:CG	1:D:609:HIS:CD2	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PRO:HG3	1:B:224:SER:OG	1.95	0.66
1:B:36:VAL:HG12	1:B:77:TYR:CE1	2.31	0.66
1:C:432:PRO:HB2	1:C:434:ARG:CG	2.26	0.66
1:A:53:ILE:HD11	1:A:58:ILE:HD11	1.73	0.66
1:B:40:GLN:O	1:B:44:ARG:CG	2.42	0.66
1:D:516:GLY:HA2	1:D:619:LEU:HD23	1.78	0.66
1:B:154:LYS:HD2	1:B:155:TYR:CE1	2.28	0.66
1:B:317:LEU:HD23	1:B:401:LEU:HD23	1.76	0.66
3:B:800:DTP:H5'1	3:B:800:DTP:O2B	1.96	0.66
1:C:627:GLN:HA	1:C:654:GLN:HE22	1.58	0.66
2:E:74:ILE:HG13	2:E:78:LYS:HE3	1.78	0.65
1:D:696:ASN:HD22	1:D:730:TYR:HB3	1.62	0.65
1:D:10:ARG:HD2	1:D:91:LYS:HE2	1.75	0.65
1:A:40:GLN:HE22	2:F:334:TRP:N	1.95	0.65
1:A:229:GLU:HG3	1:A:257:ASN:HD22	1.61	0.65
1:A:459:ILE:HB	1:A:503:ALA:HA	1.77	0.65
1:C:154:LYS:HG2	1:C:155:TYR:HD1	1.62	0.65
1:C:7:VAL:CG2	1:C:17:ILE:CG1	2.75	0.65
1:C:621:PRO:HD3	1:C:694:SER:CB	2.25	0.65
1:D:301:ALA:CB	1:D:438:LEU:HD11	2.26	0.65
1:A:206:SER:OG	1:A:625:SER:HB3	1.96	0.65
1:D:489:LEU:HB3	1:D:513:LEU:HD22	1.77	0.65
1:C:208:PRO:HD3	1:C:464:LEU:CD1	2.26	0.65
1:C:33:LEU:HD13	1:C:80:LEU:HB2	1.77	0.65
1:C:268:ILE:HD13	3:C:900:DTP:C8	2.27	0.65
1:D:217:THR:OG1	1:D:219:THR:HG22	1.97	0.65
1:D:260:ARG:NH1	1:D:448:PRO:HG3	2.12	0.65
1:D:560:LYS:HG2	1:D:609:HIS:CG	2.31	0.65
1:C:427:ASP:HB3	1:C:430:ILE:CD1	2.26	0.65
2:E:118:HIS:CE1	2:E:234:ILE:HG23	2.32	0.65
2:F:76:ASN:HD21	2:F:211:SER:HA	1.62	0.65
2:G:76:ASN:HD21	2:G:211:SER:HA	1.62	0.65
1:C:320:LYS:HB3	1:C:409:THR:HG21	1.77	0.65
1:D:427:ASP:OD1	1:D:428:PRO:CD	2.40	0.65
1:D:290:LYS:NZ	1:D:297:VAL:O	2.30	0.64
2:G:5:PHE:HE1	2:G:24:ASN:O	1.80	0.64
2:G:74:ILE:HG13	2:G:78:LYS:HE3	1.79	0.64
1:A:441:GLU:CD	1:A:620:MET:CB	2.65	0.64
2:F:171:GLY:O	2:F:184:VAL:HG11	1.97	0.64
2:F:203:LEU:HG	2:F:207:ARG:HD2	1.79	0.64
2:H:171:GLY:O	2:H:184:VAL:HG11	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LYS:H	1:A:585:LYS:HD3	1.61	0.64
1:C:281:PHE:CZ	3:C:900:DTP:H2'1	2.31	0.64
1:D:430:ILE:CG2	1:D:570:GLU:CG	2.76	0.64
1:C:6:LEU:HB2	1:C:51:ASP:HA	1.79	0.64
1:B:320:LYS:HE3	1:B:411:ARG:CG	2.26	0.64
1:B:206:SER:OG	1:B:625:SER:HB3	1.97	0.64
2:E:307:TYR:O	2:E:311:ILE:HG22	1.98	0.64
1:A:307:PRO:HG2	1:A:310:HIS:HB2	1.78	0.64
1:B:441:GLU:HA	1:B:692:SER:O	1.98	0.64
2:G:203:LEU:HG	2:G:207:ARG:HD2	1.80	0.64
2:G:45:SER:HB3	2:H:49:ARG:HH12	1.61	0.64
2:H:99:ILE:HD13	2:H:105:GLU:HA	1.80	0.64
2:H:365:VAL:HG12	2:H:366:ASP:H	1.62	0.64
1:A:260:ARG:NH1	1:A:448:PRO:HG3	2.13	0.64
1:C:284:HIS:HA	1:D:287:THR:HB	1.79	0.64
2:G:218:PHE:CZ	2:G:296:MET:SD	2.91	0.64
2:G:307:TYR:O	2:G:311:ILE:HG22	1.97	0.64
1:A:131:MET:SD	1:A:193:VAL:HG11	2.39	0.63
2:F:307:TYR:O	2:F:311:ILE:HG22	1.98	0.63
2:H:118:HIS:CE1	2:H:234:ILE:HG23	2.33	0.63
1:B:8:THR:CB	1:B:54:LYS:HA	2.28	0.63
1:C:215:VAL:O	1:C:216:ARG:HD3	1.97	0.63
2:H:307:TYR:O	2:H:311:ILE:HG22	1.98	0.63
1:C:260:ARG:NH1	1:C:448:PRO:HG3	2.14	0.63
1:B:443:ALA:H	1:B:691:GLN:HG2	1.62	0.63
3:B:900:DTP:H5'1	3:B:900:DTP:H8	1.81	0.63
1:C:432:PRO:HB2	1:C:434:ARG:HG3	1.80	0.63
1:C:276:THR:HB	3:C:900:DTP:C2	2.28	0.63
1:B:294:GLN:C	1:B:296:GLY:H	2.02	0.63
1:B:34:HIS:O	1:B:35:ASN:HB3	1.98	0.63
1:B:618:ALA:CB	1:B:691:GLN:CB	2.77	0.63
1:C:693:ILE:HG22	1:C:694:SER:N	2.12	0.63
1:D:40:GLN:OE1	2:E:334:TRP:CG	2.52	0.63
1:D:233:SER:HA	3:D:900:DTP:C5'	2.29	0.63
1:B:6:LEU:CB	1:B:52:GLY:H	2.07	0.63
1:D:475:LEU:HD21	1:D:543:THR:HG23	1.79	0.63
1:B:8:THR:HB	1:B:54:LYS:HA	1.79	0.63
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.14	0.63
1:D:228:ILE:HD12	1:D:244:ILE:HG12	1.81	0.63
2:E:12:GLN:NE2	2:E:23:VAL:HG13	2.14	0.63
1:B:712:GLN:HE22	2:H:370:LEU:HG	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:VAL:O	1:C:216:ARG:CD	2.47	0.62
1:D:370:ALA:HA	1:D:428:PRO:HB2	1.81	0.62
2:E:76:ASN:HD21	2:E:211:SER:HA	1.62	0.62
2:G:99:ILE:HD13	2:G:105:GLU:HA	1.81	0.62
1:A:151:LEU:HD23	1:A:155:TYR:CG	2.34	0.62
1:C:227:LEU:CB	1:C:435:GLN:NE2	2.59	0.62
1:A:320:LYS:HE3	1:A:411:ARG:CB	2.30	0.62
1:A:285:PHE:O	1:A:289:VAL:HG23	2.00	0.62
1:B:474:ASN:H	1:B:474:ASN:HD22	1.47	0.62
1:B:131:MET:SD	1:B:193:VAL:HG11	2.40	0.62
1:B:260:ARG:NH1	1:B:448:PRO:HG3	2.14	0.62
1:D:524:LEU:HB3	1:D:529:LYS:O	2.00	0.62
2:E:218:PHE:CZ	2:E:296:MET:SD	2.93	0.62
2:H:207:ARG:HH22	2:H:282:GLN:NE2	1.98	0.62
1:A:441:GLU:HB2	1:A:619:LEU:O	1.99	0.62
1:A:723:LYS:HG3	2:F:375:LEU:OXT	2.00	0.62
1:C:465:SER:O	1:C:516:GLY:N	2.23	0.62
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.81	0.62
1:A:150:GLN:O	1:A:154:LYS:HG3	1.99	0.62
1:A:463:THR:HG23	1:A:492:LEU:CD2	2.27	0.62
1:D:249:SER:HB3	1:D:292:CYS:SG	2.39	0.62
2:H:83:LEU:HD22	2:H:203:LEU:HD21	1.81	0.62
2:E:198:MET:SD	2:E:249:LEU:HD13	2.39	0.62
2:F:53:VAL:HG11	2:F:230:ILE:HG13	1.82	0.62
2:G:171:GLY:O	2:G:184:VAL:HG11	2.00	0.62
1:D:189:ARG:HG2	1:D:189:ARG:NH1	2.14	0.62
1:D:520:PHE:HB3	1:D:635:ILE:HA	1.80	0.62
1:A:227:LEU:HD23	1:A:435:GLN:HG3	1.80	0.61
2:E:49:ARG:O	2:E:52:GLU:HG2	1.99	0.61
1:A:474:ASN:H	1:A:474:ASN:HD22	1.48	0.61
2:E:207:ARG:HH22	2:E:282:GLN:NE2	1.99	0.61
2:F:218:PHE:CZ	2:F:296:MET:SD	2.93	0.61
2:G:83:LEU:HD22	2:G:203:LEU:HD21	1.82	0.61
1:C:125:GLU:HG2	1:C:129:LYS:HE2	1.82	0.61
1:C:524:LEU:HB3	1:C:529:LYS:O	2.00	0.61
1:C:530:ARG:HH11	1:C:667:GLU:HB2	1.65	0.61
1:C:246:LYS:HZ3	1:D:234:LEU:C	2.02	0.61
1:D:694:SER:O	1:D:696:ASN:ND2	2.33	0.61
1:A:224:SER:O	1:A:252:ALA:HA	1.99	0.61
1:C:573:TYR:HE1	1:C:578:LEU:HD23	1.65	0.61
2:E:311:ILE:HG23	2:E:312:THR:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ARG:O	2:F:52:GLU:HG2	2.00	0.61
2:F:74:ILE:HG13	2:F:78:LYS:HE3	1.81	0.61
2:H:203:LEU:HG	2:H:207:ARG:HD2	1.81	0.61
1:D:189:ARG:HH11	1:D:189:ARG:CG	2.13	0.61
1:C:276:THR:O	1:D:294:GLN:HG3	2.00	0.61
1:D:53:ILE:CD1	1:D:58:ILE:HD11	2.31	0.61
2:H:49:ARG:O	2:H:52:GLU:HG2	2.01	0.61
1:A:215:VAL:O	1:A:216:ARG:CG	2.49	0.61
1:B:221:GLN:NE2	1:B:250:GLN:HG2	2.16	0.61
1:D:115:TYR:HA	1:D:216:ARG:O	2.01	0.61
1:D:348:LEU:HB3	2:E:371:SER:HA	1.81	0.61
1:A:154:LYS:HA	1:A:160:ARG:HH22	1.64	0.61
1:B:320:LYS:HE3	1:B:411:ARG:HG3	1.81	0.61
1:D:122:ASP:O	1:D:189:ARG:NH2	2.33	0.61
1:A:221:GLN:NE2	1:A:250:GLN:HG2	2.16	0.61
1:A:442:ILE:HG22	1:A:444:LEU:HG	1.81	0.61
1:B:10:ARG:HG2	1:B:55:THR:HG21	1.82	0.61
1:D:290:LYS:HG3	1:D:296:GLY:O	2.00	0.61
1:D:669:LEU:HD11	1:D:698:ASN:ND2	2.15	0.61
2:H:74:ILE:HG13	2:H:78:LYS:HE3	1.81	0.61
1:A:233:SER:OG	1:A:236:SER:HB3	1.99	0.61
1:A:246:LYS:HG2	1:B:238:ASN:HD21	1.66	0.61
1:B:319:LEU:O	1:B:329:ARG:HD2	2.00	0.61
1:B:6:LEU:HD12	1:B:51:ASP:CB	2.30	0.61
1:B:18:ASN:O	3:B:800:DTP:H2	2.01	0.61
2:F:118:HIS:CE1	2:F:234:ILE:HG23	2.35	0.61
1:A:55:THR:HA	1:A:58:ILE:HG13	1.80	0.61
1:D:15:GLU:HG2	3:D:800:DTP:N6	2.16	0.61
1:C:211:ILE:O	1:C:215:VAL:HG23	2.00	0.60
1:D:573:TYR:HE1	1:D:578:LEU:HD23	1.65	0.60
2:F:18:PHE:O	2:F:19:PHE:HB2	2.01	0.60
2:G:99:ILE:HD11	2:G:108:VAL:HG21	1.82	0.60
1:B:36:VAL:CG1	1:B:77:TYR:CE2	2.85	0.60
1:B:696:ASN:ND2	1:B:730:TYR:HB3	2.16	0.60
2:G:118:HIS:CE1	2:G:234:ILE:HG23	2.36	0.60
2:H:53:VAL:HG11	2:H:230:ILE:HG13	1.83	0.60
1:C:228:ILE:HD12	1:C:244:ILE:HG12	1.82	0.60
1:D:694:SER:O	1:D:730:TYR:CB	2.48	0.60
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.84	0.60
1:C:115:TYR:HA	1:C:216:ARG:O	2.02	0.60
1:C:619:LEU:CD1	1:C:693:ILE:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:N	1:A:210:PRO:HD2	2.17	0.60
1:C:465:SER:HB3	1:C:515:ILE:HG12	1.83	0.60
1:B:209:THR:N	1:B:210:PRO:HD2	2.17	0.60
1:C:619:LEU:HB3	1:C:693:ILE:HA	1.83	0.60
1:D:186:ARG:NH2	1:D:189:ARG:HH22	1.87	0.60
2:G:53:VAL:HG11	2:G:230:ILE:HG13	1.83	0.60
1:A:68:ASP:HA	1:A:653:ARG:NH1	2.16	0.60
2:F:91:PRO:HB2	2:F:112:ALA:HB2	1.83	0.60
2:G:98:LEU:HD21	2:G:164:THR:HG23	1.83	0.60
2:G:18:PHE:O	2:G:19:PHE:HB2	2.01	0.60
2:G:311:ILE:HG23	2:G:312:THR:N	2.16	0.60
1:B:437:ASN:HD21	1:B:441:GLU:CD	2.05	0.60
1:C:425:PRO:HB2	1:C:615:THR:HG22	1.83	0.60
1:C:128:PHE:HA	1:C:131:MET:HE3	1.84	0.59
1:C:294:GLN:HB2	1:C:298:ARG:HD2	1.83	0.59
1:C:407:ALA:HA	1:C:732:GLN:OE1	2.02	0.59
1:D:670:TRP:CZ2	1:D:735:ARG:HB2	2.37	0.59
2:E:98:LEU:HD21	2:E:164:THR:HG23	1.84	0.59
2:E:53:VAL:HG11	2:E:230:ILE:HG13	1.84	0.59
2:F:101:ILE:HG13	2:F:104:LEU:HB3	1.84	0.59
2:F:99:ILE:HD13	2:F:105:GLU:HA	1.82	0.59
2:H:99:ILE:HD11	2:H:108:VAL:HG21	1.84	0.59
1:B:185:PRO:CG	1:B:188:THR:OG1	2.39	0.59
1:B:320:LYS:O	1:B:321:ASN:C	2.41	0.59
1:D:53:ILE:HD11	1:D:58:ILE:HD11	1.83	0.59
2:E:23:VAL:HG22	2:E:100:SER:O	2.02	0.59
2:H:18:PHE:O	2:H:19:PHE:HB2	2.02	0.59
1:A:150:GLN:OE1	1:A:154:LYS:HE3	2.01	0.59
1:A:53:ILE:HD12	1:A:58:ILE:CD1	2.30	0.59
1:B:285:PHE:O	1:B:289:VAL:HG23	2.01	0.59
1:B:689:ILE:HG22	1:B:691:GLN:O	2.01	0.59
1:D:301:ALA:HB1	1:D:438:LEU:CD1	2.30	0.59
2:G:317:GLN:HB2	2:G:323:LEU:HD21	1.84	0.59
1:A:441:GLU:HG2	1:A:442:ILE:N	2.18	0.59
1:A:403:MET:HE2	1:A:714:LEU:HB3	1.83	0.59
1:B:276:THR:CB	3:B:900:DTP:H2	2.32	0.59
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.82	0.59
1:D:7:VAL:N	1:D:15:GLU:O	2.35	0.59
1:D:301:ALA:CB	1:D:438:LEU:CD1	2.80	0.59
1:D:530:ARG:HH11	1:D:667:GLU:HB2	1.67	0.59
2:H:302:ASP:O	2:H:306:GLN:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:LEU:HD11	1:C:613:ASN:HD21	1.65	0.59
1:D:21:LYS:HD2	3:D:800:DTP:C2	2.32	0.59
1:D:459:ILE:HB	1:D:503:ALA:HA	1.84	0.59
2:E:91:PRO:O	2:E:95:LEU:HB2	2.03	0.59
2:E:99:ILE:HD13	2:E:105:GLU:HA	1.83	0.59
2:G:91:PRO:HB2	2:G:112:ALA:HB2	1.84	0.59
2:H:311:ILE:HG23	2:H:312:THR:N	2.16	0.59
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.03	0.59
1:D:290:LYS:HE2	1:D:332:HIS:HB3	1.82	0.59
1:A:227:LEU:C	1:A:435:GLN:HE22	2.05	0.59
1:A:469:LEU:HD12	1:A:520:PHE:HA	1.85	0.59
1:B:171:PHE:O	1:B:175:LEU:HD12	2.02	0.59
2:F:302:ASP:O	2:F:306:GLN:HG2	2.02	0.59
2:F:207:ARG:HH22	2:F:282:GLN:NE2	2.01	0.59
1:D:403:MET:HE2	1:D:714:LEU:HB3	1.85	0.59
1:D:430:ILE:CG2	1:D:570:GLU:HB3	2.33	0.59
2:F:83:LEU:HD22	2:F:203:LEU:HD21	1.84	0.59
2:F:98:LEU:HD21	2:F:164:THR:HG23	1.84	0.59
2:H:57:ARG:HG2	2:H:60:ILE:HD11	1.84	0.59
2:E:302:ASP:O	2:E:306:GLN:HG2	2.03	0.59
2:G:49:ARG:O	2:G:52:GLU:HG2	2.02	0.59
2:H:92:ASN:O	2:H:96:LEU:HB2	2.03	0.59
1:A:254:ILE:O	1:A:302:ALA:HB1	2.02	0.58
1:B:403:MET:HE2	1:B:714:LEU:HB3	1.85	0.58
1:C:189:ARG:O	1:C:193:VAL:HG23	2.03	0.58
1:C:21:LYS:HB2	3:C:800:DTP:C2	2.32	0.58
1:D:407:ALA:HA	1:D:732:GLN:OE1	2.03	0.58
1:D:55:THR:HG21	3:D:800:DTP:O1B	2.03	0.58
1:A:461:LEU:HD11	1:A:503:ALA:HB1	1.86	0.58
1:B:276:THR:N	3:B:900:DTP:H2	2.16	0.58
1:B:8:THR:OG1	1:B:54:LYS:HA	2.03	0.58
1:C:426:PHE:HE1	1:C:510:ARG:HE	1.50	0.58
1:D:30:ALA:HA	1:D:33:LEU:HD12	1.84	0.58
2:E:221:ARG:HH12	2:E:296:MET:HG2	1.68	0.58
2:G:302:ASP:O	2:G:306:GLN:HG2	2.03	0.58
1:B:215:VAL:O	1:B:216:ARG:CB	2.51	0.58
1:B:442:ILE:HG22	1:B:444:LEU:HG	1.85	0.58
1:D:427:ASP:HB3	1:D:430:ILE:HG13	1.86	0.58
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.38	0.58
2:F:221:ARG:HH12	2:F:296:MET:HG2	1.68	0.58
2:G:198:MET:HG2	2:G:249:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASN:CG	1:D:246:LYS:HE2	2.23	0.58
1:D:50:TYR:O	1:D:53:ILE:HG23	2.03	0.58
2:F:311:ILE:HG23	2:F:312:THR:N	2.18	0.58
2:G:91:PRO:O	2:G:95:LEU:HB2	2.04	0.58
1:A:171:PHE:O	1:A:175:LEU:HD12	2.03	0.58
1:C:368:PHE:CE2	1:C:417:VAL:HG21	2.38	0.58
1:D:365:TYR:O	1:D:368:PHE:HB3	2.03	0.58
1:B:282:TYR:HA	1:B:285:PHE:HD2	1.69	0.58
1:B:276:THR:H	3:B:900:DTP:H2	1.69	0.58
1:C:459:ILE:HB	1:C:503:ALA:HA	1.86	0.58
1:C:465:SER:CB	1:C:515:ILE:HA	2.34	0.58
1:D:196:PHE:HD1	1:D:484:LEU:HB3	1.68	0.58
1:D:551:LEU:O	1:D:616:LEU:HD11	2.03	0.58
2:E:101:ILE:HG13	2:E:104:LEU:HB3	1.85	0.58
2:H:296:MET:O	2:H:299:LEU:O	2.22	0.58
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.84	0.58
1:C:622:SER:HB2	1:C:625:SER:CB	2.33	0.58
1:C:693:ILE:HG22	1:C:694:SER:H	1.68	0.58
1:D:622:SER:HB2	1:D:625:SER:CB	2.32	0.58
2:E:8:THR:CG2	2:E:9:LYS:N	2.67	0.58
2:F:317:GLN:HB2	2:F:323:LEU:HD21	1.86	0.58
1:B:320:LYS:CB	1:B:409:THR:HG21	2.29	0.58
1:D:694:SER:O	1:D:730:TYR:HB3	2.03	0.58
1:A:10:ARG:HE	1:A:91:LYS:HZ1	1.51	0.58
1:B:42:GLU:OE1	2:H:298:GLY:HA2	2.03	0.58
1:B:56:SER:O	1:B:60:GLU:HG2	2.04	0.58
1:D:62:ILE:HG13	1:D:63:ILE:N	2.19	0.58
2:F:99:ILE:HD11	2:F:108:VAL:HG21	1.86	0.58
2:F:92:ASN:O	2:F:96:LEU:HB2	2.04	0.58
2:H:198:MET:SD	2:H:249:LEU:HD13	2.44	0.58
1:A:62:ILE:HG13	1:A:63:ILE:N	2.18	0.57
1:A:10:ARG:HG3	1:A:91:LYS:HE2	1.85	0.57
1:C:72:ARG:HG2	1:C:642:VAL:HG23	1.85	0.57
2:E:198:MET:HG2	2:E:249:LEU:HD22	1.85	0.57
1:C:297:VAL:O	1:C:297:VAL:CG1	2.51	0.57
1:C:62:ILE:HG13	1:C:63:ILE:N	2.19	0.57
1:C:441:GLU:HA	1:C:692:SER:O	2.05	0.57
2:E:317:GLN:HB2	2:E:323:LEU:HD21	1.85	0.57
1:C:54:LYS:O	1:C:58:ILE:HG12	2.04	0.57
2:E:305:CYS:O	2:E:309:GLU:HG3	2.04	0.57
2:G:165:SER:O	2:G:169:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.40	0.57
2:G:57:ARG:HG2	2:G:60:ILE:HD11	1.86	0.57
1:A:254:ILE:O	1:A:302:ALA:CB	2.52	0.57
1:A:439:CYS:HB3	1:A:441:GLU:CD	2.23	0.57
1:A:543:THR:O	1:A:547:ILE:HG13	2.04	0.57
1:D:18:ASN:HD22	1:D:21:LYS:HE3	1.69	0.57
1:D:520:PHE:CB	1:D:635:ILE:HA	2.34	0.57
1:D:712:GLN:HE22	2:E:370:LEU:HG	1.69	0.57
2:G:296:MET:O	2:G:299:LEU:O	2.23	0.57
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.87	0.57
1:D:227:LEU:HB3	1:D:435:GLN:NE2	2.20	0.57
2:F:57:ARG:HG2	2:F:60:ILE:HD11	1.87	0.57
2:G:101:ILE:HG13	2:G:104:LEU:HB3	1.86	0.57
1:A:44:ARG:NH1	1:A:69:LEU:CD2	2.57	0.57
1:B:101:ALA:HB3	1:B:104:ASP:OD2	2.04	0.57
1:B:258:ALA:HB1	1:B:261:ILE:HD12	1.86	0.57
1:C:619:LEU:HD13	1:C:693:ILE:HD13	1.86	0.57
1:D:465:SER:O	1:D:515:ILE:HA	2.05	0.57
2:H:305:CYS:O	2:H:309:GLU:HG3	2.05	0.57
1:A:101:ALA:HB3	1:A:104:ASP:OD2	2.05	0.57
1:C:208:PRO:HB3	1:C:464:LEU:CD2	2.35	0.57
1:C:208:PRO:HB3	1:C:464:LEU:HD21	1.86	0.57
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.87	0.57
1:D:128:PHE:HA	1:D:131:MET:HE3	1.86	0.57
1:D:560:LYS:HD2	1:D:609:HIS:NE2	2.19	0.57
2:G:190:LYS:HB3	2:G:261:MET:SD	2.44	0.57
2:G:160:LEU:HD21	2:G:193:LEU:HD22	1.87	0.57
2:G:207:ARG:HH22	2:G:282:GLN:NE2	2.03	0.57
1:B:369:PHE:O	1:B:421:ASN:CG	2.43	0.57
1:B:439:CYS:O	1:B:440:LEU:HB2	2.03	0.57
1:C:44:ARG:NE	1:C:44:ARG:HA	2.20	0.57
1:D:441:GLU:HA	1:D:692:SER:O	2.05	0.57
1:D:18:ASN:H	3:D:800:DTP:H2	1.68	0.57
2:E:245:THR:HA	2:E:248:MET:HE3	1.86	0.57
2:E:3:THR:OG1	2:E:5:PHE:O	2.20	0.57
2:F:197:LEU:HB2	2:F:249:LEU:HD21	1.87	0.57
1:A:234:LEU:HG	3:A:900:DTP:H2'2	1.87	0.57
1:B:618:ALA:CB	1:B:691:GLN:HB2	2.29	0.57
1:C:18:ASN:HD22	1:C:21:LYS:HE3	1.70	0.57
1:C:348:LEU:HB3	2:G:371:SER:HA	1.85	0.57
2:E:296:MET:O	2:E:299:LEU:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:221:ARG:HH12	2:G:296:MET:HG2	1.69	0.57
1:A:439:CYS:CB	1:A:441:GLU:CD	2.74	0.56
1:C:209:THR:N	1:C:210:PRO:HD2	2.20	0.56
1:C:280:PRO:CB	1:D:291:SER:O	2.51	0.56
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.40	0.56
1:C:441:GLU:HG3	1:C:620:MET:HB3	1.87	0.56
1:D:209:THR:N	1:D:210:PRO:HD2	2.20	0.56
1:D:341:LYS:HG2	1:D:722:TYR:OH	2.03	0.56
2:E:45:SER:HB3	2:F:49:ARG:HH12	1.69	0.56
2:E:8:THR:HG22	2:E:9:LYS:N	2.18	0.56
2:F:296:MET:O	2:F:299:LEU:O	2.23	0.56
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.86	0.56
1:A:173:TYR:CZ	1:A:201:SER:HA	2.40	0.56
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.87	0.56
1:C:93:ALA:HB1	1:C:166:TYR:O	2.05	0.56
2:G:305:CYS:O	2:G:309:GLU:HG3	2.05	0.56
2:H:101:ILE:HG13	2:H:104:LEU:HB3	1.88	0.56
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.41	0.56
2:H:160:LEU:HD21	2:H:193:LEU:HD22	1.87	0.56
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.86	0.56
1:A:21:LYS:O	1:A:25:VAL:HG23	2.05	0.56
1:B:317:LEU:O	1:B:405:GLU:HG3	2.06	0.56
1:B:441:GLU:O	1:B:692:SER:O	2.24	0.56
1:D:621:PRO:HD3	1:D:694:SER:CB	2.35	0.56
2:F:311:ILE:HD11	2:F:315:ARG:HE	1.69	0.56
2:G:92:ASN:O	2:G:96:LEU:HB2	2.05	0.56
1:B:62:ILE:HG13	1:B:63:ILE:N	2.19	0.56
1:C:529:LYS:HB3	1:C:536:ALA:HB2	1.88	0.56
1:C:639:ARG:HH22	1:C:733:ASN:HB3	1.71	0.56
2:F:198:MET:HG2	2:F:249:LEU:HD22	1.87	0.56
2:H:317:GLN:HB2	2:H:323:LEU:HD21	1.87	0.56
1:A:19:LEU:HA	1:A:22:ILE:CD1	2.36	0.56
1:A:215:VAL:O	1:A:216:ARG:HG2	2.05	0.56
1:B:231:GLY:HA2	1:B:260:ARG:HD3	1.87	0.56
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.88	0.56
1:C:7:VAL:HG22	1:C:17:ILE:CG1	2.34	0.56
1:C:467:PHE:HB2	1:C:517:VAL:HG12	1.86	0.56
2:F:91:PRO:O	2:F:95:LEU:HB2	2.06	0.56
2:G:304:LEU:O	2:G:308:VAL:HG23	2.06	0.56
1:A:320:LYS:HB3	1:A:409:THR:HG21	1.87	0.56
1:B:68:ASP:HA	1:B:653:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LYS:HD2	3:C:800:DTP:C6	2.35	0.56
1:C:530:ARG:NH1	1:C:667:GLU:HB2	2.20	0.56
1:D:39:SER:O	1:D:43:LEU:HG	2.06	0.56
2:E:12:GLN:HE21	2:E:23:VAL:HG13	1.69	0.56
2:H:255:GLY:CA	2:H:262:ALA:HB2	2.36	0.56
1:A:217:THR:OG1	1:A:219:THR:HG22	2.06	0.56
1:B:417:VAL:O	1:B:421:ASN:ND2	2.38	0.56
1:D:6:LEU:CA	1:D:14:THR:HG22	2.36	0.56
2:E:91:PRO:HB2	2:E:112:ALA:HB2	1.87	0.56
1:A:215:VAL:O	1:A:216:ARG:CB	2.53	0.56
1:A:439:CYS:SG	1:A:621:PRO:CD	2.92	0.56
1:B:106:VAL:O	1:B:110:VAL:HG23	2.05	0.56
1:B:154:LYS:HA	1:B:160:ARG:NH2	2.16	0.56
1:B:173:TYR:CE2	1:B:201:SER:HA	2.41	0.56
1:B:229:GLU:HG3	1:B:257:ASN:ND2	2.20	0.56
1:C:154:LYS:HG2	1:C:155:TYR:CD1	2.41	0.56
1:D:430:ILE:CG2	1:D:570:GLU:CB	2.83	0.56
1:D:639:ARG:HH22	1:D:733:ASN:HB3	1.71	0.56
2:H:198:MET:HG2	2:H:249:LEU:HD22	1.87	0.56
1:C:154:LYS:HA	1:C:160:ARG:HH22	1.71	0.56
1:C:215:VAL:O	1:C:216:ARG:HG2	2.06	0.56
1:D:72:ARG:HG2	1:D:642:VAL:HG23	1.86	0.56
1:D:93:ALA:HB1	1:D:166:TYR:O	2.05	0.56
2:F:165:SER:O	2:F:169:LEU:HG	2.06	0.56
2:G:198:MET:SD	2:G:249:LEU:HD13	2.46	0.56
1:B:233:SER:C	3:B:900:DTP:H3'	2.26	0.55
1:C:439:CYS:HB2	1:C:441:GLU:OE1	2.06	0.55
1:C:467:PHE:CE2	1:C:515:ILE:HG21	2.41	0.55
1:C:403:MET:HE2	1:C:714:LEU:HB3	1.87	0.55
2:E:196:CYS:O	2:E:200:VAL:HG23	2.06	0.55
2:E:49:ARG:HH12	2:F:45:SER:HB3	1.72	0.55
1:A:670:TRP:CE2	1:A:735:ARG:HB2	2.41	0.55
1:A:618:ALA:HA	1:A:689:ILE:CG2	2.36	0.55
1:B:10:ARG:HE	1:B:91:LYS:NZ	2.03	0.55
1:C:719:LEU:HB3	2:G:373:PHE:CD2	2.40	0.55
1:D:189:ARG:HH11	1:D:189:ARG:HG2	1.70	0.55
1:D:44:ARG:HE	1:D:44:ARG:HA	1.71	0.55
1:D:18:ASN:H	3:D:800:DTP:C2	2.19	0.55
2:E:306:GLN:HB3	2:E:328:ARG:NH1	2.20	0.55
2:F:255:GLY:CA	2:F:262:ALA:HB2	2.36	0.55
1:B:469:LEU:HD12	1:B:520:PHE:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:ASN:O	2:E:96:LEU:HB2	2.05	0.55
2:F:330:ASN:HB3	2:F:333:PRO:HG3	1.88	0.55
2:H:95:LEU:O	2:H:99:ILE:HG13	2.06	0.55
1:B:463:THR:HG23	1:B:492:LEU:HD23	1.88	0.55
1:D:530:ARG:NH1	1:D:667:GLU:HB2	2.22	0.55
2:E:57:ARG:HG2	2:E:60:ILE:HD11	1.87	0.55
2:G:89:ARG:O	2:G:93:VAL:HG23	2.07	0.55
2:H:190:LYS:HB3	2:H:261:MET:SD	2.46	0.55
1:A:282:TYR:HA	1:A:285:PHE:HD2	1.71	0.55
1:B:173:TYR:CZ	1:B:201:SER:HA	2.42	0.55
1:B:254:ILE:O	1:B:302:ALA:HB1	2.05	0.55
1:B:35:ASN:ND2	1:B:35:ASN:O	2.39	0.55
1:C:465:SER:HB3	1:C:515:ILE:HA	1.88	0.55
1:C:520:PHE:CB	1:C:635:ILE:HA	2.36	0.55
1:D:106:VAL:O	1:D:110:VAL:HG23	2.06	0.55
1:D:530:ARG:HB2	1:D:533:ASP:OD2	2.07	0.55
2:E:99:ILE:HD11	2:E:108:VAL:HG21	1.87	0.55
2:E:190:LYS:HB3	2:E:261:MET:SD	2.47	0.55
2:F:305:CYS:O	2:F:309:GLU:HG3	2.04	0.55
2:H:91:PRO:HB2	2:H:112:ALA:HB2	1.87	0.55
2:H:98:LEU:HD21	2:H:164:THR:HG23	1.87	0.55
1:A:173:TYR:CE2	1:A:201:SER:HA	2.42	0.55
1:A:619:LEU:HD12	1:A:693:ILE:CG1	2.37	0.55
1:C:196:PHE:CD1	1:C:484:LEU:HB3	2.40	0.55
2:G:255:GLY:CA	2:G:262:ALA:HB2	2.37	0.55
1:A:181:PHE:O	1:A:189:ARG:HD2	2.07	0.55
1:A:185:PRO:HB2	1:A:187:GLU:CG	2.37	0.55
1:A:278:CYS:HB3	1:A:282:TYR:CE1	2.41	0.55
1:B:254:ILE:O	1:B:302:ALA:HA	2.07	0.55
1:B:45:SER:OG	1:B:61:THR:HG22	2.06	0.55
1:D:685:MET:O	1:D:689:ILE:HG12	2.07	0.55
2:G:49:ARG:HH12	2:H:45:SER:HB3	1.72	0.55
2:G:8:THR:HG22	2:G:9:LYS:N	2.22	0.55
1:B:102:LEU:HD23	1:B:128:PHE:O	2.07	0.55
1:B:6:LEU:O	1:B:53:ILE:HG22	2.07	0.55
1:C:106:VAL:O	1:C:110:VAL:HG23	2.07	0.55
2:E:95:LEU:O	2:E:99:ILE:HG13	2.07	0.55
2:H:91:PRO:O	2:H:95:LEU:HB2	2.06	0.55
1:B:403:MET:CE	1:B:714:LEU:HB3	2.36	0.55
1:B:515:ILE:O	1:B:618:ALA:O	2.24	0.55
1:D:40:GLN:O	1:D:44:ARG:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:CYS:HB2	1:D:441:GLU:OE1	2.07	0.55
1:D:441:GLU:HG3	1:D:619:LEU:O	2.06	0.55
1:A:106:VAL:O	1:A:110:VAL:HG23	2.07	0.55
1:A:242:SER:HB3	1:B:238:ASN:HB3	1.89	0.55
1:A:689:ILE:CG2	1:A:691:GLN:O	2.51	0.55
1:A:7:VAL:CG2	1:A:15:GLU:O	2.54	0.55
1:C:281:PHE:HZ	3:C:900:DTP:H2'1	1.73	0.55
2:F:160:LEU:HD21	2:F:193:LEU:HD22	1.87	0.55
2:F:273:TYR:O	2:F:277:VAL:HG23	2.07	0.55
1:A:10:ARG:HH22	1:A:88:HIS:CE1	2.26	0.54
1:C:432:PRO:HG2	1:C:434:ARG:NH1	2.21	0.54
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.89	0.54
1:C:619:LEU:CD1	1:C:693:ILE:HG12	2.37	0.54
1:D:529:LYS:HB3	1:D:536:ALA:HB2	1.88	0.54
1:D:560:LYS:HD3	1:D:609:HIS:CD2	2.41	0.54
1:A:244:ILE:HG12	1:A:254:ILE:HG21	1.90	0.54
1:B:21:LYS:O	1:B:25:VAL:HG23	2.07	0.54
1:B:403:MET:HB2	1:B:711:MET:HE1	1.89	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.06	0.54
1:C:287:THR:CB	1:D:284:HIS:HA	2.37	0.54
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.88	0.54
1:D:430:ILE:CD1	1:D:570:GLU:HA	2.37	0.54
1:B:217:THR:OG1	1:B:219:THR:HG22	2.08	0.54
1:B:647:SER:HB2	1:B:652:LEU:HD11	1.89	0.54
1:D:368:PHE:CD2	1:D:369:PHE:CZ	2.95	0.54
1:D:678:TYR:OH	1:D:695:ALA:CB	2.56	0.54
2:E:273:TYR:O	2:E:277:VAL:HG23	2.08	0.54
2:H:196:CYS:O	2:H:200:VAL:HG23	2.07	0.54
2:H:306:GLN:HB3	2:H:328:ARG:NH1	2.22	0.54
1:C:234:LEU:C	1:D:246:LYS:HZ3	2.11	0.54
1:C:685:MET:O	1:C:689:ILE:HG12	2.07	0.54
1:D:290:LYS:CE	1:D:332:HIS:HB3	2.37	0.54
2:E:160:LEU:HD21	2:E:193:LEU:HD22	1.87	0.54
2:H:206:ILE:HG12	2:H:315:ARG:HG3	1.90	0.54
1:A:238:ASN:HB3	1:B:242:SER:HB3	1.89	0.54
1:B:254:ILE:O	1:B:302:ALA:CB	2.55	0.54
1:C:154:LYS:CG	1:C:155:TYR:HD1	2.20	0.54
1:D:425:PRO:HG2	1:D:615:THR:HG22	1.88	0.54
2:H:165:SER:O	2:H:169:LEU:HG	2.07	0.54
1:C:87:PHE:HE1	3:C:800:DTP:O2A	1.90	0.54
2:F:306:GLN:HB3	2:F:328:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:HG3	1:A:257:ASN:ND2	2.21	0.54
1:A:254:ILE:O	1:A:302:ALA:HA	2.07	0.54
1:B:304:LEU:HD23	1:B:305:PHE:N	2.23	0.54
2:F:190:LYS:HB3	2:F:261:MET:SD	2.47	0.54
1:A:483:ILE:O	1:A:487:ARG:HB2	2.08	0.54
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.42	0.54
1:B:483:ILE:O	1:B:487:ARG:HB2	2.08	0.54
1:B:511:ARG:HH11	1:B:511:ARG:HG2	1.73	0.54
1:C:432:PRO:CG	1:C:434:ARG:HH11	2.21	0.54
1:D:6:LEU:HD23	1:D:14:THR:HG21	1.89	0.54
2:E:255:GLY:CA	2:E:262:ALA:HB2	2.37	0.54
2:G:197:LEU:HB2	2:G:249:LEU:HD21	1.89	0.54
1:C:719:LEU:HD22	2:G:375:LEU:HD21	1.89	0.54
2:H:129:ILE:HG13	2:H:130:VAL:HG13	1.89	0.54
2:G:141:VAL:HG11	2:H:9:LYS:HA	1.90	0.54
1:A:228:ILE:HG21	1:A:240:THR:HG23	1.90	0.54
1:A:231:GLY:HA2	1:A:260:ARG:HD3	1.90	0.54
1:A:321:ASN:ND2	1:A:323:ARG:O	2.41	0.54
1:C:208:PRO:CD	1:C:464:LEU:CD1	2.85	0.54
1:C:520:PHE:O	1:C:523:TYR:HB3	2.08	0.54
1:C:530:ARG:HB2	1:C:533:ASP:OD2	2.08	0.54
1:D:545:GLU:OE1	1:D:595:LEU:HA	2.08	0.54
1:D:233:SER:HA	3:D:900:DTP:O5'	2.08	0.54
2:F:163:MET:HB3	2:F:189:LEU:HD13	1.90	0.54
2:F:196:CYS:O	2:F:200:VAL:HG23	2.07	0.54
2:F:227:ASN:O	2:F:231:ILE:HG12	2.08	0.54
2:G:306:GLN:HB3	2:G:328:ARG:NH1	2.23	0.54
1:C:565:CYS:SG	1:C:568:PHE:HB2	2.47	0.54
1:D:151:LEU:HA	1:D:155:TYR:HB2	1.90	0.54
1:D:18:ASN:N	3:D:800:DTP:H2	2.22	0.54
2:E:129:ILE:HG13	2:E:130:VAL:HG13	1.89	0.54
2:G:273:TYR:O	2:G:277:VAL:HG23	2.08	0.54
1:B:689:ILE:CG2	1:B:691:GLN:O	2.56	0.53
1:D:228:ILE:CG2	1:D:240:THR:HG23	2.39	0.53
1:A:544:PHE:CZ	1:A:685:MET:HG2	2.34	0.53
1:A:7:VAL:HG11	3:A:800:DTP:N6	2.22	0.53
1:C:185:PRO:HG2	1:C:188:THR:HG1	1.72	0.53
1:C:425:PRO:CB	1:C:615:THR:HG22	2.37	0.53
1:C:92:LYS:HD3	1:C:165:ILE:HD12	1.88	0.53
1:D:642:VAL:HG22	1:D:655:VAL:HG22	1.90	0.53
2:E:36:PHE:CZ	2:E:104:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:VAL:HG11	2:F:9:LYS:HA	1.89	0.53
2:G:330:ASN:HB3	2:G:333:PRO:HG3	1.89	0.53
2:H:197:LEU:HB2	2:H:249:LEU:HD21	1.89	0.53
1:A:54:LYS:HB2	1:A:57:ASP:OD2	2.07	0.53
1:C:107:VAL:O	1:C:111:GLU:HG3	2.09	0.53
1:D:565:CYS:SG	1:D:568:PHE:HB2	2.48	0.53
2:H:5:PHE:CD1	2:H:24:ASN:O	2.61	0.53
1:A:670:TRP:CH2	1:A:735:ARG:HB2	2.43	0.53
1:B:542:LYS:HG3	1:B:596:HIS:CD2	2.43	0.53
2:F:5:PHE:CD1	2:F:24:ASN:O	2.61	0.53
2:H:273:TYR:O	2:H:277:VAL:HG23	2.08	0.53
1:A:125:GLU:O	1:A:129:LYS:HG3	2.08	0.53
1:B:290:LYS:CG	1:B:296:GLY:O	2.57	0.53
1:B:552:LEU:HB3	1:B:602:LEU:HD21	1.91	0.53
1:C:701:PRO:O	1:C:707:GLY:HA2	2.09	0.53
1:D:430:ILE:HG22	1:D:570:GLU:OE1	2.09	0.53
1:D:701:PRO:O	1:D:707:GLY:HA2	2.08	0.53
2:G:8:THR:CG2	2:G:9:LYS:N	2.72	0.53
1:A:102:LEU:O	1:A:106:VAL:HG23	2.08	0.53
1:B:418:ASP:HA	1:B:421:ASN:HD22	1.73	0.53
1:C:613:ASN:CG	1:C:616:LEU:HD21	2.28	0.53
1:D:226:VAL:HG21	1:D:247:TYR:CG	2.44	0.53
2:G:169:LEU:HD22	2:H:166:TYR:CE2	2.43	0.53
1:B:517:VAL:O	1:B:634:GLY:HA2	2.09	0.53
2:E:78:LYS:HE2	2:E:136:VAL:HG13	1.91	0.53
2:G:78:LYS:HE2	2:G:136:VAL:HG13	1.91	0.53
1:A:140:ASP:OD1	1:A:169:ALA:HB3	2.09	0.53
1:A:317:LEU:O	1:A:405:GLU:HG3	2.09	0.53
1:B:7:VAL:HG23	1:B:17:ILE:HG12	1.89	0.53
1:C:403:MET:HB2	1:C:711:MET:HE3	1.90	0.53
1:C:544:PHE:HA	1:C:547:ILE:HD12	1.90	0.53
2:H:36:PHE:CZ	2:H:104:LEU:HD13	2.44	0.53
1:B:137:HIS:HA	1:B:170:GLN:HG3	1.89	0.53
1:C:474:ASN:OD1	1:C:476:ASP:HB2	2.09	0.53
1:C:510:ARG:HG2	1:C:567:TRP:CE3	2.41	0.53
1:C:545:GLU:OE1	1:C:595:LEU:HA	2.08	0.53
1:D:317:LEU:HD23	1:D:401:LEU:HD23	1.90	0.53
2:G:196:CYS:O	2:G:200:VAL:HG23	2.07	0.53
1:B:102:LEU:O	1:B:106:VAL:HG23	2.09	0.53
1:C:226:VAL:HG21	1:C:247:TYR:CG	2.44	0.53
1:C:430:ILE:CG2	1:C:570:GLU:OE1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:TRP:CH2	1:C:735:ARG:HB2	2.44	0.53
1:D:107:VAL:O	1:D:111:GLU:HG3	2.08	0.53
1:D:364:LEU:HD23	1:D:378:LEU:CB	2.38	0.53
1:D:92:LYS:HD3	1:D:165:ILE:HD12	1.91	0.53
1:A:102:LEU:HD23	1:A:128:PHE:O	2.08	0.52
1:A:152:GLU:O	1:A:158:GLN:NE2	2.42	0.52
1:A:242:SER:HA	1:B:238:ASN:OD1	2.09	0.52
1:A:320:LYS:HE3	1:A:411:ARG:HB2	1.91	0.52
1:A:317:LEU:HD23	1:A:401:LEU:CD2	2.39	0.52
1:B:140:ASP:OD1	1:B:169:ALA:HB3	2.09	0.52
1:B:293:SER:CB	1:B:298:ARG:O	2.53	0.52
1:C:642:VAL:HG22	1:C:655:VAL:HG22	1.91	0.52
1:C:87:PHE:CE1	3:C:800:DTP:O2A	2.62	0.52
2:H:227:ASN:O	2:H:231:ILE:HG12	2.09	0.52
1:A:18:ASN:N	3:A:800:DTP:H2	2.22	0.52
1:A:276:THR:HG21	1:B:292:CYS:HA	1.90	0.52
2:E:206:ILE:HG12	2:E:315:ARG:HG3	1.91	0.52
2:E:304:LEU:O	2:E:308:VAL:HG23	2.08	0.52
1:B:125:GLU:O	1:B:129:LYS:HG3	2.08	0.52
1:B:140:ASP:HA	1:B:143:PHE:CE2	2.43	0.52
1:C:573:TYR:CE1	1:C:578:LEU:HD23	2.44	0.52
1:D:21:LYS:O	1:D:25:VAL:HG23	2.08	0.52
1:D:403:MET:HB2	1:D:711:MET:HE3	1.90	0.52
1:D:519:ASN:HB2	1:D:631:ALA:HB1	1.90	0.52
1:D:464:LEU:HD13	1:D:620:MET:HG3	1.90	0.52
1:D:620:MET:HB2	1:D:621:PRO:HD2	1.90	0.52
2:F:78:LYS:HE2	2:F:136:VAL:HG13	1.91	0.52
1:B:286:GLN:CD	1:B:332:HIS:HB2	2.29	0.52
1:B:618:ALA:CB	1:B:691:GLN:HB3	2.39	0.52
1:B:82:ALA:O	1:B:86:ILE:HG12	2.09	0.52
1:C:38:ILE:O	1:C:42:GLU:HG3	2.09	0.52
1:D:316:LEU:HA	1:D:319:LEU:HG	1.92	0.52
1:D:510:ARG:HG2	1:D:567:TRP:CE3	2.39	0.52
2:G:175:HIS:CD2	2:H:178:ASN:HD21	2.28	0.52
2:H:89:ARG:O	2:H:93:VAL:HG23	2.09	0.52
1:B:290:LYS:HG3	1:B:296:GLY:O	2.09	0.52
1:C:317:LEU:HD23	1:C:401:LEU:HD23	1.90	0.52
1:C:432:PRO:CG	1:C:434:ARG:NH1	2.72	0.52
2:F:198:MET:SD	2:F:249:LEU:HD13	2.50	0.52
2:F:95:LEU:O	2:F:99:ILE:HG13	2.09	0.52
1:A:10:ARG:HE	1:A:91:LYS:CE	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:O	1:B:252:ALA:HA	2.10	0.52
1:C:464:LEU:HD12	1:C:464:LEU:O	2.10	0.52
1:D:189:ARG:O	1:D:193:VAL:CG2	2.49	0.52
1:D:638:PRO:O	1:D:668:LEU:HA	2.10	0.52
2:G:206:ILE:HG12	2:G:315:ARG:HG3	1.92	0.52
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.25	0.52
1:C:463:THR:CG2	1:C:489:LEU:HD22	2.35	0.52
1:C:617:SER:OG	1:C:690:ASP:N	2.27	0.52
2:E:197:LEU:HB2	2:E:249:LEU:HD21	1.90	0.52
2:F:304:LEU:O	2:F:308:VAL:HG23	2.08	0.52
2:G:129:ILE:HG13	2:G:130:VAL:HG13	1.90	0.52
2:G:163:MET:HB3	2:G:189:LEU:HD13	1.92	0.52
2:H:330:ASN:HB3	2:H:333:PRO:HG3	1.92	0.52
1:A:403:MET:CE	1:A:714:LEU:HB3	2.39	0.52
1:D:136:ASP:HB3	1:D:139:ARG:NE	2.25	0.52
1:D:286:GLN:CD	1:D:332:HIS:HB2	2.29	0.52
1:A:403:MET:HB2	1:A:711:MET:HE1	1.92	0.52
1:A:478:LEU:HB2	1:A:550:TYR:CD2	2.45	0.52
1:B:244:ILE:CG2	1:B:254:ILE:HG13	2.24	0.52
1:B:303:THR:HG23	1:B:334:ASP:C	2.30	0.52
1:B:474:ASN:N	1:B:474:ASN:HD22	2.06	0.52
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.92	0.52
1:C:206:SER:CA	1:C:466:ALA:HB3	2.38	0.52
1:D:368:PHE:CZ	1:D:417:VAL:HG21	2.45	0.52
2:E:89:ARG:O	2:E:93:VAL:HG23	2.10	0.52
1:A:140:ASP:HA	1:A:143:PHE:CE2	2.45	0.52
1:A:553:LYS:O	1:A:557:GLU:HG2	2.10	0.52
1:A:647:SER:HB2	1:A:652:LEU:HD11	1.92	0.52
1:A:678:TYR:O	1:A:682:VAL:HG23	2.10	0.52
1:A:91:LYS:HD2	3:A:800:DTP:O2A	2.10	0.52
1:C:638:PRO:O	1:C:668:LEU:HA	2.10	0.52
1:D:279:ILE:HB	1:D:280:PRO:HD3	1.92	0.52
1:D:544:PHE:HA	1:D:547:ILE:HD12	1.91	0.52
1:A:279:ILE:HD12	1:A:319:LEU:HD21	1.92	0.51
1:A:322:ASN:HA	1:A:331:ARG:HE	1.75	0.51
1:A:384:LYS:N	1:A:384:LYS:HD2	2.25	0.51
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.45	0.51
1:A:474:ASN:HD22	1:A:474:ASN:N	2.07	0.51
1:A:517:VAL:O	1:A:634:GLY:HA2	2.10	0.51
1:A:6:LEU:HB2	1:A:52:GLY:N	2.24	0.51
1:C:131:MET:HA	1:C:134:PHE:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD12	2:G:295:SER:O	2.10	0.51
1:C:228:ILE:CG2	1:C:240:THR:HG23	2.40	0.51
1:C:371:ASP:HB3	1:C:374:GLU:HB3	1.93	0.51
1:C:364:LEU:HD23	1:C:378:LEU:CB	2.38	0.51
1:D:189:ARG:CG	1:D:189:ARG:NH1	2.72	0.51
1:A:515:ILE:O	1:A:618:ALA:O	2.29	0.51
1:A:622:SER:HB2	1:A:625:SER:HB2	1.92	0.51
1:B:244:ILE:HG12	1:B:254:ILE:HG21	1.92	0.51
1:B:678:TYR:O	1:B:682:VAL:HG23	2.10	0.51
1:B:670:TRP:CZ2	1:B:735:ARG:HB2	2.46	0.51
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.92	0.51
1:C:151:LEU:HD23	1:C:155:TYR:CD2	2.45	0.51
1:C:147:ALA:CB	1:C:628:ILE:HA	2.41	0.51
1:D:293:SER:HB2	1:D:298:ARG:O	2.07	0.51
1:A:219:THR:HA	1:B:269:ARG:HH22	1.74	0.51
1:A:59:HIS:CD2	3:A:800:DTP:H4'	2.46	0.51
1:B:305:PHE:CZ	1:B:436:SER:HB3	2.45	0.51
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.93	0.51
1:D:542:LYS:HG3	1:D:596:HIS:CD2	2.45	0.51
2:E:258:ASP:OD1	2:E:259:PRO:HD2	2.11	0.51
1:C:426:PHE:O	1:C:572:THR:HG23	2.10	0.51
1:C:180:LEU:HD13	1:C:488:ALA:HB1	1.92	0.51
1:C:686:GLN:HG2	1:C:725:GLY:O	2.11	0.51
1:D:147:ALA:CB	1:D:628:ILE:HA	2.40	0.51
1:A:137:HIS:HA	1:A:170:GLN:HG3	1.92	0.51
1:C:188:THR:O	1:C:192:TYR:HD2	1.92	0.51
2:F:206:ILE:HG12	2:F:315:ARG:HG3	1.91	0.51
1:A:247:TYR:OH	1:A:461:LEU:HD21	2.10	0.51
1:A:44:ARG:HG3	1:A:69:LEU:HD21	1.93	0.51
1:B:278:CYS:HB3	1:B:282:TYR:CE1	2.45	0.51
1:C:245:VAL:HB	1:D:238:ASN:HD21	1.76	0.51
1:D:305:PHE:CZ	1:D:436:SER:HB3	2.45	0.51
2:H:145:GLN:HG2	2:H:289:TYR:CG	2.46	0.51
1:A:304:LEU:HD23	1:A:305:PHE:N	2.25	0.51
1:A:441:GLU:CD	1:A:620:MET:HB3	2.31	0.51
1:B:119:LEU:HD21	1:B:179:CYS:SG	2.50	0.51
1:B:384:LYS:N	1:B:384:LYS:HD2	2.24	0.51
1:B:544:PHE:CE2	1:B:685:MET:HG2	2.46	0.51
1:B:686:GLN:HG2	1:B:725:GLY:O	2.11	0.51
1:C:513:LEU:HD12	1:C:616:LEU:CD2	2.35	0.51
1:C:543:THR:O	1:C:547:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:HD22	1:C:76:ASP:HB3	1.92	0.51
1:D:573:TYR:CE1	1:D:578:LEU:HD23	2.44	0.51
1:A:347:LEU:O	2:F:367:THR:HG21	2.11	0.51
2:G:227:ASN:O	2:G:231:ILE:HG12	2.10	0.51
1:A:421:ASN:HB3	1:A:428:PRO:HB3	1.93	0.51
1:A:442:ILE:CG2	1:A:444:LEU:HG	2.40	0.51
1:A:469:LEU:HB3	1:A:523:TYR:CD1	2.45	0.51
1:B:253:GLY:C	1:B:254:ILE:HD13	2.32	0.51
1:B:553:LYS:O	1:B:557:GLU:HG2	2.10	0.51
1:B:643:SER:C	1:B:644:ILE:HD12	2.32	0.51
1:C:151:LEU:HG	1:C:628:ILE:HD12	1.93	0.51
1:D:215:VAL:O	1:D:216:ARG:CB	2.58	0.51
1:D:293:SER:HB3	1:D:298:ARG:O	2.09	0.51
1:D:560:LYS:HD3	1:D:609:HIS:ND1	2.22	0.51
2:E:311:ILE:HD11	2:E:315:ARG:HE	1.75	0.51
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.92	0.51
2:F:36:PHE:CZ	2:F:104:LEU:HD13	2.45	0.51
1:A:8:THR:HG21	1:A:54:LYS:HG2	1.93	0.51
1:B:619:LEU:HB2	1:B:693:ILE:HG23	1.92	0.51
1:D:686:GLN:HG2	1:D:725:GLY:O	2.10	0.51
2:E:330:ASN:HB3	2:E:333:PRO:HG3	1.92	0.51
2:F:89:ARG:O	2:F:93:VAL:HG23	2.11	0.51
2:G:95:LEU:O	2:G:99:ILE:HG13	2.11	0.51
1:A:606:ILE:HG23	1:A:611:LEU:HG	1.92	0.51
1:B:247:TYR:OH	1:B:461:LEU:HD21	2.10	0.51
1:C:136:ASP:HB3	1:C:139:ARG:NE	2.25	0.51
1:D:131:MET:HA	1:D:134:PHE:CD2	2.45	0.51
2:H:332:ILE:HB	2:H:334:TRP:NE1	2.26	0.51
1:A:19:LEU:CD1	2:F:295:SER:O	2.59	0.50
1:A:253:GLY:C	1:A:254:ILE:HD13	2.31	0.50
1:A:55:THR:O	1:A:58:ILE:CG1	2.59	0.50
1:B:322:ASN:HA	1:B:331:ARG:HE	1.75	0.50
1:B:723:LYS:HD2	2:H:373:PHE:CZ	2.45	0.50
1:C:208:PRO:CD	1:C:464:LEU:HD11	2.41	0.50
1:C:515:ILE:HD12	1:C:551:LEU:HD22	1.92	0.50
1:D:474:ASN:OD1	1:D:476:ASP:HB2	2.12	0.50
1:D:180:LEU:HD13	1:D:488:ALA:HB1	1.92	0.50
2:G:175:HIS:HD2	2:H:178:ASN:HD21	1.59	0.50
1:A:276:THR:HB	3:A:900:DTP:H2	1.93	0.50
1:A:320:LYS:CD	1:A:411:ARG:HB2	2.40	0.50
1:A:50:TYR:H	1:A:53:ILE:HG21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:HA	1:D:151:LEU:HD12	1.94	0.50
2:F:74:ILE:O	2:F:78:LYS:HG3	2.11	0.50
2:H:311:ILE:HD11	2:H:315:ARG:HE	1.76	0.50
1:A:46:HIS:HE1	2:F:220:GLU:O	1.94	0.50
1:A:686:GLN:HG2	1:A:725:GLY:O	2.10	0.50
1:B:680:GLN:O	1:B:684:ILE:HG13	2.11	0.50
1:C:293:SER:CB	1:C:298:ARG:O	2.59	0.50
1:C:286:GLN:CD	1:C:332:HIS:HB2	2.31	0.50
2:E:178:ASN:HD21	2:F:175:HIS:CD2	2.29	0.50
2:F:129:ILE:HG13	2:F:130:VAL:HG13	1.92	0.50
2:G:311:ILE:HD11	2:G:315:ARG:HE	1.75	0.50
1:A:196:PHE:O	1:A:200:VAL:HG22	2.11	0.50
1:A:441:GLU:OE1	1:A:620:MET:CB	2.54	0.50
1:C:313:VAL:HG13	1:C:314:GLU:N	2.26	0.50
1:C:55:THR:HB	3:C:800:DTP:H8	1.92	0.50
1:D:303:THR:HG21	1:D:440:LEU:HD21	1.94	0.50
2:F:332:ILE:HB	2:F:334:TRP:NE1	2.25	0.50
2:H:163:MET:HB3	2:H:189:LEU:HD13	1.93	0.50
1:B:103:TYR:O	1:B:107:VAL:HG23	2.12	0.50
1:C:430:ILE:HG22	1:C:431:ALA:N	2.26	0.50
1:D:313:VAL:HG13	1:D:314:GLU:N	2.27	0.50
2:E:332:ILE:HB	2:E:334:TRP:NE1	2.27	0.50
2:G:5:PHE:CD1	2:G:24:ASN:O	2.65	0.50
2:H:304:LEU:O	2:H:308:VAL:HG23	2.11	0.50
1:A:227:LEU:CA	1:A:435:GLN:NE2	2.73	0.50
1:B:53:ILE:O	1:B:53:ILE:HG23	2.11	0.50
1:C:135:ILE:HA	1:C:197:TYR:CZ	2.46	0.50
1:C:316:LEU:HA	1:C:319:LEU:HG	1.92	0.50
2:G:36:PHE:CZ	2:G:104:LEU:HD13	2.47	0.50
1:A:151:LEU:HD23	1:A:155:TYR:CD2	2.47	0.50
1:A:618:ALA:HB2	1:A:691:GLN:CB	2.32	0.50
1:A:82:ALA:O	1:A:86:ILE:HG12	2.10	0.50
1:D:135:ILE:HD11	1:D:174:ILE:HG21	1.93	0.50
1:D:368:PHE:HD2	1:D:369:PHE:CZ	2.29	0.50
1:D:55:THR:OG1	3:D:800:DTP:H5'1	2.11	0.50
1:A:680:GLN:O	1:A:684:ILE:HG13	2.11	0.50
1:B:469:LEU:HB3	1:B:523:TYR:CD1	2.46	0.50
1:C:619:LEU:CD1	1:C:693:ILE:CD1	2.90	0.50
1:C:656:VAL:HG23	1:C:659:TYR:HB2	1.94	0.50
2:E:255:GLY:CA	2:E:258:ASP:O	2.57	0.50
1:A:153:GLY:O	1:A:160:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:SER:HB2	1:B:625:SER:HB2	1.94	0.50
1:C:303:THR:HG21	1:C:440:LEU:HD21	1.94	0.50
2:E:23:VAL:HG22	2:E:100:SER:C	2.32	0.50
2:F:160:LEU:HD21	2:F:193:LEU:CD2	2.41	0.50
2:E:175:HIS:CD2	2:F:178:ASN:HD21	2.29	0.50
2:G:160:LEU:HD21	2:G:193:LEU:CD2	2.41	0.50
1:B:35:ASN:O	1:B:35:ASN:CG	2.50	0.49
1:D:469:LEU:HB3	1:D:523:TYR:CD1	2.47	0.49
1:D:656:VAL:HG23	1:D:659:TYR:HB2	1.93	0.49
2:E:74:ILE:O	2:E:78:LYS:HG3	2.11	0.49
2:F:147:GLN:O	2:F:151:GLU:N	2.45	0.49
2:G:55:VAL:HG12	2:G:226:GLY:HA3	1.94	0.49
2:H:147:GLN:O	2:H:151:GLU:N	2.46	0.49
1:A:224:SER:O	1:A:252:ALA:CA	2.60	0.49
1:A:463:THR:CG2	1:A:492:LEU:CD2	2.78	0.49
1:C:619:LEU:CD1	1:C:693:ILE:HG23	2.32	0.49
1:D:33:LEU:HD22	1:D:76:ASP:HB3	1.93	0.49
1:C:348:LEU:O	2:G:371:SER:HB3	2.12	0.49
2:H:78:LYS:HE2	2:H:136:VAL:HG13	1.93	0.49
1:A:103:TYR:O	1:A:107:VAL:HG23	2.13	0.49
1:A:254:ILE:O	1:A:302:ALA:CA	2.60	0.49
1:A:247:TYR:CZ	1:A:461:LEU:HD21	2.47	0.49
1:C:276:THR:CB	3:C:900:DTP:H2	2.39	0.49
1:D:227:LEU:HD23	1:D:435:GLN:HG3	1.93	0.49
1:D:514:GLY:HA2	1:D:618:ALA:HB2	1.91	0.49
1:D:519:ASN:HA	1:D:632:THR:H	1.77	0.49
1:D:681:LEU:O	1:D:685:MET:HG3	2.13	0.49
1:A:228:ILE:CG2	1:A:240:THR:HG23	2.42	0.49
1:A:227:LEU:CB	1:A:435:GLN:HE21	2.17	0.49
1:A:669:LEU:HD11	1:A:698:ASN:ND2	2.28	0.49
1:B:324:GLY:HA3	1:B:329:ARG:NH2	2.28	0.49
1:B:645:LYS:NZ	1:B:645:LYS:HB2	2.27	0.49
1:D:543:THR:O	1:D:547:ILE:HG13	2.11	0.49
2:H:74:ILE:O	2:H:78:LYS:HG3	2.12	0.49
1:A:40:GLN:HE22	2:F:334:TRP:H	1.60	0.49
1:B:196:PHE:O	1:B:200:VAL:HG22	2.12	0.49
1:A:269:ARG:HH22	1:B:219:THR:HA	1.77	0.49
1:C:247:TYR:O	1:C:252:ALA:HB3	2.13	0.49
1:D:114:LYS:HE2	1:D:166:TYR:CE2	2.47	0.49
1:D:433:VAL:HG11	1:D:443:ALA:HB1	1.94	0.49
1:D:54:LYS:O	1:D:58:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:332:ILE:HB	2:G:334:TRP:NE1	2.28	0.49
1:A:552:LEU:HB3	1:A:602:LEU:HD21	1.93	0.49
1:B:478:LEU:HB2	1:B:550:TYR:CD2	2.47	0.49
1:B:696:ASN:N	1:B:696:ASN:HD22	2.11	0.49
1:C:342:LEU:HD21	1:C:379:TYR:CD2	2.47	0.49
1:C:469:LEU:HB3	1:C:523:TYR:CD1	2.47	0.49
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.48	0.49
1:C:154:LYS:CG	1:C:155:TYR:CD1	2.96	0.49
1:C:583:TYR:HD2	1:C:587:LEU:HD12	1.77	0.49
1:D:135:ILE:HA	1:D:197:TYR:CZ	2.47	0.49
2:E:160:LEU:HD21	2:E:193:LEU:CD2	2.43	0.49
1:A:520:PHE:CB	1:A:635:ILE:HA	2.43	0.49
1:B:107:VAL:O	1:B:111:GLU:HG3	2.11	0.49
1:A:238:ASN:OD1	1:B:242:SER:HA	2.12	0.49
1:B:520:PHE:CB	1:B:635:ILE:HA	2.43	0.49
1:C:542:LYS:HG3	1:C:596:HIS:CD2	2.46	0.49
1:D:368:PHE:HD2	1:D:369:PHE:CE1	2.31	0.49
1:A:144:SER:O	1:A:148:VAL:HG23	2.12	0.49
1:A:119:LEU:HD21	1:A:179:CYS:SG	2.53	0.49
1:B:134:PHE:HB3	1:B:194:LYS:HG3	1.95	0.49
1:B:214:GLY:O	1:B:215:VAL:C	2.50	0.49
1:C:379:TYR:O	1:C:383:GLU:HG3	2.13	0.49
1:D:517:VAL:O	1:D:634:GLY:HA2	2.12	0.49
2:E:155:SER:O	2:E:159:GLU:HG3	2.13	0.49
2:E:55:VAL:HG12	2:E:226:GLY:HA3	1.94	0.49
2:G:155:SER:O	2:G:159:GLU:HG3	2.13	0.49
1:C:43:LEU:HD12	2:G:334:TRP:CD1	2.48	0.49
1:A:37:SER:HB3	1:A:40:GLN:HG2	1.93	0.49
1:A:618:ALA:HA	1:A:689:ILE:HG23	1.93	0.49
1:B:227:LEU:HB3	1:B:435:GLN:NE2	2.28	0.49
1:B:441:GLU:HG2	1:B:442:ILE:CG1	2.33	0.49
1:B:606:ILE:HG23	1:B:611:LEU:HG	1.94	0.49
1:C:248:VAL:HG11	1:C:289:VAL:HA	1.95	0.49
2:E:227:ASN:O	2:E:231:ILE:HG12	2.13	0.49
2:H:147:GLN:NE2	2:H:147:GLN:HA	2.27	0.49
2:H:204:GLU:OE2	2:H:241:HIS:HB3	2.13	0.49
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.95	0.49
1:A:244:ILE:CG2	1:A:254:ILE:HG13	2.24	0.48
1:B:361:VAL:O	1:B:364:LEU:HB2	2.13	0.48
1:C:40:GLN:HG2	1:C:44:ARG:HG3	1.95	0.48
1:D:103:TYR:O	1:D:107:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:TYR:O	1:D:383:GLU:HG3	2.12	0.48
1:D:437:ASN:HB3	1:D:442:ILE:HB	1.94	0.48
1:D:689:ILE:CG2	1:D:691:GLN:H	2.25	0.48
2:H:155:SER:O	2:H:159:GLU:HG3	2.13	0.48
1:A:151:LEU:CA	1:A:155:TYR:HB2	2.35	0.48
1:D:248:VAL:HG11	1:D:289:VAL:HA	1.95	0.48
1:D:151:LEU:HG	1:D:628:ILE:HD12	1.94	0.48
1:D:94:TYR:CD1	1:D:100:PRO:CD	2.96	0.48
2:G:145:GLN:HG2	2:G:289:TYR:CG	2.49	0.48
2:H:160:LEU:HD21	2:H:193:LEU:CD2	2.42	0.48
1:B:290:LYS:HE3	1:B:332:HIS:HB3	1.95	0.48
1:B:532:SER:HA	1:B:677:GLY:HA3	1.95	0.48
1:D:367:ALA:O	1:D:371:ASP:O	2.31	0.48
2:E:147:GLN:O	2:E:151:GLU:N	2.47	0.48
1:A:437:ASN:HD21	1:A:439:CYS:CB	2.05	0.48
1:C:103:TYR:O	1:C:107:VAL:HG23	2.13	0.48
1:C:437:ASN:HB3	1:C:442:ILE:HB	1.93	0.48
1:C:301:ALA:HB1	1:C:438:LEU:HD11	1.95	0.48
1:D:692:SER:OG	1:D:728:THR:HG23	2.14	0.48
2:G:147:GLN:HA	2:G:147:GLN:NE2	2.29	0.48
2:G:245:THR:HA	2:G:248:MET:HE3	1.95	0.48
1:C:42:GLU:OE1	2:G:298:GLY:N	2.46	0.48
1:A:312:GLU:O	1:A:316:LEU:HG	2.12	0.48
1:A:324:GLY:HA3	1:A:329:ARG:NH2	2.29	0.48
1:A:645:LYS:HB2	1:A:645:LYS:NZ	2.29	0.48
1:B:144:SER:O	1:B:148:VAL:HG23	2.14	0.48
1:B:254:ILE:O	1:B:302:ALA:CA	2.61	0.48
1:C:233:SER:HA	3:C:900:DTP:O5'	2.13	0.48
1:D:583:TYR:HD2	1:D:587:LEU:HD12	1.77	0.48
1:B:441:GLU:HG2	1:B:442:ILE:N	2.29	0.48
1:B:430:ILE:HG21	1:B:570:GLU:HG2	1.94	0.48
1:C:208:PRO:CB	1:C:464:LEU:CD1	2.60	0.48
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.95	0.48
2:G:74:ILE:O	2:G:78:LYS:HG3	2.14	0.48
1:C:148:VAL:HA	1:C:151:LEU:HD12	1.94	0.48
1:C:458:GLU:OE1	1:C:567:TRP:CZ3	2.67	0.48
1:D:125:GLU:O	1:D:129:LYS:HG3	2.13	0.48
1:D:403:MET:CE	1:D:714:LEU:HB3	2.44	0.48
1:D:572:THR:HB	1:D:577:ILE:HB	1.95	0.48
1:D:644:ILE:HA	1:D:652:LEU:O	2.14	0.48
2:E:35:ILE:HG23	2:E:36:PHE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:ASN:OD1	2:F:109:GLU:HG2	2.13	0.48
2:F:245:THR:HA	2:F:248:MET:HE3	1.94	0.48
2:G:9:LYS:HD3	2:H:142:THR:HG23	1.94	0.48
1:A:383:GLU:O	1:A:390:LYS:HE2	2.14	0.48
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.95	0.48
1:A:696:ASN:HD22	1:A:696:ASN:N	2.11	0.48
1:C:86:ILE:HD11	1:C:148:VAL:HG22	1.95	0.48
1:C:294:GLN:CB	1:C:298:ARG:HD2	2.43	0.48
1:D:668:LEU:HB2	1:D:671:GLU:HG3	1.96	0.48
1:D:693:ILE:HG22	1:D:694:SER:N	2.28	0.48
2:E:163:MET:HB3	2:E:189:LEU:HD13	1.95	0.48
2:E:118:HIS:ND1	2:E:234:ILE:HG23	2.28	0.48
2:G:92:ASN:OD1	2:G:109:GLU:HG2	2.14	0.48
2:G:204:GLU:OE2	2:G:241:HIS:HB3	2.14	0.48
1:A:132:ASP:HA	1:A:135:ILE:HD12	1.96	0.48
1:A:182:SER:HA	1:A:189:ARG:HE	1.79	0.48
1:A:441:GLU:OE1	1:A:621:PRO:HD2	2.14	0.48
1:A:55:THR:CB	3:A:800:DTP:H8	2.42	0.48
1:B:231:GLY:N	1:B:236:SER:OG	2.46	0.48
1:B:312:GLU:O	1:B:316:LEU:HG	2.13	0.48
1:B:644:ILE:HG13	1:B:653:ARG:HG2	1.95	0.48
2:H:122:TYR:O	2:H:126:ILE:HG13	2.14	0.48
1:A:6:LEU:HB2	1:A:52:GLY:H	1.79	0.48
1:D:342:LEU:HD21	1:D:379:TYR:CD2	2.49	0.48
1:D:689:ILE:HG22	1:D:691:GLN:O	2.12	0.48
2:E:145:GLN:HG2	2:E:289:TYR:CG	2.49	0.48
2:G:147:GLN:O	2:G:151:GLU:N	2.47	0.48
1:A:361:VAL:O	1:A:364:LEU:HB2	2.13	0.47
1:B:19:LEU:HA	1:B:22:ILE:CD1	2.44	0.47
1:B:317:LEU:HD23	1:B:401:LEU:CD2	2.42	0.47
1:C:94:TYR:CD1	1:C:100:PRO:HG3	2.49	0.47
2:F:206:ILE:O	2:F:210:VAL:HG23	2.14	0.47
1:A:87:PHE:HE1	3:A:800:DTP:O2A	1.97	0.47
1:C:441:GLU:CA	1:C:692:SER:O	2.62	0.47
1:D:618:ALA:O	1:D:620:MET:HE3	2.12	0.47
2:F:126:ILE:O	2:F:130:VAL:HG22	2.14	0.47
2:F:84:ASP:HA	2:F:87:GLN:HB2	1.96	0.47
2:G:9:LYS:HD3	2:H:142:THR:CG2	2.44	0.47
2:H:255:GLY:HA2	2:H:262:ALA:HB2	1.96	0.47
1:A:107:VAL:O	1:A:111:GLU:HG3	2.14	0.47
1:C:437:ASN:O	1:C:440:LEU:HD22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:VAL:HG12	2:F:226:GLY:HA3	1.97	0.47
2:G:204:GLU:HG2	2:G:238:GLU:OE2	2.14	0.47
1:A:532:SER:HA	1:A:677:GLY:HA3	1.96	0.47
1:B:51:ASP:O	1:B:51:ASP:OD2	2.32	0.47
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.72	0.47
2:F:145:GLN:HG2	2:F:289:TYR:CG	2.49	0.47
2:H:102:PRO:HG2	2:H:103:GLU:OE1	2.14	0.47
1:A:490:ASP:CG	1:A:511:ARG:HH21	2.18	0.47
1:B:303:THR:HG23	1:B:334:ASP:O	2.14	0.47
1:B:180:LEU:HD13	1:B:488:ALA:HB1	1.96	0.47
1:C:186:ARG:HH21	1:C:189:ARG:NH2	2.08	0.47
1:C:668:LEU:HB2	1:C:671:GLU:HG3	1.96	0.47
1:D:561:GLU:HG2	1:D:562:GLN:HG3	1.96	0.47
2:E:8:THR:O	2:F:141:VAL:HG11	2.14	0.47
2:G:255:GLY:HA2	2:G:262:ALA:HB2	1.96	0.47
1:A:231:GLY:N	1:A:236:SER:OG	2.45	0.47
1:A:560:LYS:HG2	1:A:609:HIS:CB	2.44	0.47
1:A:644:ILE:HG13	1:A:653:ARG:HG2	1.95	0.47
1:B:181:PHE:O	1:B:189:ARG:HD2	2.15	0.47
1:C:285:PHE:O	1:C:289:VAL:HG23	2.15	0.47
1:C:287:THR:HB	1:D:284:HIS:ND1	2.30	0.47
1:C:309:TRP:O	1:C:355:LEU:HA	2.14	0.47
1:C:403:MET:CE	1:C:714:LEU:HB3	2.45	0.47
1:C:558:LEU:HD11	1:C:562:GLN:NE2	2.30	0.47
1:C:689:ILE:CG2	1:C:691:GLN:H	2.26	0.47
1:C:7:VAL:HG21	1:C:17:ILE:HG12	1.91	0.47
1:D:441:GLU:CB	1:D:619:LEU:O	2.59	0.47
1:D:441:GLU:CA	1:D:692:SER:O	2.63	0.47
1:C:125:GLU:O	1:C:129:LYS:HG3	2.14	0.47
1:D:15:GLU:HG3	1:D:16:ARG:N	2.28	0.47
1:D:519:ASN:CB	1:D:631:ALA:HB1	2.45	0.47
2:E:266:GLU:OE2	2:E:269:LYS:HD2	2.15	0.47
2:F:255:GLY:HA2	2:F:262:ALA:HB2	1.95	0.47
2:G:126:ILE:O	2:G:130:VAL:HG22	2.15	0.47
2:H:204:GLU:HG2	2:H:238:GLU:OE2	2.15	0.47
1:A:320:LYS:HE3	1:A:411:ARG:HB3	1.96	0.47
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.47
1:A:63:ILE:HD13	1:A:85:ALA:HA	1.97	0.47
1:B:244:ILE:O	1:B:248:VAL:HG13	2.15	0.47
1:B:459:ILE:HB	1:B:503:ALA:CA	2.44	0.47
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG23	1:C:167:GLU:OE2	2.14	0.47
1:C:681:LEU:O	1:C:685:MET:HG3	2.14	0.47
1:C:619:LEU:CD1	1:C:693:ILE:CG1	2.93	0.47
1:D:44:ARG:HG3	1:D:69:LEU:HD21	1.96	0.47
2:E:93:VAL:HG13	2:F:97:PRO:HG3	1.97	0.47
1:B:309:TRP:O	1:B:355:LEU:HA	2.14	0.47
1:B:339:ILE:O	1:B:416:ASN:HA	2.15	0.47
1:B:51:ASP:OD2	1:B:51:ASP:C	2.52	0.47
1:B:603:ARG:O	1:B:607:LYS:HB2	2.15	0.47
1:C:567:TRP:O	1:C:569:ASN:N	2.48	0.47
1:D:25:VAL:HG21	3:D:800:DTP:O3'	2.15	0.47
2:H:1:ALA:HB3	2:H:168:HIS:CA	2.42	0.47
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.50	0.47
1:D:247:TYR:O	1:D:252:ALA:HB3	2.15	0.47
2:F:155:SER:O	2:F:159:GLU:HG3	2.15	0.47
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.95	0.47
1:A:431:ALA:HB1	1:A:445:PRO:CB	2.44	0.47
1:B:10:ARG:HD3	1:B:55:THR:CG2	2.45	0.47
1:C:234:LEU:HD22	1:D:246:LYS:HD3	1.96	0.47
1:C:264:LEU:HD13	1:C:276:THR:O	2.15	0.47
1:D:85:ALA:O	1:D:89:LEU:HG	2.15	0.47
2:G:206:ILE:O	2:G:210:VAL:HG23	2.15	0.47
2:G:48:TRP:CZ3	2:G:50:PRO:HG3	2.49	0.47
2:H:205:ALA:HB1	2:H:315:ARG:HD2	1.97	0.47
1:A:42:GLU:O	2:F:297:ILE:CD1	2.63	0.46
1:B:59:HIS:O	1:B:62:ILE:HG12	2.15	0.46
1:C:135:ILE:HG23	1:C:170:GLN:HB3	1.97	0.46
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.96	0.46
2:E:147:GLN:HA	2:E:147:GLN:NE2	2.30	0.46
1:B:294:GLN:C	1:B:296:GLY:N	2.69	0.46
1:B:383:GLU:O	1:B:390:LYS:HE2	2.15	0.46
1:B:463:THR:HG22	1:B:489:LEU:HD22	1.97	0.46
1:C:585:LYS:HD3	1:C:585:LYS:N	2.23	0.46
1:D:458:GLU:OE1	1:D:567:TRP:CZ3	2.69	0.46
2:F:122:TYR:O	2:F:126:ILE:HG13	2.15	0.46
2:H:118:HIS:ND1	2:H:234:ILE:HG23	2.30	0.46
1:A:233:SER:OG	1:A:236:SER:N	2.40	0.46
1:A:258:ALA:O	1:A:260:ARG:N	2.49	0.46
1:A:304:LEU:HB3	1:A:335:TYR:HD1	1.81	0.46
1:A:371:ASP:HB3	1:A:374:GLU:HB3	1.97	0.46
1:A:342:LEU:HD23	1:A:375:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD13	1:A:488:ALA:HB1	1.97	0.46
1:B:140:ASP:HA	1:B:143:PHE:CD2	2.51	0.46
1:B:560:LYS:HG2	1:B:609:HIS:CB	2.45	0.46
1:C:617:SER:O	1:C:690:ASP:HB2	2.15	0.46
2:E:126:ILE:O	2:E:130:VAL:HG22	2.15	0.46
2:F:103:GLU:HG2	2:F:104:LEU:N	2.30	0.46
2:H:55:VAL:HG12	2:H:226:GLY:HA3	1.96	0.46
1:A:394:LYS:NZ	1:A:394:LYS:HB2	2.30	0.46
1:A:603:ARG:O	1:A:607:LYS:HB2	2.14	0.46
1:B:146:ALA:HB3	1:B:654:GLN:NE2	2.31	0.46
1:B:258:ALA:O	1:B:260:ARG:N	2.49	0.46
1:B:519:ASN:HA	1:B:632:THR:H	1.81	0.46
1:D:135:ILE:HG23	1:D:170:GLN:HB3	1.97	0.46
1:D:176:VAL:HG22	1:D:215:VAL:HB	1.97	0.46
1:D:350:GLY:HA3	2:E:367:THR:HG21	1.98	0.46
1:D:55:THR:HG1	3:D:800:DTP:H5'1	1.80	0.46
1:A:202:THR:OG1	1:A:204:LYS:HD3	2.15	0.46
1:A:253:GLY:O	1:A:254:ILE:HD13	2.16	0.46
1:C:572:THR:HB	1:C:577:ILE:HB	1.97	0.46
1:D:86:ILE:HD11	1:D:148:VAL:HG22	1.96	0.46
1:D:185:PRO:HB2	1:D:187:GLU:CG	2.45	0.46
1:D:567:TRP:O	1:D:569:ASN:N	2.49	0.46
2:F:1:ALA:HB3	2:F:168:HIS:CA	2.43	0.46
2:F:260:GLU:O	2:F:264:ILE:HG13	2.15	0.46
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.51	0.46
1:A:706:SER:HB2	1:A:708:LYS:CD	2.46	0.46
1:B:320:LYS:CD	1:B:411:ARG:HB2	2.46	0.46
1:B:431:ALA:HB1	1:B:445:PRO:CB	2.46	0.46
1:C:233:SER:HA	3:C:900:DTP:PA	2.56	0.46
1:C:317:LEU:O	1:C:405:GLU:HG3	2.15	0.46
1:C:40:GLN:O	1:C:44:ARG:N	2.43	0.46
1:D:102:LEU:O	1:D:106:VAL:HG23	2.16	0.46
1:C:246:LYS:NZ	1:D:234:LEU:HB3	2.30	0.46
1:D:583:TYR:CB	1:D:687:LYS:HG3	2.46	0.46
1:D:6:LEU:O	1:D:14:THR:HG23	2.15	0.46
2:E:122:TYR:O	2:E:126:ILE:HG13	2.15	0.46
2:E:204:GLU:OE2	2:E:241:HIS:HB3	2.16	0.46
2:E:260:GLU:O	2:E:264:ILE:HG13	2.16	0.46
2:F:239:ALA:O	2:F:242:LEU:HG	2.15	0.46
2:H:126:ILE:O	2:H:130:VAL:HG22	2.15	0.46
1:B:228:ILE:HG21	1:B:240:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:THR:O	1:C:582:THR:HB	2.15	0.46
2:E:136:VAL:O	2:E:140:ILE:HG13	2.16	0.46
1:A:353:ILE:HB	1:A:393:VAL:HG23	1.98	0.46
1:B:172:LEU:O	1:B:176:VAL:HG23	2.16	0.46
1:C:680:GLN:O	1:C:684:ILE:HG13	2.16	0.46
1:C:85:ALA:O	1:C:89:LEU:HG	2.15	0.46
1:D:264:LEU:HD13	1:D:276:THR:O	2.15	0.46
1:D:53:ILE:HG13	1:D:58:ILE:CD1	2.44	0.46
2:F:203:LEU:HA	2:F:207:ARG:HD2	1.98	0.46
2:G:166:TYR:CE2	2:H:169:LEU:HD22	2.50	0.46
1:A:172:LEU:O	1:A:176:VAL:HG23	2.16	0.46
1:A:214:GLY:O	1:A:215:VAL:C	2.53	0.46
1:C:102:LEU:O	1:C:106:VAL:HG23	2.16	0.46
1:C:215:VAL:O	1:C:216:ARG:CB	2.64	0.46
1:D:240:THR:O	1:D:244:ILE:HG13	2.16	0.46
2:F:147:GLN:HA	2:F:147:GLN:NE2	2.30	0.46
2:G:260:GLU:O	2:G:264:ILE:HG13	2.16	0.46
2:H:48:TRP:CZ3	2:H:50:PRO:HG3	2.51	0.46
1:A:244:ILE:O	1:A:248:VAL:HG13	2.15	0.46
1:A:357:SER:HB3	1:A:360:ASP:OD2	2.16	0.46
1:B:182:SER:HA	1:B:189:ARG:HE	1.80	0.46
1:B:706:SER:HB2	1:B:708:LYS:CD	2.45	0.46
1:C:137:HIS:HA	1:C:170:GLN:HG3	1.98	0.46
1:C:339:ILE:HD12	1:C:414:ILE:HG23	1.98	0.46
1:C:520:PHE:O	1:C:523:TYR:CB	2.63	0.46
1:C:692:SER:OG	1:C:728:THR:HG23	2.16	0.46
1:D:152:GLU:O	1:D:158:GLN:NE2	2.48	0.46
1:D:309:TRP:O	1:D:355:LEU:HA	2.15	0.46
1:D:437:ASN:O	1:D:440:LEU:HD22	2.16	0.46
1:D:544:PHE:CE2	1:D:685:MET:HG2	2.51	0.46
1:D:696:ASN:N	1:D:696:ASN:ND2	2.62	0.46
2:E:255:GLY:HA2	2:E:262:ALA:HB2	1.97	0.46
1:A:365:TYR:O	1:A:368:PHE:HB3	2.16	0.45
1:A:41:VAL:HG22	1:A:69:LEU:CD1	2.44	0.45
1:A:440:LEU:N	1:A:440:LEU:CD2	2.78	0.45
1:B:253:GLY:O	1:B:254:ILE:HD13	2.16	0.45
1:B:365:TYR:O	1:B:368:PHE:HB3	2.17	0.45
1:B:371:ASP:HB3	1:B:374:GLU:HB3	1.98	0.45
1:B:511:ARG:NH1	1:B:511:ARG:HG2	2.30	0.45
1:B:681:LEU:O	1:B:685:MET:HG3	2.16	0.45
1:C:226:VAL:HG21	1:C:247:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:THR:O	1:D:219:THR:N	2.49	0.45
2:E:46:PHE:O	2:E:48:TRP:HD1	1.99	0.45
2:E:97:PRO:HG3	2:F:93:VAL:HG13	1.98	0.45
2:G:103:GLU:HG2	2:G:104:LEU:N	2.30	0.45
2:G:118:HIS:ND1	2:G:234:ILE:HG23	2.31	0.45
2:G:239:ALA:O	2:G:242:LEU:HG	2.16	0.45
2:H:260:GLU:O	2:H:264:ILE:HG13	2.16	0.45
2:H:276:PHE:HB3	2:H:316:MET:SD	2.56	0.45
1:A:233:SER:OG	1:A:236:SER:HB2	2.15	0.45
1:A:59:HIS:NE2	3:A:800:DTP:H4'	2.30	0.45
1:B:202:THR:OG1	1:B:204:LYS:HD3	2.17	0.45
1:B:327:GLY:C	1:B:328:ASN:HD22	2.19	0.45
1:B:418:ASP:HA	1:B:421:ASN:ND2	2.31	0.45
1:B:619:LEU:CB	1:B:693:ILE:HG23	2.46	0.45
1:C:59:HIS:CD2	3:C:800:DTP:H4'	2.50	0.45
2:F:266:GLU:OE2	2:F:269:LYS:HD2	2.17	0.45
1:A:511:ARG:HG2	1:A:511:ARG:HH11	1.81	0.45
1:C:310:HIS:O	1:C:355:LEU:HB3	2.17	0.45
1:C:644:ILE:HA	1:C:652:LEU:O	2.16	0.45
1:D:137:HIS:HA	1:D:170:GLN:HG3	1.97	0.45
1:D:217:THR:O	1:D:218:PRO:C	2.55	0.45
1:D:320:LYS:HE2	1:D:333:MET:O	2.17	0.45
2:E:28:TYR:CD2	2:F:120:ARG:HA	2.51	0.45
2:F:136:VAL:O	2:F:140:ILE:HG13	2.16	0.45
2:F:309:GLU:HB3	2:F:325:PHE:HB3	1.99	0.45
1:A:106:VAL:HG21	1:A:128:PHE:CE1	2.52	0.45
1:A:146:ALA:HB3	1:A:654:GLN:NE2	2.31	0.45
1:C:242:SER:O	1:D:238:ASN:ND2	2.50	0.45
1:C:56:SER:O	1:C:59:HIS:HB2	2.17	0.45
1:C:689:ILE:HG22	1:C:691:GLN:O	2.11	0.45
1:D:339:ILE:HD12	1:D:414:ILE:HG23	1.97	0.45
2:E:103:GLU:HG2	2:E:104:LEU:N	2.31	0.45
1:B:341:LYS:HE3	2:H:375:LEU:HB2	1.98	0.45
1:A:430:ILE:HG21	1:A:570:GLU:HG2	1.98	0.45
1:A:68:ASP:HA	1:A:653:ARG:HH12	1.78	0.45
1:B:34:HIS:O	1:B:36:VAL:HG22	2.17	0.45
1:C:465:SER:CB	1:C:489:LEU:HD11	2.47	0.45
1:C:619:LEU:HD13	1:C:693:ILE:CG1	2.47	0.45
1:C:693:ILE:CG2	1:C:694:SER:N	2.79	0.45
2:H:266:GLU:OE2	2:H:269:LYS:HD2	2.16	0.45
1:A:309:TRP:O	1:A:355:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:CD2	2:F:298:GLY:HA3	2.45	0.45
1:C:136:ASP:HB3	1:C:139:ARG:HE	1.82	0.45
1:C:613:ASN:HB2	1:C:616:LEU:HG	1.98	0.45
2:F:204:GLU:HG2	2:F:238:GLU:OE2	2.16	0.45
1:A:339:ILE:O	1:A:416:ASN:HA	2.16	0.45
1:A:512:THR:O	1:A:513:LEU:HD23	2.16	0.45
1:A:696:ASN:HD21	1:A:730:TYR:HB3	1.81	0.45
1:B:342:LEU:HD23	1:B:375:PHE:HE2	1.81	0.45
1:B:552:LEU:HD12	1:B:599:TRP:HZ3	1.82	0.45
1:C:544:PHE:CE2	1:C:685:MET:HG2	2.52	0.45
2:E:239:ALA:O	2:E:242:LEU:HG	2.17	0.45
2:E:34:ASP:O	2:E:38:LYS:HG3	2.17	0.45
2:F:284:LYS:HE3	2:F:325:PHE:CE1	2.52	0.45
2:H:92:ASN:OD1	2:H:109:GLU:HG2	2.17	0.45
1:A:519:ASN:HA	1:A:632:THR:H	1.81	0.45
1:A:643:SER:C	1:A:644:ILE:HD12	2.37	0.45
1:B:682:VAL:HA	1:B:685:MET:HE3	1.97	0.45
1:C:135:ILE:HA	1:C:197:TYR:CE2	2.52	0.45
1:C:583:TYR:CB	1:C:687:LYS:HG3	2.47	0.45
1:D:422:THR:O	1:D:582:THR:HB	2.17	0.45
1:D:558:LEU:HD11	1:D:562:GLN:NE2	2.32	0.45
1:D:670:TRP:CZ3	1:D:735:ARG:HB2	2.52	0.45
2:E:175:HIS:HD2	2:F:178:ASN:HD21	1.65	0.45
2:G:284:LYS:HE3	2:G:325:PHE:CE1	2.52	0.45
2:H:136:VAL:O	2:H:140:ILE:HG13	2.16	0.45
2:H:203:LEU:O	2:H:207:ARG:HB2	2.17	0.45
1:C:441:GLU:O	1:C:692:SER:O	2.34	0.45
1:C:510:ARG:HB2	1:C:512:THR:HG23	1.99	0.45
1:C:98:GLU:HA	1:C:99:PRO:HD3	1.81	0.45
1:D:680:GLN:O	1:D:684:ILE:HG13	2.17	0.45
2:F:46:PHE:O	2:F:48:TRP:HD1	1.99	0.45
2:G:120:ARG:HA	2:H:28:TYR:CD2	2.52	0.45
1:A:438:LEU:O	1:A:440:LEU:CD2	2.59	0.45
1:A:696:ASN:OD1	1:A:731:TYR:HB2	2.17	0.45
1:B:339:ILE:HG22	1:B:340:ASN:N	2.32	0.45
1:B:40:GLN:O	1:B:44:ARG:N	2.32	0.45
1:B:706:SER:HB2	1:B:708:LYS:HD2	1.99	0.45
1:D:6:LEU:CA	1:D:14:THR:CG2	2.94	0.45
1:D:524:LEU:HD22	1:D:529:LYS:HB2	1.97	0.45
1:D:585:LYS:N	1:D:585:LYS:HD3	2.23	0.45
1:D:33:LEU:CD1	1:D:80:LEU:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:276:PHE:HB3	2:G:316:MET:SD	2.57	0.45
1:A:134:PHE:HB3	1:A:194:LYS:HG3	1.99	0.44
1:A:140:ASP:HA	1:A:143:PHE:CD2	2.52	0.44
1:A:59:HIS:CE1	3:A:800:DTP:O2A	2.71	0.44
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.99	0.44
1:B:512:THR:O	1:B:513:LEU:HD23	2.17	0.44
1:D:254:ILE:HG22	1:D:255:GLY:N	2.32	0.44
2:G:122:TYR:O	2:G:126:ILE:HG13	2.16	0.44
2:G:136:VAL:O	2:G:140:ILE:HG13	2.17	0.44
2:H:103:GLU:HG2	2:H:104:LEU:N	2.32	0.44
2:H:365:VAL:HG12	2:H:366:ASP:N	2.30	0.44
1:A:348:LEU:O	2:F:371:SER:HB3	2.17	0.44
1:A:682:VAL:HA	1:A:685:MET:HE3	1.98	0.44
1:B:222:PHE:HD2	1:B:496:GLN:HB3	1.81	0.44
1:B:55:THR:HA	1:B:58:ILE:HG12	1.98	0.44
1:C:240:THR:O	1:C:244:ILE:HG13	2.17	0.44
1:C:431:ALA:CB	1:C:445:PRO:HB3	2.32	0.44
1:C:500:ILE:HG22	1:C:502:ALA:H	1.83	0.44
2:F:76:ASN:HD21	2:F:211:SER:CA	2.30	0.44
2:G:203:LEU:HA	2:G:207:ARG:HD2	1.98	0.44
1:A:241:SER:O	1:A:245:VAL:HG23	2.18	0.44
1:A:545:GLU:HA	1:A:688:PHE:CE2	2.53	0.44
1:B:357:SER:HB3	1:B:360:ASP:OD2	2.17	0.44
1:B:556:ASN:O	1:B:560:LYS:HG3	2.17	0.44
1:B:63:ILE:HD13	1:B:85:ALA:HA	1.99	0.44
1:C:167:GLU:OE2	1:C:216:ARG:NH2	2.47	0.44
1:D:6:LEU:HB3	1:D:14:THR:CG2	2.47	0.44
1:D:585:LYS:CD	1:D:585:LYS:H	2.25	0.44
1:D:538:ASN:HB3	1:D:593:GLU:OE1	2.18	0.44
2:H:284:LYS:HE3	2:H:325:PHE:CE1	2.52	0.44
1:A:327:GLY:C	1:A:328:ASN:HD22	2.20	0.44
1:A:697:THR:OG1	1:A:732:GLN:HG3	2.18	0.44
1:B:188:THR:HB	1:B:192:TYR:HE2	1.82	0.44
1:B:479:GLU:O	1:B:483:ILE:HG13	2.18	0.44
1:D:694:SER:O	1:D:730:TYR:HB2	2.16	0.44
2:E:284:LYS:HE3	2:E:325:PHE:CE1	2.52	0.44
1:D:348:LEU:HD22	2:E:370:LEU:O	2.18	0.44
1:A:712:GLN:NE2	2:F:370:LEU:HG	2.21	0.44
2:F:48:TRP:CZ3	2:F:50:PRO:HG3	2.52	0.44
2:H:203:LEU:HA	2:H:207:ARG:HD2	1.98	0.44
1:C:307:PRO:HG2	1:C:310:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:VAL:HG21	1:D:247:TYR:CD1	2.53	0.44
1:D:75:PRO:O	1:D:78:GLN:HB2	2.18	0.44
2:F:204:GLU:OE2	2:F:241:HIS:HB3	2.18	0.44
2:G:205:ALA:HB1	2:G:315:ARG:HD2	2.00	0.44
2:H:273:TYR:OH	2:H:324:PRO:HB3	2.17	0.44
1:A:339:ILE:HG22	1:A:340:ASN:N	2.32	0.44
1:A:685:MET:O	1:A:689:ILE:HG12	2.18	0.44
1:B:670:TRP:CH2	1:B:735:ARG:HB2	2.53	0.44
1:C:254:ILE:HG22	1:C:255:GLY:N	2.32	0.44
1:C:320:LYS:HE2	1:C:333:MET:O	2.17	0.44
1:D:307:PRO:HG2	1:D:310:HIS:HB2	2.00	0.44
2:G:309:GLU:HB3	2:G:325:PHE:HB3	1.99	0.44
1:A:232:ASP:OD2	1:A:262:ARG:NH2	2.50	0.44
1:B:320:LYS:HD2	1:B:411:ARG:HB2	2.00	0.44
1:C:172:LEU:O	1:C:176:VAL:HG23	2.18	0.44
1:C:553:LYS:HA	1:C:602:LEU:HD11	2.00	0.44
1:A:46:HIS:CE1	2:F:220:GLU:O	2.71	0.44
1:A:232:ASP:OD2	1:A:262:ARG:NE	2.49	0.44
1:A:439:CYS:O	1:A:440:LEU:CB	2.58	0.44
1:A:706:SER:HB2	1:A:708:LYS:HD2	2.00	0.44
1:C:155:TYR:OH	1:C:624:THR:HG21	2.14	0.44
1:D:228:ILE:HG21	1:D:240:THR:HG23	1.99	0.44
1:D:350:GLY:CA	2:E:367:THR:HG21	2.48	0.44
1:D:441:GLU:CG	1:D:620:MET:HB3	2.46	0.44
2:E:206:ILE:O	2:E:210:VAL:HG23	2.17	0.44
2:H:149:ARG:HH21	2:H:283:GLU:CD	2.20	0.44
1:A:510:ARG:HB3	1:A:510:ARG:HE	1.60	0.44
1:B:304:LEU:HB3	1:B:335:TYR:HD1	1.83	0.44
1:B:44:ARG:HA	1:B:44:ARG:NE	2.31	0.44
1:C:244:ILE:HG23	1:C:254:ILE:HG13	2.00	0.44
1:C:500:ILE:HD12	1:C:500:ILE:N	2.32	0.44
1:C:538:ASN:HB3	1:C:593:GLU:OE1	2.17	0.44
1:D:317:LEU:O	1:D:405:GLU:HG3	2.18	0.44
2:E:166:TYR:CE2	2:F:169:LEU:HD22	2.53	0.44
2:G:209:TYR:HA	2:G:212:PHE:CD2	2.53	0.44
2:G:266:GLU:OE2	2:G:269:LYS:HD2	2.17	0.44
1:B:230:CYS:SG	1:B:237:ILE:HA	2.58	0.43
1:B:290:LYS:HG2	1:B:296:GLY:O	2.18	0.43
1:B:55:THR:HG23	1:B:56:SER:N	2.33	0.43
1:D:102:LEU:HD23	1:D:128:PHE:O	2.18	0.43
1:D:136:ASP:HB3	1:D:139:ARG:HE	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ILE:HG22	1:D:240:THR:HG23	1.99	0.43
1:D:248:VAL:C	1:D:250:GLN:H	2.22	0.43
1:D:313:VAL:O	1:D:317:LEU:HB2	2.18	0.43
2:F:96:LEU:HB2	2:F:97:PRO:HD3	1.99	0.43
1:A:222:PHE:HD2	1:A:496:GLN:HB3	1.82	0.43
1:C:640:GLY:HA2	1:C:668:LEU:HD22	2.00	0.43
1:D:172:LEU:O	1:D:176:VAL:HG23	2.18	0.43
2:G:18:PHE:O	2:G:19:PHE:CB	2.66	0.43
2:H:209:TYR:HA	2:H:212:PHE:CD2	2.53	0.43
1:A:59:HIS:HA	1:A:62:ILE:HG12	1.99	0.43
1:B:152:GLU:HG2	1:B:152:GLU:O	2.17	0.43
1:B:644:ILE:HA	1:B:652:LEU:O	2.18	0.43
1:B:668:LEU:HB2	1:B:671:GLU:HG3	2.00	0.43
1:B:697:THR:OG1	1:B:732:GLN:HG3	2.18	0.43
1:C:75:PRO:O	1:C:78:GLN:HB2	2.18	0.43
1:D:520:PHE:O	1:D:523:TYR:HB3	2.17	0.43
1:D:514:GLY:HA3	1:D:618:ALA:HB3	1.90	0.43
1:D:695:ALA:C	1:D:696:ASN:HD22	2.21	0.43
2:F:171:GLY:O	2:F:184:VAL:CG1	2.65	0.43
2:F:18:PHE:O	2:F:19:PHE:CB	2.66	0.43
2:F:96:LEU:CB	2:F:97:PRO:HD3	2.47	0.43
2:H:206:ILE:O	2:H:210:VAL:HG23	2.18	0.43
2:H:46:PHE:O	2:H:48:TRP:HD1	2.01	0.43
1:A:131:MET:HA	1:A:134:PHE:CD2	2.53	0.43
1:A:439:CYS:HG	1:A:620:MET:HB2	1.83	0.43
1:A:549:TYR:CD1	1:A:602:LEU:HD22	2.54	0.43
1:B:106:VAL:HG21	1:B:128:PHE:CE1	2.53	0.43
1:B:189:ARG:O	1:B:193:VAL:HG23	2.18	0.43
1:B:244:ILE:O	1:B:248:VAL:HG22	2.17	0.43
1:B:320:LYS:HD3	1:B:409:THR:HB	2.00	0.43
1:D:18:ASN:O	3:D:800:DTP:H2	2.17	0.43
2:E:309:GLU:HB3	2:E:325:PHE:HB3	2.00	0.43
2:G:96:LEU:HB2	2:G:97:PRO:HD3	2.00	0.43
2:H:239:ALA:O	2:H:242:LEU:HG	2.18	0.43
2:H:309:GLU:HB3	2:H:325:PHE:HB3	2.00	0.43
1:A:459:ILE:HB	1:A:503:ALA:CA	2.44	0.43
1:A:681:LEU:O	1:A:685:MET:HG3	2.18	0.43
1:B:132:ASP:HA	1:B:135:ILE:HD12	1.99	0.43
1:B:131:MET:HA	1:B:134:PHE:CD2	2.54	0.43
1:B:179:CYS:HB2	1:B:215:VAL:HG12	2.00	0.43
1:B:423:HIS:HB2	1:B:582:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:THR:OG1	1:D:204:LYS:HD3	2.19	0.43
1:D:500:ILE:HG22	1:D:502:ALA:H	1.81	0.43
2:E:92:ASN:OD1	2:E:109:GLU:HG2	2.18	0.43
2:H:221:ARG:NH1	2:H:296:MET:HG2	2.30	0.43
2:H:297:ILE:O	2:H:297:ILE:HG13	2.18	0.43
2:H:76:ASN:HD21	2:H:211:SER:CA	2.29	0.43
1:A:556:ASN:O	1:A:560:LYS:HG3	2.18	0.43
1:A:730:TYR:O	1:A:731:TYR:C	2.57	0.43
1:B:394:LYS:NZ	1:B:394:LYS:HB2	2.33	0.43
1:C:151:LEU:CA	1:C:155:TYR:HB2	2.41	0.43
1:C:543:THR:HG22	1:C:547:ILE:HD11	2.01	0.43
1:D:320:LYS:HE2	1:D:334:ASP:HA	2.01	0.43
1:D:500:ILE:HD12	1:D:500:ILE:N	2.33	0.43
1:D:640:GLY:HA2	1:D:668:LEU:HD22	2.01	0.43
1:D:678:TYR:CZ	1:D:695:ALA:HB1	2.54	0.43
2:E:204:GLU:HG2	2:E:238:GLU:OE2	2.18	0.43
2:E:166:TYR:CZ	2:F:169:LEU:HD13	2.53	0.43
1:A:238:ASN:HB3	1:B:242:SER:CB	2.49	0.43
1:B:348:LEU:HB3	2:H:371:SER:HA	2.00	0.43
1:C:361:VAL:HG23	1:C:361:VAL:O	2.19	0.43
1:D:244:ILE:HG23	1:D:254:ILE:HG13	1.99	0.43
1:D:474:ASN:N	1:D:474:ASN:HD22	2.17	0.43
1:A:43:LEU:HD21	2:F:298:GLY:HA3	2.00	0.43
1:A:560:LYS:HG2	1:A:609:HIS:HB3	1.99	0.43
1:B:353:ILE:HB	1:B:393:VAL:HG23	2.01	0.43
1:B:40:GLN:NE2	2:H:334:TRP:HB3	2.33	0.43
1:B:442:ILE:HD13	1:B:691:GLN:OE1	2.19	0.43
1:C:465:SER:HB3	1:C:515:ILE:CG2	2.43	0.43
1:D:56:SER:O	1:D:59:HIS:HB2	2.18	0.43
2:E:1:ALA:HB3	2:E:168:HIS:CA	2.37	0.43
2:E:205:ALA:HB1	2:E:315:ARG:HD2	2.01	0.43
2:F:125:ILE:O	2:F:129:ILE:HG12	2.18	0.43
2:G:178:ASN:HD21	2:H:175:HIS:HD2	1.65	0.43
1:A:339:ILE:HD12	1:A:414:ILE:HG23	2.00	0.43
1:A:544:PHE:CZ	1:A:685:MET:CG	3.00	0.43
1:B:283:LYS:HG3	1:B:330:VAL:HG22	2.01	0.43
1:B:474:ASN:HD21	1:B:477:GLU:HG3	1.83	0.43
1:B:8:THR:O	1:B:55:THR:HB	2.18	0.43
1:C:524:LEU:HD22	1:C:529:LYS:HB2	2.00	0.43
1:D:135:ILE:HA	1:D:197:TYR:CE2	2.53	0.43
1:D:361:VAL:O	1:D:361:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:GLU:O	1:D:692:SER:O	2.36	0.43
2:E:149:ARG:HH21	2:E:283:GLU:CD	2.21	0.43
2:G:102:PRO:HG2	2:G:103:GLU:OE1	2.19	0.43
1:A:147:ALA:HB1	1:A:628:ILE:HA	2.00	0.43
1:A:425:PRO:HG2	1:A:690:ASP:HB3	2.01	0.43
1:B:561:GLU:HG2	1:B:561:GLU:O	2.18	0.43
2:F:115:GLU:OE1	2:F:115:GLU:HA	2.19	0.43
2:F:118:HIS:ND1	2:F:234:ILE:HG23	2.32	0.43
1:A:19:LEU:HD12	2:F:295:SER:O	2.18	0.43
1:A:474:ASN:HD21	1:A:477:GLU:HG3	1.84	0.42
1:B:83:ARG:HG2	1:B:141:MET:HG3	2.01	0.42
1:B:92:LYS:HG2	1:B:92:LYS:O	2.19	0.42
1:C:553:LYS:O	1:C:557:GLU:HG2	2.19	0.42
1:C:55:THR:OG1	3:C:800:DTP:O4'	2.31	0.42
1:D:510:ARG:HB2	1:D:512:THR:HG23	2.00	0.42
1:D:514:GLY:C	1:D:618:ALA:HB3	2.39	0.42
2:E:213:ALA:O	2:E:334:TRP:HH2	2.01	0.42
2:F:311:ILE:HD11	2:F:315:ARG:NE	2.33	0.42
2:G:46:PHE:O	2:G:48:TRP:HD1	2.01	0.42
1:A:303:THR:HA	1:A:334:ASP:O	2.19	0.42
1:A:479:GLU:O	1:A:483:ILE:HG13	2.19	0.42
1:A:644:ILE:HA	1:A:652:LEU:O	2.18	0.42
1:B:155:TYR:OH	1:B:624:THR:CG2	2.67	0.42
1:B:36:VAL:CG1	1:B:77:TYR:CD2	3.03	0.42
1:C:467:PHE:CE2	1:C:515:ILE:CG2	3.02	0.42
1:D:172:LEU:CD2	1:D:212:MET:HE2	2.49	0.42
1:D:286:GLN:OE1	1:D:332:HIS:HB2	2.19	0.42
1:D:430:ILE:HG21	1:D:570:GLU:HA	2.01	0.42
2:F:104:LEU:O	2:F:108:VAL:HG23	2.19	0.42
2:G:92:ASN:HB3	2:H:92:ASN:HB3	2.01	0.42
2:H:76:ASN:O	2:H:80:GLN:HG3	2.19	0.42
1:A:37:SER:HB3	1:A:40:GLN:CG	2.49	0.42
1:A:353:ILE:N	1:A:393:VAL:O	2.51	0.42
1:A:552:LEU:HD12	1:A:599:TRP:HZ3	1.84	0.42
1:B:490:ASP:CG	1:B:511:ARG:HH21	2.21	0.42
1:C:532:SER:OG	1:C:673:PRO:HD2	2.20	0.42
1:D:444:LEU:HA	1:D:445:PRO:HD3	1.90	0.42
1:D:620:MET:SD	1:D:620:MET:N	2.92	0.42
1:D:696:ASN:HD21	1:D:730:TYR:HB3	1.76	0.42
2:E:92:ASN:HB3	2:F:92:ASN:HB3	2.00	0.42
2:G:28:TYR:CD2	2:H:120:ARG:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:CE1	1:B:288:ALA:HB2	2.54	0.42
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.00	0.42
1:C:320:LYS:HE2	1:C:334:ASP:HA	2.00	0.42
1:C:619:LEU:HB3	1:C:693:ILE:HG23	2.01	0.42
1:D:94:TYR:CG	1:D:100:PRO:HD3	2.54	0.42
2:F:203:LEU:O	2:F:207:ARG:HB2	2.19	0.42
2:F:300:ASN:OD1	2:F:302:ASP:HB2	2.20	0.42
2:G:178:ASN:HD21	2:H:175:HIS:CD2	2.37	0.42
1:A:320:LYS:CE	1:A:411:ARG:HB2	2.49	0.42
1:A:334:ASP:OD1	1:A:411:ARG:HB3	2.20	0.42
1:A:50:TYR:H	1:A:53:ILE:CG2	2.32	0.42
1:A:618:ALA:HB2	1:A:691:GLN:CD	2.39	0.42
1:B:147:ALA:HB1	1:B:628:ILE:HA	2.01	0.42
1:B:240:THR:O	1:B:244:ILE:HG13	2.19	0.42
1:B:304:LEU:N	1:B:334:ASP:O	2.53	0.42
1:B:54:LYS:HE2	1:B:57:ASP:OD2	2.20	0.42
1:B:640:GLY:HA2	1:B:668:LEU:HD22	2.01	0.42
1:C:94:TYR:CG	1:C:100:PRO:HD3	2.55	0.42
1:C:520:PHE:HB3	1:C:635:ILE:HA	2.01	0.42
1:C:91:LYS:HG2	1:C:91:LYS:O	2.19	0.42
2:E:203:LEU:O	2:E:207:ARG:HB2	2.20	0.42
2:G:1:ALA:HB3	2:G:168:HIS:CA	2.41	0.42
2:G:213:ALA:O	2:G:334:TRP:HH2	2.03	0.42
2:G:96:LEU:CB	2:G:97:PRO:HD3	2.50	0.42
1:B:478:LEU:HD13	1:B:547:ILE:HA	2.01	0.42
1:B:565:CYS:SG	1:B:568:PHE:HB2	2.59	0.42
1:C:228:ILE:HG22	1:C:240:THR:HG23	2.01	0.42
1:C:693:ILE:CG2	1:C:694:SER:H	2.31	0.42
1:D:140:ASP:OD1	1:D:169:ALA:HB3	2.20	0.42
1:D:172:LEU:HD21	1:D:212:MET:HE2	2.01	0.42
1:D:553:LYS:HA	1:D:602:LEU:HD11	2.01	0.42
2:E:96:LEU:HB2	2:E:97:PRO:HD3	2.00	0.42
2:F:276:PHE:HB3	2:F:316:MET:SD	2.59	0.42
2:G:11:ASP:OD1	2:G:13:LEU:HB2	2.19	0.42
2:G:31:GLN:HG2	2:G:37:GLU:HB2	2.02	0.42
1:A:179:CYS:HB2	1:A:215:VAL:HG12	2.00	0.42
1:A:641:TYR:O	1:A:655:VAL:HA	2.20	0.42
1:B:139:ARG:NH1	1:B:202:THR:HG23	2.34	0.42
1:B:210:PRO:HG3	1:B:224:SER:HG	1.83	0.42
1:C:154:LYS:HD2	1:C:209:THR:CG2	2.49	0.42
1:C:172:LEU:CD2	1:C:212:MET:HE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LEU:HA	1:C:445:PRO:HD3	1.90	0.42
1:C:617:SER:OG	1:C:690:ASP:OD2	2.38	0.42
1:C:7:VAL:CG2	1:C:17:ILE:HG13	2.49	0.42
2:E:102:PRO:HG2	2:E:103:GLU:OE1	2.19	0.42
2:E:203:LEU:HA	2:E:207:ARG:HD2	2.02	0.42
2:E:42:LYS:HE3	2:E:46:PHE:CZ	2.55	0.42
2:E:5:PHE:CE1	2:E:24:ASN:CG	2.93	0.42
2:E:76:ASN:HD21	2:E:211:SER:CA	2.31	0.42
2:E:96:LEU:HA	2:E:99:ILE:HD12	2.01	0.42
2:F:209:TYR:HA	2:F:212:PHE:CD2	2.54	0.42
1:A:240:THR:O	1:A:244:ILE:HG13	2.20	0.42
1:A:7:VAL:HG11	3:A:800:DTP:C5	2.49	0.42
1:C:140:ASP:OD1	1:C:169:ALA:HB3	2.20	0.42
1:C:467:PHE:O	1:C:518:ILE:N	2.37	0.42
1:C:520:PHE:O	1:C:521:ALA:C	2.58	0.42
1:D:304:LEU:HD23	1:D:305:PHE:N	2.35	0.42
1:D:310:HIS:O	1:D:355:LEU:HB3	2.18	0.42
1:D:467:PHE:CE1	1:D:481:LEU:HB3	2.54	0.42
1:D:518:ILE:HD12	1:D:631:ALA:HB3	2.02	0.42
1:D:543:THR:HG22	1:D:547:ILE:HD11	2.02	0.42
2:E:11:ASP:OD1	2:E:13:LEU:HB2	2.19	0.42
2:E:335:ILE:O	2:E:339:LEU:HG	2.18	0.42
2:F:213:ALA:O	2:F:334:TRP:HH2	2.03	0.42
2:F:244:GLY:O	2:F:248:MET:HG3	2.20	0.42
2:H:191:LYS:HG3	2:H:264:ILE:HG23	2.02	0.42
1:A:519:ASN:CB	1:A:631:ALA:HB1	2.50	0.42
1:B:228:ILE:CG2	1:B:240:THR:HG23	2.49	0.42
1:B:258:ALA:C	1:B:260:ARG:H	2.23	0.42
1:B:317:LEU:HA	1:B:317:LEU:HD12	1.89	0.42
1:B:303:THR:CG2	1:B:334:ASP:O	2.67	0.42
1:B:406:ARG:O	1:B:410:GLY:HA2	2.20	0.42
1:C:228:ILE:HG21	1:C:240:THR:HG23	2.00	0.42
1:C:436:SER:OG	1:C:440:LEU:HD13	2.20	0.42
1:C:33:LEU:CD1	1:C:80:LEU:HB2	2.46	0.42
1:D:367:ALA:C	1:D:369:PHE:N	2.73	0.42
1:D:91:LYS:O	1:D:91:LYS:HG2	2.20	0.42
2:E:125:ILE:O	2:E:129:ILE:HG12	2.20	0.42
2:E:165:SER:HB3	2:F:165:SER:HB3	2.02	0.42
2:E:187:ARG:NH1	2:E:260:GLU:HG3	2.35	0.42
2:F:149:ARG:HD2	2:F:286:TRP:HB2	2.02	0.42
1:C:723:LYS:HG3	2:G:375:LEU:OXT	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:HB3	1:A:197:TYR:HD1	1.84	0.42
1:A:75:PRO:O	1:A:78:GLN:HB2	2.19	0.42
1:B:136:ASP:OD2	1:B:139:ARG:HG3	2.18	0.42
1:B:560:LYS:HG2	1:B:609:HIS:HB3	2.01	0.42
1:C:248:VAL:C	1:C:250:GLN:H	2.23	0.42
1:C:482:ALA:O	1:C:486:VAL:CG2	2.68	0.42
1:C:482:ALA:O	1:C:486:VAL:HG23	2.20	0.42
1:D:410:GLY:O	1:D:411:ARG:HD2	2.20	0.42
1:D:498:TYR:CB	1:D:504:LYS:HB2	2.50	0.42
2:H:96:LEU:HB2	2:H:97:PRO:HD3	2.01	0.42
1:A:645:LYS:HG2	1:A:646:ALA:N	2.35	0.41
1:B:519:ASN:CB	1:B:631:ALA:HB1	2.50	0.41
1:C:169:ALA:O	1:C:172:LEU:HB3	2.20	0.41
1:C:410:GLY:O	1:C:411:ARG:HD2	2.20	0.41
1:D:560:LYS:HD3	1:D:609:HIS:CG	2.55	0.41
1:D:643:SER:O	1:D:653:ARG:HA	2.20	0.41
2:E:35:ILE:HG23	2:E:36:PHE:H	1.84	0.41
2:E:96:LEU:CB	2:E:97:PRO:HD3	2.50	0.41
2:H:96:LEU:CB	2:H:97:PRO:HD3	2.50	0.41
1:A:478:LEU:HD13	1:A:547:ILE:HA	2.02	0.41
1:B:334:ASP:OD1	1:B:411:ARG:HB3	2.20	0.41
1:B:339:ILE:HD12	1:B:414:ILE:HG23	2.02	0.41
1:B:639:ARG:O	1:B:668:LEU:HB3	2.19	0.41
1:C:50:TYR:O	1:C:51:ASP:C	2.56	0.41
1:D:260:ARG:HH12	1:D:448:PRO:HG3	1.85	0.41
1:A:463:THR:O	1:A:489:LEU:HD22	2.20	0.41
1:B:146:ALA:HB2	1:B:654:GLN:HB2	2.02	0.41
1:B:241:SER:O	1:B:245:VAL:HG23	2.19	0.41
1:B:686:GLN:NE2	1:B:727:LYS:HE3	2.35	0.41
1:C:152:GLU:HG2	1:C:152:GLU:O	2.20	0.41
1:C:430:ILE:HG21	1:C:570:GLU:CG	2.50	0.41
1:C:619:LEU:HD13	1:C:693:ILE:CD1	2.50	0.41
1:D:275:HIS:ND1	3:D:900:DTP:H1'	2.35	0.41
2:E:209:TYR:HA	2:E:212:PHE:CD2	2.55	0.41
2:E:300:ASN:OD1	2:E:302:ASP:HB2	2.21	0.41
2:F:76:ASN:O	2:F:80:GLN:HG3	2.20	0.41
2:G:171:GLY:O	2:G:184:VAL:CG1	2.66	0.41
2:G:76:ASN:O	2:G:80:GLN:HG3	2.20	0.41
2:H:18:PHE:O	2:H:19:PHE:CB	2.66	0.41
2:H:31:GLN:HG2	2:H:37:GLU:HB2	2.02	0.41
1:A:139:ARG:NH1	1:A:202:THR:HG23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG13	1:A:314:GLU:N	2.36	0.41
1:B:160:ARG:HA	1:B:160:ARG:HD3	1.91	0.41
1:B:619:LEU:HD12	1:B:693:ILE:CD1	2.51	0.41
1:C:202:THR:OG1	1:C:204:LYS:HD3	2.19	0.41
1:D:521:ALA:HB3	1:D:632:THR:HG21	2.02	0.41
2:G:115:GLU:HA	2:G:115:GLU:OE1	2.21	0.41
2:G:125:ILE:O	2:G:129:ILE:HG12	2.20	0.41
1:A:413:TYR:HB3	1:A:729:LEU:O	2.21	0.41
1:A:583:TYR:CB	1:A:687:LYS:HG3	2.51	0.41
1:B:353:ILE:N	1:B:393:VAL:O	2.52	0.41
1:B:442:ILE:CG2	1:B:444:LEU:HG	2.50	0.41
1:B:549:TYR:CD1	1:B:602:LEU:HD22	2.55	0.41
1:C:246:LYS:HZ3	1:D:234:LEU:HB3	1.85	0.41
1:C:515:ILE:HD12	1:C:551:LEU:CD2	2.50	0.41
1:C:425:PRO:CG	1:C:615:THR:HG22	2.50	0.41
1:D:169:ALA:O	1:D:172:LEU:HB3	2.21	0.41
1:D:224:SER:O	1:D:252:ALA:HA	2.20	0.41
1:D:437:ASN:OD1	1:D:441:GLU:OE1	2.39	0.41
2:E:276:PHE:HB3	2:E:316:MET:SD	2.60	0.41
2:G:203:LEU:O	2:G:207:ARG:HB2	2.19	0.41
1:A:258:ALA:C	1:A:260:ARG:H	2.22	0.41
1:B:641:TYR:O	1:B:655:VAL:HA	2.21	0.41
1:B:644:ILE:HD12	1:B:644:ILE:N	2.36	0.41
1:C:227:LEU:HB3	1:C:435:GLN:HE21	1.72	0.41
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.21	0.41
1:C:304:LEU:HD23	1:C:305:PHE:N	2.36	0.41
1:C:313:VAL:O	1:C:317:LEU:HB2	2.19	0.41
1:D:367:ALA:HB1	1:D:375:PHE:HB2	2.02	0.41
1:D:463:THR:CG2	1:D:489:LEU:HD22	2.46	0.41
1:D:556:ASN:ND2	1:D:609:HIS:HB2	2.27	0.41
2:E:332:ILE:HG22	2:E:334:TRP:HE1	1.85	0.41
2:E:48:TRP:CZ3	2:E:50:PRO:HG3	2.55	0.41
2:G:297:ILE:O	2:G:297:ILE:HG13	2.21	0.41
2:G:9:LYS:CA	2:H:141:VAL:HG11	2.45	0.41
1:A:284:HIS:HA	1:B:287:THR:CB	2.50	0.41
1:A:565:CYS:HA	1:A:566:PRO:HD3	1.96	0.41
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.49	0.41
1:A:92:LYS:O	1:A:92:LYS:HG2	2.20	0.41
1:C:224:SER:O	1:C:252:ALA:HA	2.21	0.41
1:C:431:ALA:HA	1:C:432:PRO:HD2	1.85	0.41
1:D:426:PHE:HE1	1:D:510:ARG:HE	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:244:GLY:O	2:E:248:MET:HG3	2.21	0.41
1:A:45:SER:O	1:A:46:HIS:C	2.59	0.41
1:A:686:GLN:CD	1:A:727:LYS:HG3	2.41	0.41
1:A:77:TYR:CD1	1:A:80:LEU:HD23	2.55	0.41
1:B:645:LYS:HG2	1:B:646:ALA:N	2.36	0.41
1:B:68:ASP:HA	1:B:653:ARG:HH12	1.85	0.41
1:C:498:TYR:CB	1:C:504:LYS:HB2	2.51	0.41
1:C:465:SER:CB	1:C:514:GLY:O	2.61	0.41
1:C:645:LYS:HG2	1:C:646:ALA:N	2.36	0.41
1:D:437:ASN:OD1	1:D:442:ILE:HG12	2.21	0.41
2:F:205:ALA:HB1	2:F:315:ARG:HD2	2.03	0.41
2:F:34:ASP:N	2:F:34:ASP:OD1	2.54	0.41
2:F:31:GLN:HG2	2:F:37:GLU:HB2	2.02	0.41
2:H:36:PHE:HZ	2:H:248:MET:HG2	1.85	0.41
2:H:278:GLN:O	2:H:282:GLN:HG3	2.21	0.41
1:A:541:HIS:O	1:A:545:GLU:HB2	2.21	0.41
1:A:619:LEU:HD12	1:A:693:ILE:CD1	2.50	0.41
1:C:34:HIS:O	1:C:36:VAL:HG13	2.21	0.41
1:C:639:ARG:NH2	1:C:733:ASN:HB3	2.33	0.41
2:H:11:ASP:OD1	2:H:13:LEU:HB2	2.20	0.41
2:H:69:GLU:HG2	2:H:296:MET:HG3	2.03	0.41
1:A:406:ARG:O	1:A:410:GLY:HA2	2.21	0.41
1:A:437:ASN:ND2	1:A:439:CYS:H	2.18	0.41
1:A:425:PRO:HB3	1:A:573:TYR:CE2	2.55	0.41
1:B:357:SER:O	1:B:358:PRO:C	2.58	0.41
1:B:441:GLU:O	1:B:692:SER:N	2.54	0.41
1:B:619:LEU:HD12	1:B:693:ILE:CG1	2.51	0.41
1:C:102:LEU:HD23	1:C:128:PHE:O	2.21	0.41
1:C:437:ASN:OD1	1:C:441:GLU:OE1	2.39	0.41
1:C:260:ARG:HH11	1:C:448:PRO:HG3	1.86	0.41
2:H:125:ILE:O	2:H:129:ILE:HG12	2.20	0.41
2:H:332:ILE:HG22	2:H:334:TRP:HE1	1.84	0.41
1:A:39:SER:O	1:A:40:GLN:C	2.58	0.41
1:B:232:ASP:OD2	1:B:262:ARG:NH2	2.53	0.41
1:B:53:ILE:O	1:B:54:LYS:O	2.39	0.41
1:B:583:TYR:CB	1:B:687:LYS:HG3	2.51	0.41
1:C:474:ASN:HD22	1:C:474:ASN:N	2.19	0.41
1:C:524:LEU:HD12	1:C:531:TYR:CE1	2.55	0.41
1:D:18:ASN:N	3:D:800:DTP:C2	2.82	0.41
1:D:524:LEU:HD12	1:D:531:TYR:CE1	2.56	0.41
1:D:553:LYS:O	1:D:557:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:TYR:CG	1:D:687:LYS:HG3	2.56	0.41
2:E:178:ASN:HD21	2:F:175:HIS:HD2	1.67	0.41
2:E:153:ILE:HD13	2:E:203:LEU:CD1	2.51	0.41
2:E:76:ASN:O	2:E:80:GLN:HG3	2.21	0.41
2:F:278:GLN:O	2:F:282:GLN:HG3	2.21	0.41
1:A:136:ASP:OD2	1:A:139:ARG:HG3	2.20	0.40
1:A:443:ALA:O	1:A:444:LEU:HD23	2.21	0.40
1:A:44:ARG:O	1:A:46:HIS:CD2	2.74	0.40
1:B:633:ASN:O	1:B:634:GLY:C	2.60	0.40
1:C:172:LEU:HD21	1:C:212:MET:HE2	2.02	0.40
1:C:354:THR:HG21	1:C:390:LYS:HD3	2.03	0.40
1:C:640:GLY:CA	1:C:668:LEU:HD22	2.51	0.40
1:D:442:ILE:HD11	1:D:464:LEU:HD21	2.01	0.40
1:D:678:TYR:O	1:D:682:VAL:HG23	2.21	0.40
2:G:364:GLU:HG3	2:G:365:VAL:N	2.36	0.40
1:A:238:ASN:HD21	1:B:246:LYS:HG2	1.86	0.40
1:A:244:ILE:O	1:A:248:VAL:HG22	2.21	0.40
1:B:174:ILE:HG23	1:B:175:LEU:N	2.36	0.40
1:B:21:LYS:HD2	3:B:800:DTP:C6	2.52	0.40
1:B:227:LEU:HD11	1:B:437:ASN:HB3	2.03	0.40
1:C:101:ALA:HB3	1:C:104:ASP:OD2	2.20	0.40
1:C:583:TYR:CG	1:C:687:LYS:HG3	2.57	0.40
1:D:55:THR:OG1	3:D:800:DTP:C5'	2.68	0.40
1:D:441:GLU:CG	1:D:619:LEU:O	2.70	0.40
2:G:36:PHE:O	2:G:39:LEU:HB2	2.22	0.40
2:G:76:ASN:HD21	2:G:211:SER:CA	2.29	0.40
2:H:244:GLY:O	2:H:248:MET:HG3	2.21	0.40
2:H:232:ARG:HD2	2:H:338:TRP:HE3	1.87	0.40
2:H:42:LYS:HE3	2:H:46:PHE:CZ	2.56	0.40
1:B:313:VAL:HG13	1:B:314:GLU:N	2.37	0.40
1:C:643:SER:O	1:C:653:ARG:HA	2.21	0.40
1:C:678:TYR:O	1:C:682:VAL:HG23	2.21	0.40
1:D:367:ALA:O	1:D:369:PHE:N	2.54	0.40
1:D:354:THR:HG21	1:D:390:LYS:HD3	2.03	0.40
2:E:158:ASP:OD1	2:F:4:THR:HG23	2.21	0.40
2:E:317:GLN:O	2:E:317:GLN:HG2	2.21	0.40
2:H:171:GLY:O	2:H:184:VAL:CG1	2.65	0.40
1:A:122:ASP:O	1:A:189:ARG:NH2	2.54	0.40
1:A:7:VAL:O	1:A:14:THR:HA	2.21	0.40
1:A:228:ILE:N	1:A:435:GLN:HE22	2.19	0.40
1:A:45:SER:HG	1:A:61:THR:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:N	1:B:155:TYR:CD1	2.90	0.40
1:C:696:ASN:ND2	1:C:730:TYR:HB3	2.36	0.40
1:D:430:ILE:HG21	1:D:570:GLU:CA	2.51	0.40
1:D:519:ASN:OD1	1:D:632:THR:HG23	2.21	0.40
1:D:532:SER:OG	1:D:673:PRO:HD2	2.20	0.40
2:G:104:LEU:O	2:G:108:VAL:HG23	2.21	0.40
2:G:93:VAL:HG13	2:H:97:PRO:HG3	2.04	0.40
2:H:300:ASN:OD1	2:H:302:ASP:HB2	2.21	0.40
1:A:283:LYS:HG3	1:A:330:VAL:HG22	2.04	0.40
1:A:735:ARG:HG2	1:A:736:ASP:N	2.36	0.40
1:B:696:ASN:OD1	1:B:731:TYR:HB2	2.21	0.40
1:B:75:PRO:O	1:B:78:GLN:HB2	2.22	0.40
2:E:6:SER:H	2:E:24:ASN:HB3	1.85	0.40
2:H:115:GLU:OE1	2:H:115:GLU:HA	2.21	0.40
2:H:68:HIS:O	2:H:72:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	730/761 (96%)	688 (94%)	37 (5%)	5 (1%)	22	62
1	B	730/761 (96%)	684 (94%)	41 (6%)	5 (1%)	22	62
1	C	730/761 (96%)	686 (94%)	41 (6%)	3 (0%)	34	72
1	D	730/761 (96%)	685 (94%)	42 (6%)	3 (0%)	34	72
2	E	344/375 (92%)	326 (95%)	18 (5%)	0	100	100
2	F	344/375 (92%)	325 (94%)	19 (6%)	0	100	100
2	G	348/375 (93%)	330 (95%)	18 (5%)	0	100	100
2	H	346/375 (92%)	329 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4302/4544 (95%)	4053 (94%)	233 (5%)	16 (0%)	34 72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	731	TYR
1	B	54	LYS
1	D	731	TYR
1	A	52	GLY
1	C	430	ILE
1	C	736	ASP
1	A	214	GLY
1	A	634	GLY
1	B	214	GLY
1	B	634	GLY
1	B	731	TYR
1	A	300	GLY
1	B	300	GLY
1	D	300	GLY
1	C	271	GLY
1	D	271	GLY

### 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	627/651 (96%)	595 (95%)	32 (5%)	24 50
1	B	627/651 (96%)	600 (96%)	27 (4%)	29 54
1	C	627/651 (96%)	602 (96%)	25 (4%)	31 56
1	D	627/651 (96%)	596 (95%)	31 (5%)	25 51
2	E	315/340 (93%)	309 (98%)	6 (2%)	57 75
2	F	315/340 (93%)	306 (97%)	9 (3%)	42 64
2	G	319/340 (94%)	312 (98%)	7 (2%)	52 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	317/340 (93%)	308 (97%)	9 (3%)	43 65
All	All	3774/3964 (95%)	3628 (96%)	146 (4%)	32 57

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	43	LEU
1	A	44	ARG
1	A	47	ILE
1	A	51	ASP
1	A	53	ILE
1	A	64	LYS
1	A	78	GLN
1	A	118	HIS
1	A	122	ASP
1	A	141	MET
1	A	149	LYS
1	A	152	GLU
1	A	154	LYS
1	A	187	GLU
1	A	189	ARG
1	A	224	SER
1	A	225	CYS
1	A	251	ARG
1	A	326	GLU
1	A	364	LEU
1	A	439	CYS
1	A	440	LEU
1	A	441	GLU
1	A	462	CYS
1	A	465	SER
1	A	474	ASN
1	A	510	ARG
1	A	585	LYS
1	A	620	MET
1	A	624	THR
1	A	730	TYR
1	B	8	THR
1	B	36	VAL
1	B	47	ILE
1	B	51	ASP

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Mol	Chain	Res	Type
1	B	54	LYS
1	B	64	LYS
1	B	78	GLN
1	B	118	HIS
1	B	122	ASP
1	B	141	MET
1	B	149	LYS
1	B	154	LYS
1	B	189	ARG
1	B	224	SER
1	B	225	CYS
1	B	251	ARG
1	B	326	GLU
1	B	333	MET
1	B	364	LEU
1	B	421	ASN
1	B	465	SER
1	B	474	ASN
1	B	510	ARG
1	B	585	LYS
1	B	616	LEU
1	B	620	MET
1	B	624	THR
1	C	8	THR
1	C	47	ILE
1	C	64	LYS
1	C	118	HIS
1	C	141	MET
1	C	149	LYS
1	C	154	LYS
1	C	188	THR
1	C	189	ARG
1	C	216	ARG
1	C	225	CYS
1	C	247	TYR
1	C	364	LEU
1	C	372	GLN
1	C	384	LYS
1	C	394	LYS
1	C	437	ASN
1	C	463	THR
1	C	465	SER

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Mol	Chain	Res	Type
1	C	474	ASN
1	C	556	ASN
1	C	585	LYS
1	C	619	LEU
1	C	625	SER
1	C	643	SER
1	D	8	THR
1	D	15	GLU
1	D	16	ARG
1	D	39	SER
1	D	47	ILE
1	D	53	ILE
1	D	64	LYS
1	D	118	HIS
1	D	141	MET
1	D	149	LYS
1	D	154	LYS
1	D	187	GLU
1	D	189	ARG
1	D	225	CYS
1	D	247	TYR
1	D	290	LYS
1	D	292	CYS
1	D	294	GLN
1	D	364	LEU
1	D	384	LYS
1	D	394	LYS
1	D	437	ASN
1	D	438	LEU
1	D	474	ASN
1	D	556	ASN
1	D	585	LYS
1	D	617	SER
1	D	620	MET
1	D	625	SER
1	D	643	SER
1	D	696	ASN
2	E	100	SER
2	E	156	TYR
2	E	208	PHE
2	E	253	ARG
2	E	297	ILE

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Mol	Chain	Res	Type
2	E	328	ARG
2	F	34	ASP
2	F	58	ASP
2	F	100	SER
2	F	156	TYR
2	F	208	PHE
2	F	232	ARG
2	F	253	ARG
2	F	297	ILE
2	F	328	ARG
2	G	34	ASP
2	G	100	SER
2	G	156	TYR
2	G	208	PHE
2	G	253	ARG
2	G	297	ILE
2	G	328	ARG
2	H	34	ASP
2	H	58	ASP
2	H	100	SER
2	H	156	TYR
2	H	208	PHE
2	H	232	ARG
2	H	253	ARG
2	H	297	ILE
2	H	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	46	HIS
1	A	78	GLN
1	A	130	GLN
1	A	221	GLN
1	A	257	ASN
1	A	321	ASN
1	A	328	ASN
1	A	435	GLN
1	A	474	ASN
1	A	654	GLN
1	A	696	ASN

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Mol	Chain	Res	Type
1	A	712	GLN
1	B	35	ASN
1	B	40	GLN
1	B	78	GLN
1	B	130	GLN
1	B	221	GLN
1	B	257	ASN
1	B	321	ASN
1	B	328	ASN
1	B	421	ASN
1	B	435	GLN
1	B	474	ASN
1	B	654	GLN
1	B	686	GLN
1	B	696	ASN
1	C	18	ASN
1	C	130	GLN
1	C	238	ASN
1	C	321	ASN
1	C	435	GLN
1	C	474	ASN
1	C	613	ASN
1	C	654	GLN
1	C	696	ASN
1	C	712	GLN
1	D	18	ASN
1	D	130	GLN
1	D	238	ASN
1	D	321	ASN
1	D	435	GLN
1	D	474	ASN
1	D	654	GLN
1	D	691	GLN
1	D	696	ASN
1	D	712	GLN
2	E	10	ASN
2	E	12	GLN
2	E	30	GLN
2	E	76	ASN
2	E	87	GLN
2	E	147	GLN
2	E	175	HIS

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Mol	Chain	Res	Type
2	E	201	ASN
2	E	247	HIS
2	E	282	GLN
2	F	21	GLN
2	F	30	GLN
2	F	76	ASN
2	F	87	GLN
2	F	147	GLN
2	F	175	HIS
2	F	201	ASN
2	F	282	GLN
2	G	30	GLN
2	G	76	ASN
2	G	87	GLN
2	G	147	GLN
2	G	175	HIS
2	G	178	ASN
2	G	201	ASN
2	G	247	HIS
2	G	282	GLN
2	H	30	GLN
2	H	76	ASN
2	H	87	GLN
2	H	147	GLN
2	H	201	ASN
2	H	247	HIS
2	H	282	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
3	DTP	C	900	-	26,32,32	1.58	5 (19%)	30,50,50	1.33	4 (13%)
3	DTP	D	900	-	26,32,32	1.63	6 (23%)	30,50,50	1.35	5 (16%)
3	DTP	C	800	-	26,32,32	1.57	5 (19%)	30,50,50	1.37	4 (13%)
3	DTP	A	800	-	26,32,32	1.59	5 (19%)	30,50,50	1.28	4 (13%)
3	DTP	B	900	-	26,32,32	1.60	6 (23%)	30,50,50	1.39	4 (13%)
3	DTP	A	900	-	26,32,32	1.58	5 (19%)	30,50,50	1.36	4 (13%)
3	DTP	B	800	-	26,32,32	1.59	5 (19%)	30,50,50	1.20	5 (16%)
3	DTP	D	800	-	26,32,32	1.62	6 (23%)	30,50,50	1.36	4 (13%)

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
3	DTP	C	900	-	-	8/18/34/34	0/3/3/3
3	DTP	D	900	-	-	2/18/34/34	0/3/3/3
3	DTP	C	800	-	-	7/18/34/34	0/3/3/3
3	DTP	A	800	-	-	8/18/34/34	0/3/3/3
3	DTP	B	900	-	-	5/18/34/34	0/3/3/3
3	DTP	A	900	-	-	3/18/34/34	0/3/3/3
3	DTP	B	800	-	-	2/18/34/34	0/3/3/3
3	DTP	D	800	-	-	6/18/34/34	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	800	DTP	O3'-C3'	-3.98	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	DTP	O3'-C3'	-3.94	1.35	1.43
3	B	800	DTP	O3'-C3'	-3.91	1.35	1.43
3	B	900	DTP	O3'-C3'	-3.91	1.35	1.43
3	C	800	DTP	O3'-C3'	-3.91	1.35	1.43
3	A	800	DTP	O3'-C3'	-3.90	1.35	1.43
3	A	900	DTP	O3'-C3'	-3.89	1.35	1.43
3	C	900	DTP	O3'-C3'	-3.86	1.35	1.43
3	A	800	DTP	C6-N6	3.59	1.47	1.34
3	B	900	DTP	C6-N6	3.58	1.47	1.34
3	C	900	DTP	C6-N6	3.57	1.47	1.34
3	D	800	DTP	C6-N6	3.57	1.47	1.34
3	C	800	DTP	C6-N6	3.56	1.47	1.34
3	D	900	DTP	C6-N6	3.55	1.47	1.34
3	B	800	DTP	C6-N6	3.54	1.47	1.34
3	A	900	DTP	C6-N6	3.50	1.46	1.34
3	B	800	DTP	C5'-C4'	-3.05	1.42	1.51
3	A	800	DTP	C5'-C4'	-2.98	1.42	1.51
3	D	800	DTP	C5'-C4'	-2.98	1.42	1.51
3	D	900	DTP	C5'-C4'	-2.96	1.42	1.51
3	A	900	DTP	C5'-C4'	-2.92	1.42	1.51
3	C	800	DTP	C5'-C4'	-2.85	1.42	1.51
3	A	800	DTP	O5'-C5'	-2.85	1.33	1.44
3	C	900	DTP	C5'-C4'	-2.83	1.42	1.51
3	D	900	DTP	O5'-C5'	-2.82	1.33	1.44
3	B	800	DTP	O5'-C5'	-2.81	1.34	1.44
3	D	800	DTP	O5'-C5'	-2.79	1.34	1.44
3	B	900	DTP	C5'-C4'	-2.78	1.42	1.51
3	B	900	DTP	O5'-C5'	-2.76	1.34	1.44
3	A	900	DTP	O5'-C5'	-2.75	1.34	1.44
3	C	900	DTP	O5'-C5'	-2.74	1.34	1.44
3	C	800	DTP	O5'-C5'	-2.67	1.34	1.44
3	D	900	DTP	C2'-C3'	-2.62	1.45	1.52
3	C	900	DTP	C2'-C3'	-2.60	1.46	1.52
3	D	800	DTP	C2'-C3'	-2.60	1.46	1.52
3	B	800	DTP	C2'-C3'	-2.55	1.46	1.52
3	A	900	DTP	C2'-C3'	-2.55	1.46	1.52
3	B	900	DTP	C2'-C3'	-2.52	1.46	1.52
3	C	800	DTP	C2'-C3'	-2.51	1.46	1.52
3	A	800	DTP	C2'-C3'	-2.45	1.46	1.52
3	D	900	DTP	C3'-C4'	-2.35	1.46	1.53
3	B	900	DTP	C3'-C4'	-2.17	1.47	1.53
3	D	800	DTP	C3'-C4'	-2.03	1.47	1.53



All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	900	DTP	PB-O3B-PG	-3.77	119.88	132.83
3	C	800	DTP	PB-O3B-PG	-3.63	120.38	132.83
3	D	900	DTP	PA-O3A-PB	-3.52	120.73	132.83
3	D	800	DTP	PA-O3A-PB	-3.48	120.89	132.83
3	A	900	DTP	PA-O3A-PB	-3.43	121.06	132.83
3	A	900	DTP	N3-C2-N1	-3.41	123.34	128.68
3	C	800	DTP	N3-C2-N1	-3.38	123.39	128.68
3	C	900	DTP	PA-O3A-PB	-3.37	121.25	132.83
3	C	900	DTP	PB-O3B-PG	-3.37	121.25	132.83
3	B	900	DTP	N3-C2-N1	-3.34	123.46	128.68
3	B	800	DTP	N3-C2-N1	-3.34	123.47	128.68
3	D	800	DTP	N3-C2-N1	-3.32	123.49	128.68
3	C	900	DTP	N3-C2-N1	-3.28	123.55	128.68
3	A	900	DTP	PB-O3B-PG	-3.25	121.69	132.83
3	A	800	DTP	N3-C2-N1	-3.23	123.63	128.68
3	A	800	DTP	PA-O3A-PB	-3.15	122.01	132.83
3	D	900	DTP	PB-O3B-PG	-3.02	122.47	132.83
3	D	800	DTP	PB-O3B-PG	-3.02	122.48	132.83
3	C	800	DTP	PA-O3A-PB	-3.00	122.54	132.83
3	D	900	DTP	N3-C2-N1	-2.98	124.01	128.68
3	B	900	DTP	O5'-C5'-C4'	2.71	118.33	108.99
3	A	800	DTP	O5'-C5'-C4'	2.59	117.90	108.99
3	C	800	DTP	O5'-C5'-C4'	2.56	117.81	108.99
3	A	800	DTP	PB-O3B-PG	-2.56	124.06	132.83
3	B	900	DTP	PA-O3A-PB	-2.55	124.08	132.83
3	C	900	DTP	O5'-C5'-C4'	2.50	117.59	108.99
3	D	800	DTP	O5'-C5'-C4'	2.44	117.40	108.99
3	A	900	DTP	O5'-C5'-C4'	2.43	117.37	108.99
3	B	800	DTP	PB-O3B-PG	-2.43	124.50	132.83
3	D	900	DTP	O5'-C5'-C4'	2.37	117.14	108.99
3	B	800	DTP	C4-C5-N7	-2.30	107.00	109.40
3	B	800	DTP	PA-O3A-PB	-2.13	125.51	132.83
3	D	900	DTP	C4-C5-N7	-2.10	107.21	109.40
3	B	800	DTP	O5'-C5'-C4'	2.01	115.90	108.99

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	900	DTP	C5'-O5'-PA-O3A
3	D	900	DTP	C3'-C4'-C5'-O5'

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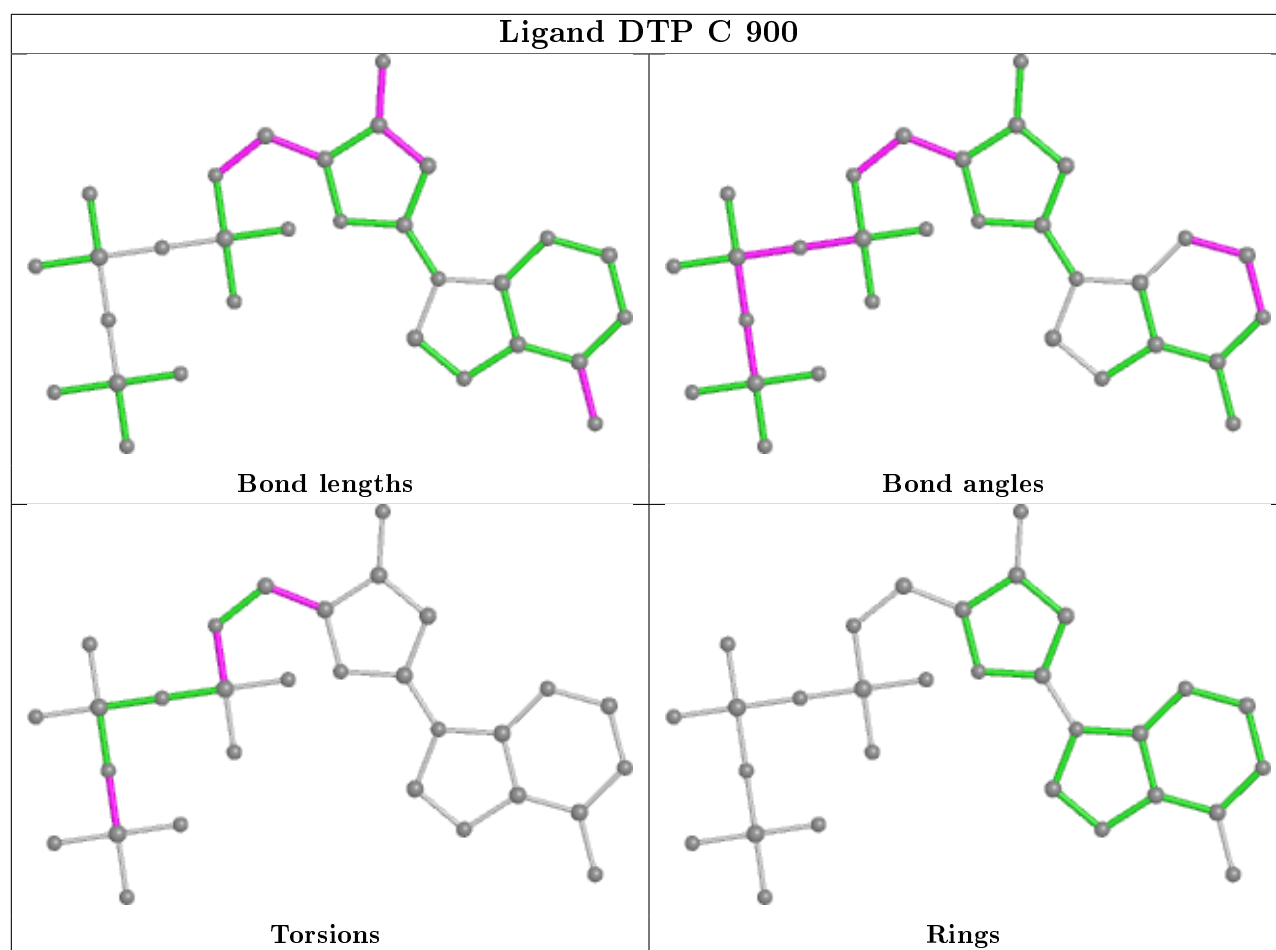
Mol	Chain	Res	Type	Atoms
3	C	800	DTP	C5'-O5'-PA-O3A
3	A	800	DTP	PB-O3B-PG-O2G
3	A	800	DTP	C5'-O5'-PA-O1A
3	A	800	DTP	C3'-C4'-C5'-O5'
3	B	900	DTP	C5'-O5'-PA-O1A
3	B	900	DTP	C5'-O5'-PA-O2A
3	B	900	DTP	C5'-O5'-PA-O3A
3	B	900	DTP	O4'-C4'-C5'-O5'
3	A	900	DTP	O4'-C4'-C5'-O5'
3	A	900	DTP	C3'-C4'-C5'-O5'
3	B	800	DTP	C5'-O5'-PA-O1A
3	D	800	DTP	C5'-O5'-PA-O3A
3	D	900	DTP	O4'-C4'-C5'-O5'
3	A	800	DTP	O4'-C4'-C5'-O5'
3	D	800	DTP	O4'-C4'-C5'-O5'
3	C	800	DTP	O4'-C4'-C5'-O5'
3	C	900	DTP	O4'-C4'-C5'-O5'
3	C	900	DTP	C3'-C4'-C5'-O5'
3	C	800	DTP	PB-O3B-PG-O1G
3	A	900	DTP	PG-O3B-PB-O1B
3	C	900	DTP	PB-O3B-PG-O1G
3	C	900	DTP	C5'-O5'-PA-O1A
3	C	900	DTP	C5'-O5'-PA-O2A
3	C	800	DTP	C5'-O5'-PA-O1A
3	C	800	DTP	C5'-O5'-PA-O2A
3	A	800	DTP	C5'-O5'-PA-O2A
3	D	800	DTP	C5'-O5'-PA-O1A
3	B	900	DTP	C3'-C4'-C5'-O5'
3	D	800	DTP	PG-O3B-PB-O1B
3	B	800	DTP	O4'-C4'-C5'-O5'
3	C	800	DTP	C3'-C4'-C5'-O5'
3	C	900	DTP	PB-O3B-PG-O2G
3	C	900	DTP	PB-O3B-PG-O3G
3	A	800	DTP	C5'-O5'-PA-O3A
3	C	800	DTP	PA-O3A-PB-O2B
3	A	800	DTP	PG-O3B-PB-O2B
3	D	800	DTP	PG-O3B-PB-O2B
3	D	800	DTP	C5'-O5'-PA-O2A
3	A	800	DTP	PG-O3B-PB-O3A

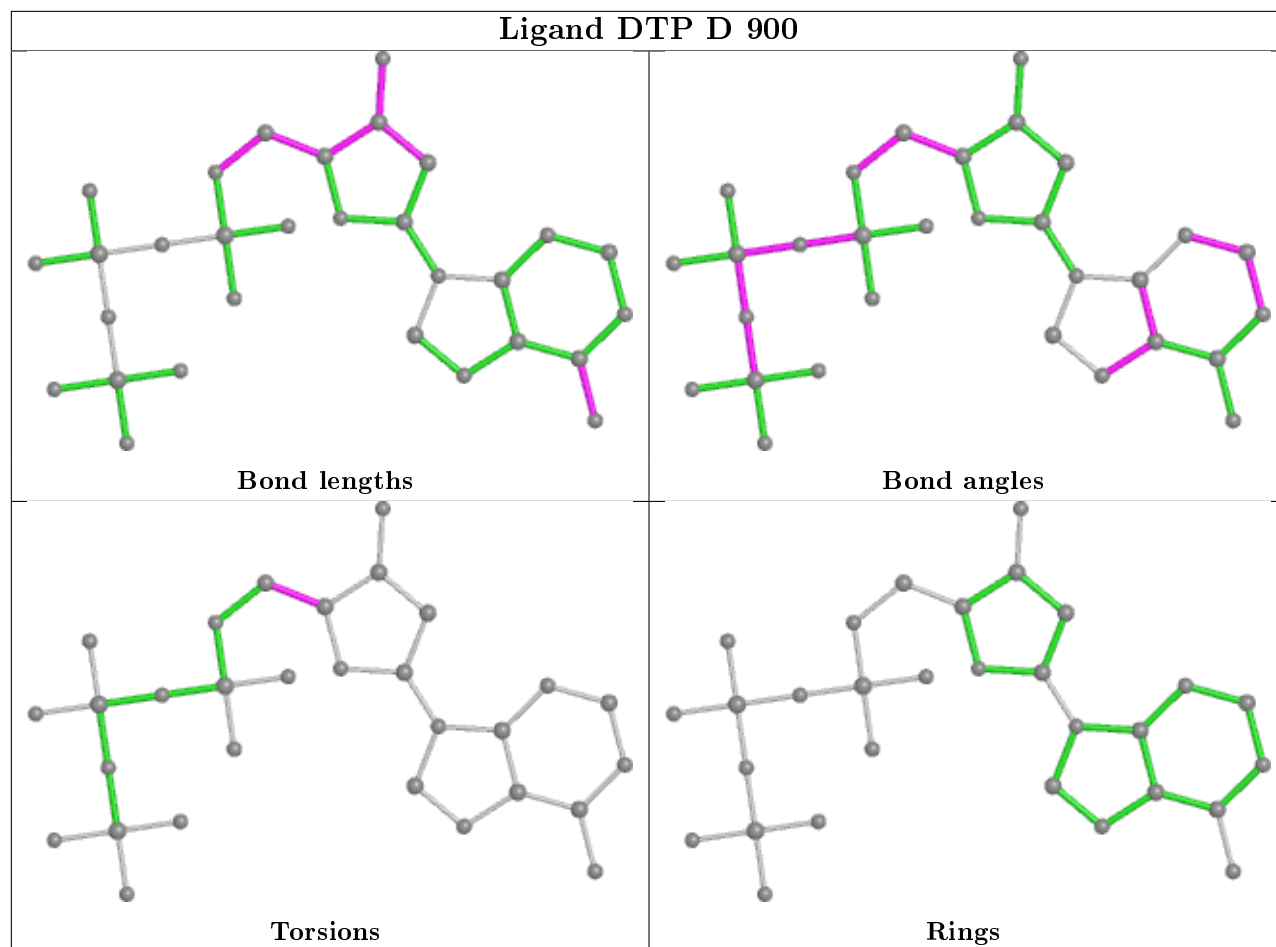
There are no ring outliers.

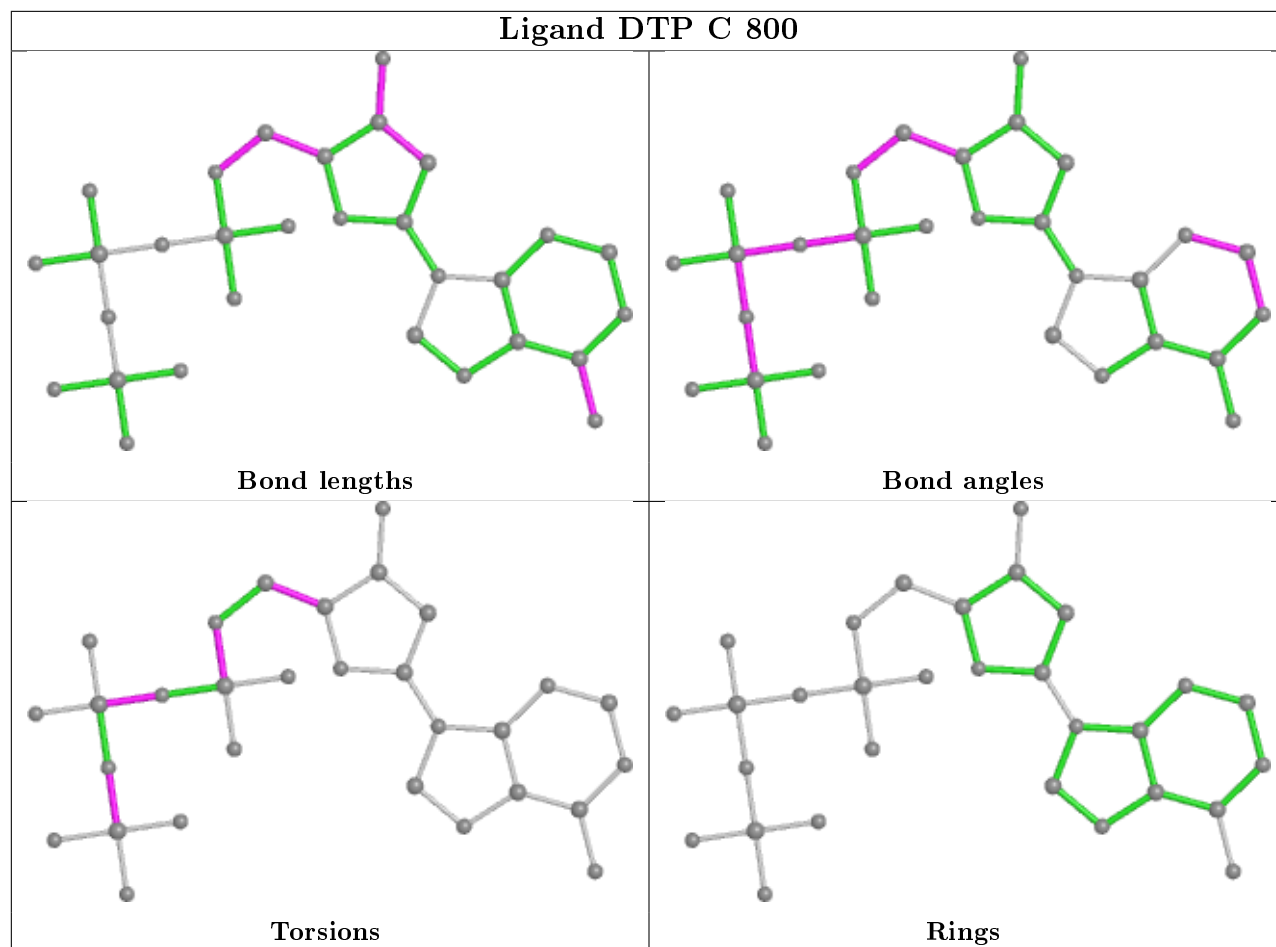
8 monomers are involved in 70 short contacts:

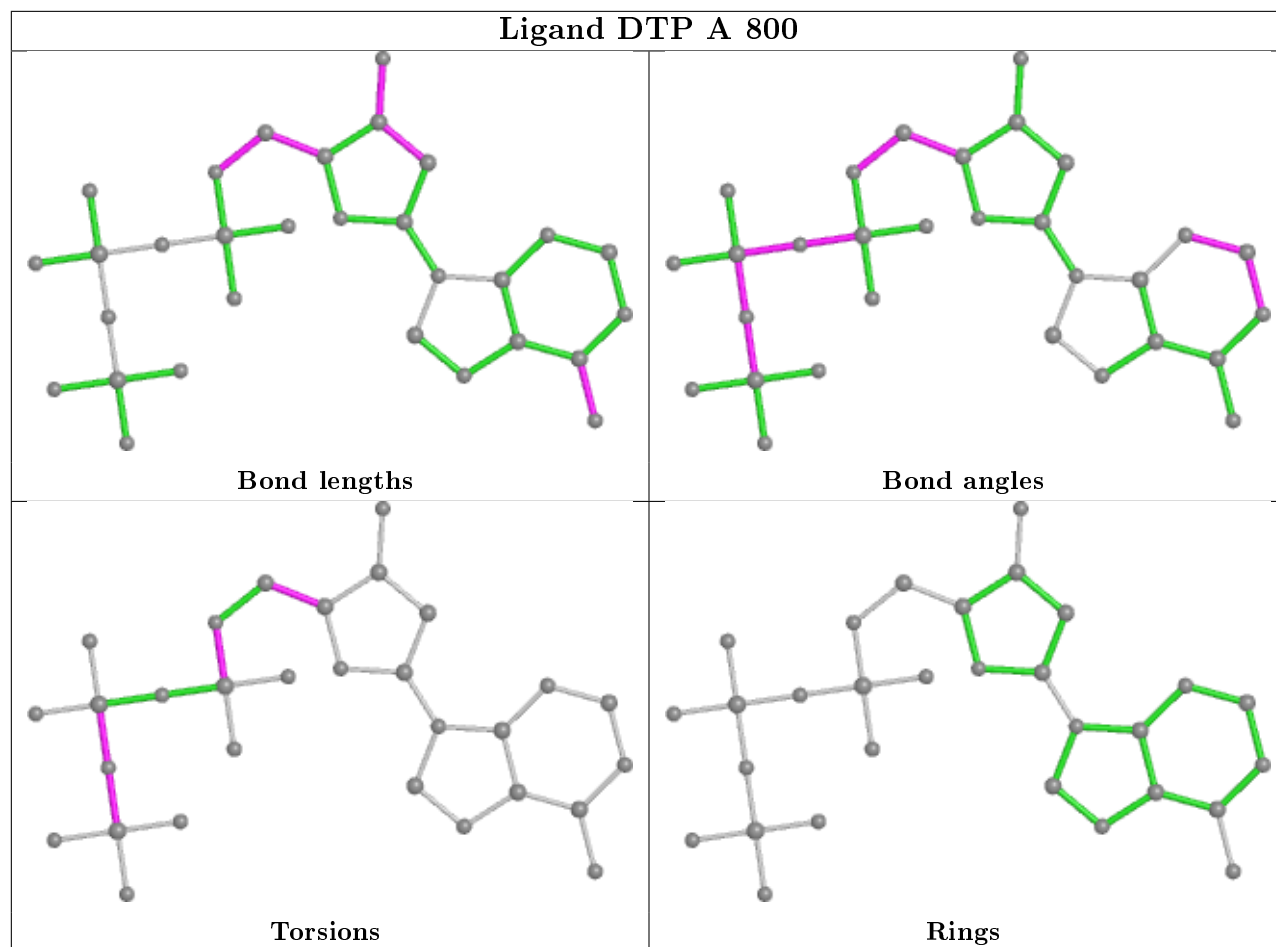
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	DTP	8	0
3	D	900	DTP	6	0
3	C	800	DTP	12	0
3	A	800	DTP	17	0
3	B	900	DTP	7	0
3	A	900	DTP	2	0
3	B	800	DTP	5	0
3	D	800	DTP	13	0

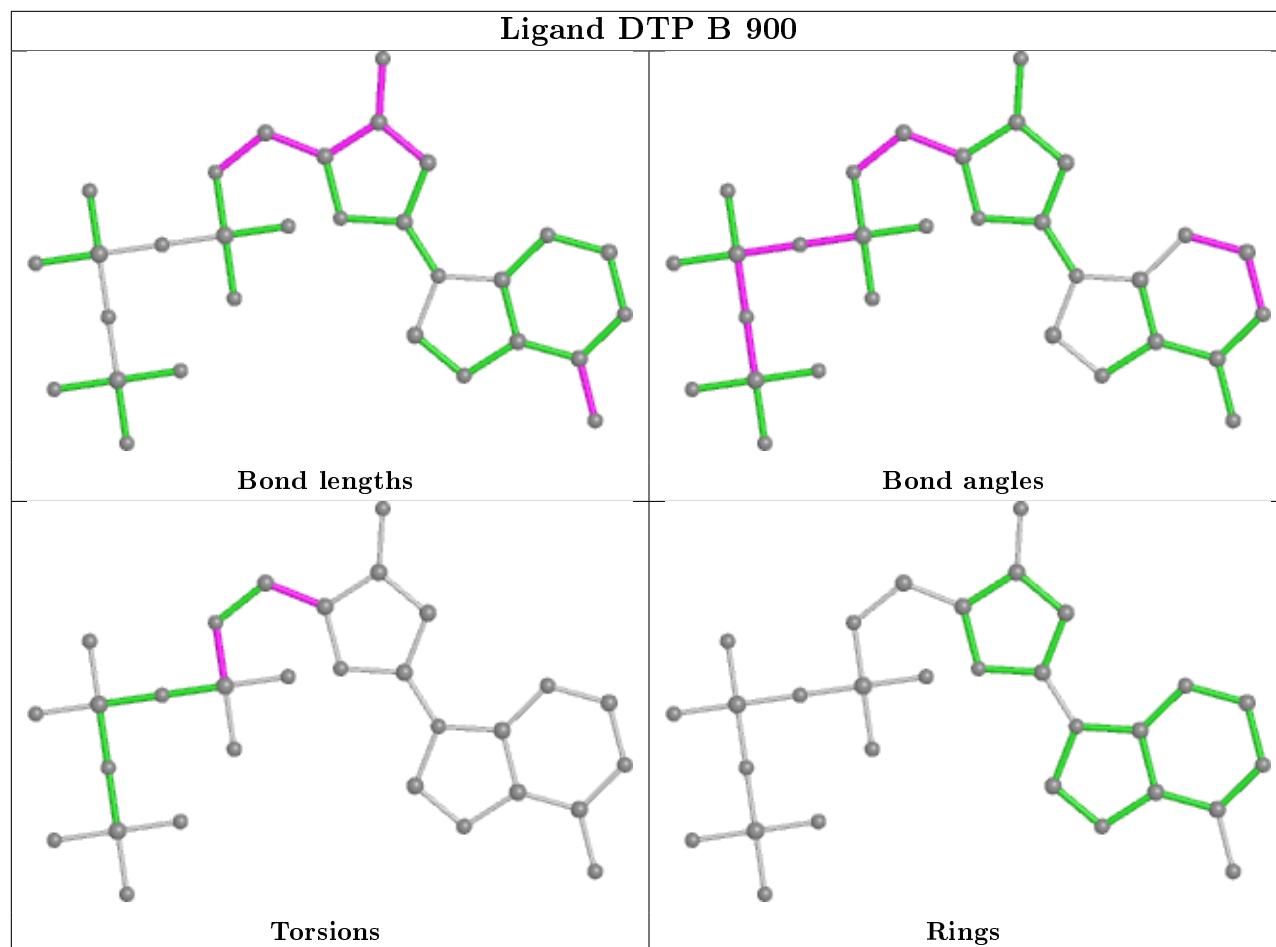
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



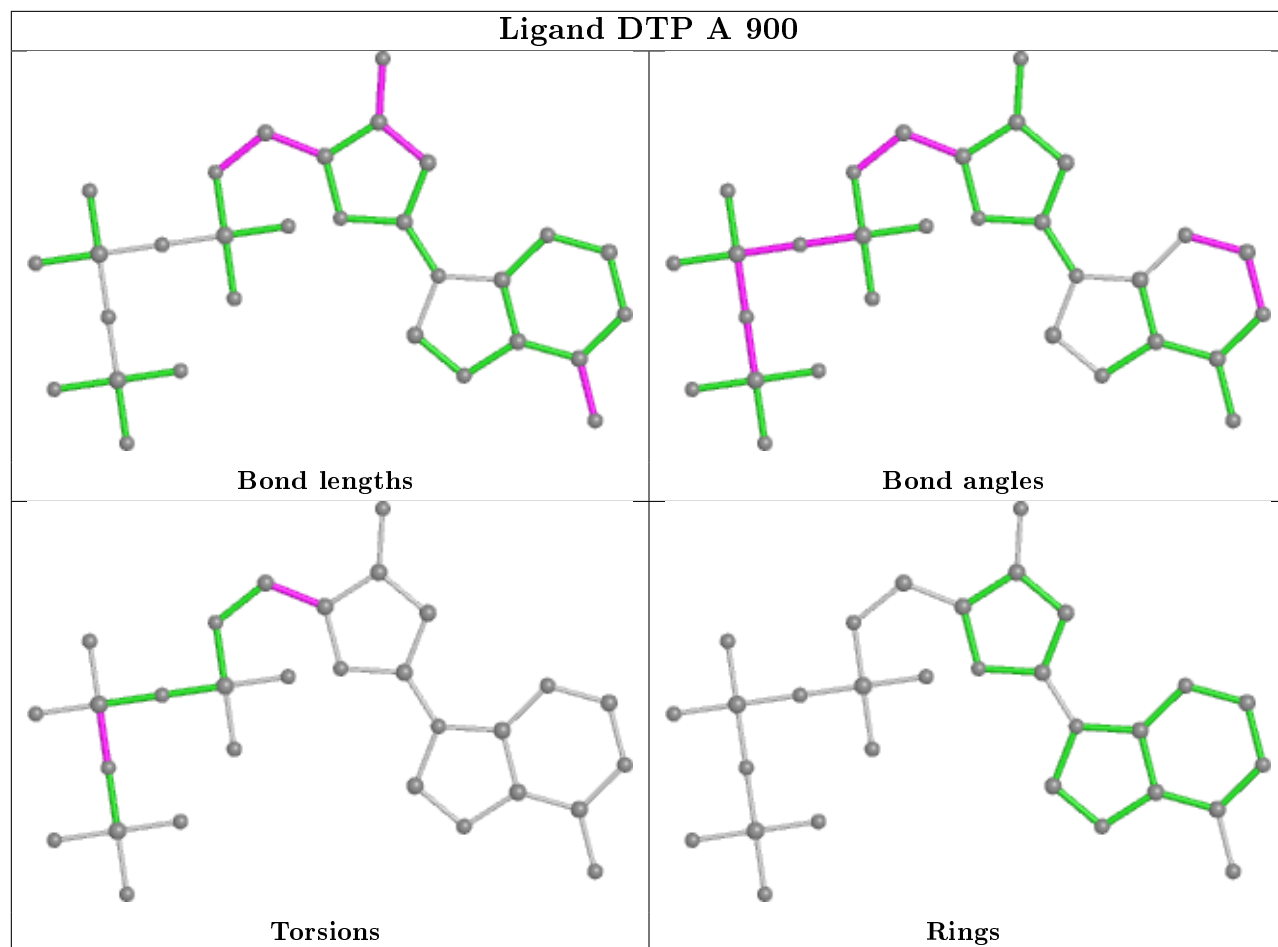


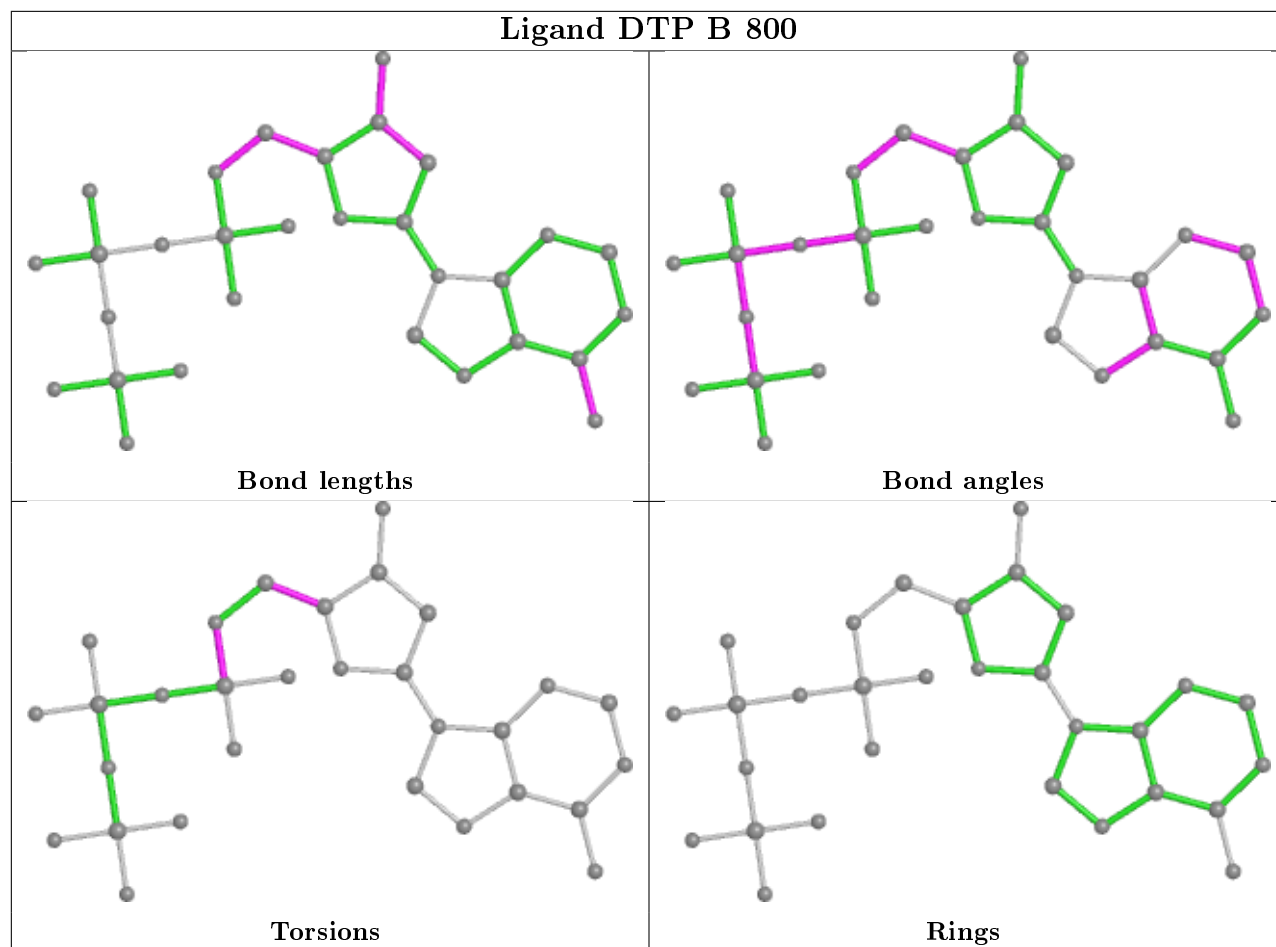


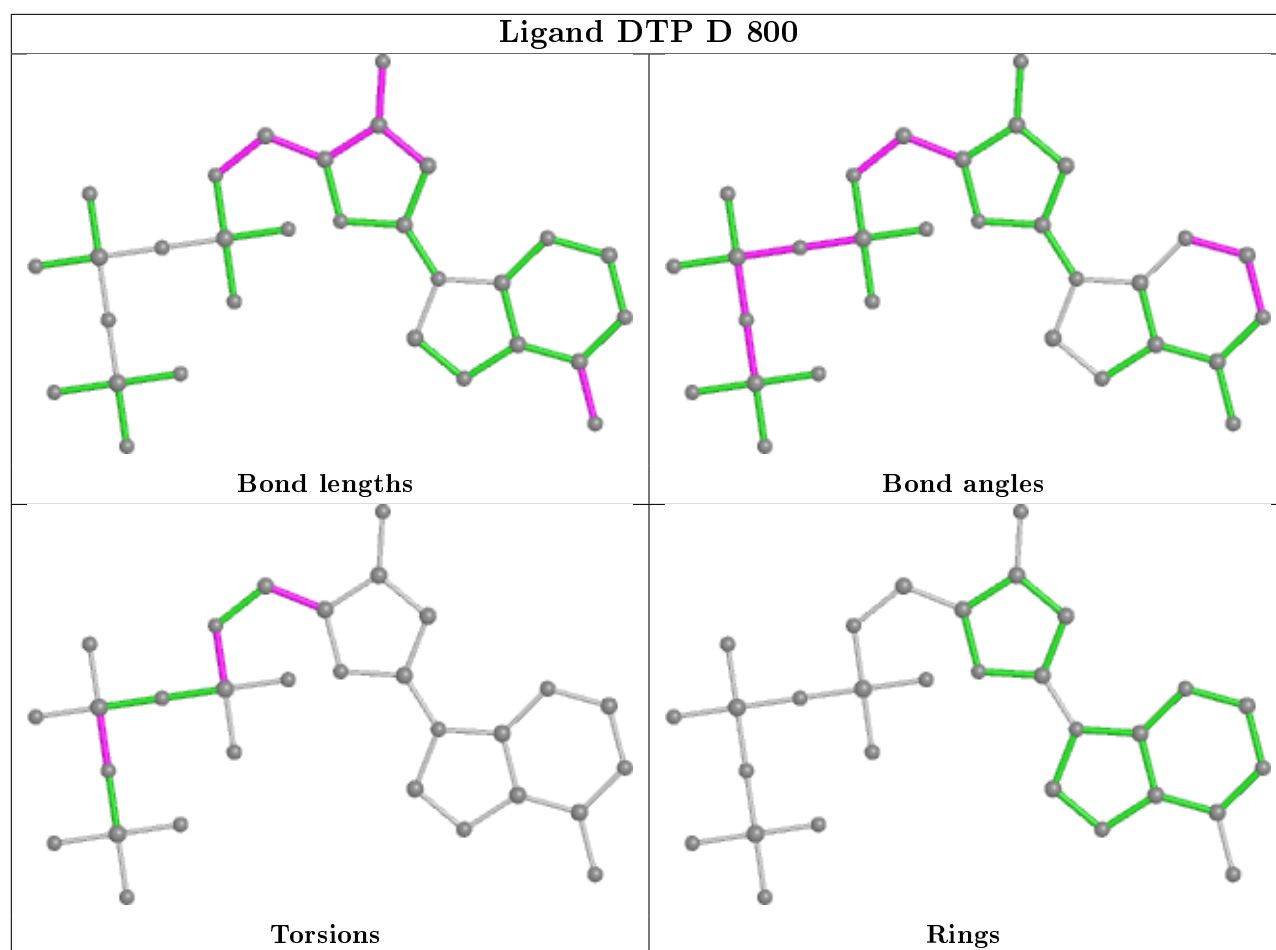












## 5.7 Other polymers [i](#)

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	732/761 (96%)	0.46	51 (6%) 16 15	157, 231, 260, 283	0
1	B	732/761 (96%)	0.51	52 (7%) 16 15	161, 232, 262, 279	0
1	C	732/761 (96%)	0.99	157 (21%) 0 2	197, 289, 342, 359	0
1	D	732/761 (96%)	1.14	167 (22%) 0 2	194, 290, 343, 359	0
2	E	348/375 (92%)	-0.00	3 (0%) 84 77	145, 207, 237, 289	0
2	F	348/375 (92%)	-0.05	2 (0%) 89 83	147, 206, 235, 285	0
2	G	352/375 (93%)	0.16	8 (2%) 60 53	147, 207, 237, 293	0
2	H	350/375 (93%)	0.07	3 (0%) 84 77	141, 203, 235, 286	0
All	All	4326/4544 (95%)	0.54	443 (10%) 6 9	141, 235, 312, 359	0

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	611	LEU	10.3
1	D	613	ASN	7.4
1	D	267	PRO	7.0
1	B	167	GLU	6.9
1	D	614	SER	6.7
1	C	100	PRO	6.5
1	D	564	ALA	6.5
1	D	462	CYS	6.5
1	D	360	ASP	6.4
1	C	621	PRO	6.2
1	C	15	GLU	6.1
1	D	383	GLU	6.0
1	D	390	LYS	6.0
1	C	266	SER	5.8
1	D	641	TYR	5.7
1	D	357	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	266	SER	5.5
1	D	389	ARG	5.4
1	D	174	ILE	5.4
1	D	181	PHE	5.3
1	D	392	ARG	5.3
1	D	167	GLU	5.3
1	D	179	CYS	5.2
1	D	178	ALA	5.1
1	C	14	THR	5.1
1	D	612	ARG	5.0
1	D	224	SER	5.0
1	D	223	SER	4.9
1	D	621	PRO	4.8
1	C	390	LYS	4.8
1	A	14	THR	4.7
1	D	225	CYS	4.7
1	A	271	GLY	4.6
1	D	56	SER	4.6
1	B	168	SER	4.6
1	D	565	CYS	4.6
1	D	253	GLY	4.6
1	C	432	PRO	4.6
1	B	171	PHE	4.5
1	C	259	GLY	4.5
1	B	166	TYR	4.4
1	D	737	GLY	4.4
1	B	667	GLU	4.4
1	D	640	GLY	4.4
1	D	510	ARG	4.4
1	C	439	CYS	4.3
1	D	698	ASN	4.3
1	D	187	GLU	4.3
1	C	216	ARG	4.2
1	C	388	ILE	4.2
1	C	622	SER	4.2
1	A	272	GLU	4.2
1	D	188	THR	4.1
1	C	263	ALA	4.1
1	D	463	THR	4.1
1	C	105	HIS	4.1
1	D	119	LEU	4.1
1	D	610	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	692	SER	4.0
1	C	119	LEU	4.0
1	C	120	LEU	4.0
1	B	165	ILE	4.0
1	D	72	ARG	4.0
1	D	356	PHE	4.0
1	C	458	GLU	3.9
1	C	620	MET	3.9
1	D	106	VAL	3.9
1	C	143	PHE	3.9
1	D	130	GLN	3.9
1	C	92	LYS	3.9
1	D	425	PRO	3.8
1	C	145	TYR	3.8
1	D	262	ARG	3.8
1	D	140	ASP	3.8
1	D	439	CYS	3.8
1	D	655	VAL	3.7
1	C	389	ARG	3.7
1	C	104	ASP	3.7
1	D	11	ASP	3.7
1	D	135	ILE	3.7
1	C	99	PRO	3.7
1	C	392	ARG	3.7
1	B	97	PHE	3.7
1	C	727	LYS	3.6
1	C	16	ARG	3.6
1	A	16	ARG	3.6
1	D	638	PRO	3.6
1	D	255	GLY	3.6
1	C	107	VAL	3.6
1	C	123	TYR	3.6
1	C	167	GLU	3.6
1	C	446	THR	3.5
1	D	252	ALA	3.5
1	C	98	GLU	3.5
1	C	436	SER	3.5
1	D	637	PRO	3.5
1	C	93	ALA	3.5
1	D	208	PRO	3.5
1	D	571	THR	3.5
1	C	694	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	182	SER	3.4
1	A	641	TYR	3.4
1	C	437	ASN	3.4
1	D	75	PRO	3.4
1	C	391	GLN	3.4
1	D	137	HIS	3.4
2	F	322	ASP	3.4
1	C	108	LYS	3.4
1	B	298	ARG	3.3
1	B	666	TYR	3.3
1	C	96	GLN	3.3
1	D	177	ALA	3.3
1	D	270	GLY	3.3
1	C	106	VAL	3.3
1	B	72	ARG	3.3
1	D	263	ALA	3.3
1	C	299	GLY	3.3
1	D	620	MET	3.3
1	C	190	LEU	3.3
1	C	737	GLY	3.3
1	B	216	ARG	3.2
1	A	622	SER	3.2
1	C	88	HIS	3.2
1	C	360	ASP	3.2
1	A	96	GLN	3.2
1	D	265	GLY	3.2
1	D	359	SER	3.2
1	D	388	ILE	3.2
1	D	105	HIS	3.2
1	A	15	GLU	3.1
1	C	358	PRO	3.1
1	C	728	THR	3.1
1	C	262	ARG	3.1
1	D	354	THR	3.1
1	D	699	TYR	3.1
1	D	622	SER	3.1
1	B	640	GLY	3.1
1	D	136	ASP	3.1
1	D	309	TRP	3.1
1	C	225	CYS	3.1
1	D	210	PRO	3.1
1	B	641	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	730	TYR	3.1
1	C	101	ALA	3.1
1	C	97	PHE	3.0
1	B	273	ALA	3.0
1	D	465	SER	3.0
1	A	270	GLY	3.0
1	D	563	GLY	3.0
1	A	94	TYR	3.0
1	C	303	THR	3.0
1	B	157	VAL	3.0
1	B	427	ASP	3.0
1	B	687	LYS	3.0
1	D	576	GLY	3.0
1	C	731	TYR	3.0
1	A	95	GLY	3.0
1	B	668	LEU	3.0
1	D	141	MET	3.0
1	D	511	ARG	3.0
1	A	165	ILE	3.0
1	C	462	CYS	3.0
1	C	265	GLY	3.0
1	D	300	GLY	3.0
1	C	10	ARG	2.9
1	D	88	HIS	2.9
1	C	116	ASP	2.9
1	C	223	SER	2.9
1	D	170	GLN	2.9
1	A	88	HIS	2.9
1	B	120	LEU	2.9
1	B	116	ASP	2.9
1	C	189	ARG	2.9
1	D	54	LYS	2.9
1	C	301	ALA	2.9
1	B	190	LEU	2.9
1	C	352	ASP	2.9
1	C	179	CYS	2.9
1	C	428	PRO	2.9
1	C	624	THR	2.9
2	G	257	ASP	2.9
1	D	165	ILE	2.9
1	C	655	VAL	2.9
1	C	421	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	99	PRO	2.9
1	D	308	MET	2.9
1	C	357	SER	2.8
1	A	269	ARG	2.8
1	C	103	TYR	2.8
1	D	139	ARG	2.8
1	C	359	SER	2.8
2	F	295	SER	2.8
1	D	572	THR	2.8
1	C	267	PRO	2.8
1	C	215	VAL	2.8
1	C	11	ASP	2.8
1	C	702	SER	2.8
1	C	295	GLY	2.8
2	G	19	PHE	2.8
1	A	667	GLU	2.7
1	B	671	GLU	2.7
1	D	437	ASN	2.7
1	D	639	ARG	2.7
1	A	614	SER	2.7
1	D	642	VAL	2.7
1	D	301	ALA	2.7
1	B	141	MET	2.7
1	C	573	TYR	2.7
1	C	144	SER	2.7
1	D	131	MET	2.7
1	C	733	ASN	2.7
1	C	128	PHE	2.7
1	A	166	TYR	2.7
1	C	510	ARG	2.7
1	C	94	TYR	2.7
1	D	123	TYR	2.7
1	C	102	LEU	2.7
1	C	178	ALA	2.6
1	C	356	PHE	2.6
1	A	58	ILE	2.6
1	B	439	CYS	2.6
1	C	323	ARG	2.6
1	D	12	GLY	2.6
1	D	327	GLY	2.6
1	D	380	THR	2.6
1	C	700	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	516	GLY	2.6
1	C	671	GLU	2.6
1	B	115	TYR	2.6
1	A	570	GLU	2.6
1	D	57	ASP	2.6
1	C	710	PRO	2.6
1	B	140	ASP	2.6
1	C	732	GLN	2.6
1	C	90	ARG	2.6
1	C	438	LEU	2.6
2	E	322	ASP	2.6
1	C	56	SER	2.6
1	B	156	LEU	2.6
1	C	445	PRO	2.6
1	D	183	ASN	2.6
1	A	426	PHE	2.6
1	C	7	VAL	2.5
1	C	429	ALA	2.5
1	D	15	GLU	2.5
1	A	144	SER	2.5
1	D	271	GLY	2.5
1	C	217	THR	2.5
1	A	17	ILE	2.5
1	D	379	TYR	2.5
1	D	668	LEU	2.5
1	D	656	VAL	2.5
1	B	145	TYR	2.5
1	D	667	GLU	2.5
1	C	370	ALA	2.5
1	B	94	TYR	2.5
1	D	8	THR	2.5
1	B	655	VAL	2.5
1	B	152	GLU	2.5
1	D	168	SER	2.5
2	G	17	MET	2.5
1	D	259	GLY	2.5
1	D	274	PHE	2.5
1	B	170	GLN	2.5
1	A	659	TYR	2.5
1	C	383	GLU	2.5
1	C	379	TYR	2.5
1	A	360	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	659	TYR	2.5
1	B	431	ALA	2.5
1	D	261	ILE	2.5
1	D	516	GLY	2.4
1	C	322	ASN	2.4
1	C	385	ASP	2.4
1	D	100	PRO	2.4
2	G	252	LEU	2.4
1	A	208	PRO	2.4
1	B	271	GLY	2.4
1	D	353	ILE	2.4
1	D	391	GLN	2.4
1	A	268	ILE	2.4
1	D	94	TYR	2.4
1	D	275	HIS	2.4
1	C	78	GLN	2.4
1	C	699	TYR	2.4
1	D	55	THR	2.4
1	A	35	ASN	2.4
1	C	138	ASP	2.4
1	A	145	TYR	2.4
1	D	562	GLN	2.4
1	B	656	VAL	2.4
1	A	273	ALA	2.4
1	B	274	PHE	2.4
1	C	76	ASP	2.4
1	D	619	LEU	2.4
1	D	505	ARG	2.4
1	B	395	ALA	2.4
1	C	182	SER	2.4
1	C	277	GLY	2.4
1	C	413	TYR	2.4
1	D	128	PHE	2.4
1	A	93	ALA	2.4
1	B	670	TRP	2.4
1	D	734	THR	2.4
1	D	514	GLY	2.4
1	A	621	PRO	2.4
1	D	358	PRO	2.4
1	D	97	PHE	2.3
1	A	206	SER	2.3
1	C	734	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	187	ARG	2.3
1	A	259	GLY	2.3
2	G	56	SER	2.3
1	D	10	ARG	2.3
1	C	183	ASN	2.3
1	C	434	ARG	2.3
1	A	6	LEU	2.3
1	A	92	LYS	2.3
1	D	171	PHE	2.3
1	C	411	ARG	2.3
1	D	705	PRO	2.3
1	C	441	GLU	2.3
1	A	356	PHE	2.3
1	C	670	TRP	2.3
1	B	531	TYR	2.3
1	A	466	ALA	2.3
1	D	464	LEU	2.3
1	D	299	GLY	2.3
1	D	193	VAL	2.3
1	C	431	ALA	2.3
1	A	655	VAL	2.3
1	C	586	ASP	2.2
1	C	91	LYS	2.2
1	C	509	GLY	2.2
1	D	427	ASP	2.2
1	A	62	ILE	2.2
1	A	257	ASN	2.2
1	A	425	PRO	2.2
1	D	617	SER	2.2
1	C	576	GLY	2.2
1	D	568	PHE	2.2
1	D	157	VAL	2.2
1	B	123	TYR	2.2
1	C	659	TYR	2.2
1	C	168	SER	2.2
1	C	142	THR	2.2
1	D	624	THR	2.2
2	E	324	PRO	2.2
1	C	447	LYS	2.2
1	D	184	TYR	2.2
1	C	387	SER	2.2
1	B	657	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	709	VAL	2.2
1	B	100	PRO	2.2
1	B	712	GLN	2.2
1	C	152	GLU	2.2
1	C	505	ARG	2.2
1	D	434	ARG	2.2
1	D	735	ARG	2.2
1	C	614	SER	2.2
1	C	273	ALA	2.2
1	C	312	GLU	2.2
1	D	197	TYR	2.2
1	D	727	LYS	2.2
1	D	14	THR	2.2
1	D	659	TYR	2.2
1	B	532	SER	2.2
1	D	381	LYS	2.2
1	D	83	ARG	2.2
1	D	618	ALA	2.2
1	C	224	SER	2.2
1	D	175	LEU	2.2
1	C	117	ASN	2.2
1	C	450	ASN	2.2
1	D	166	TYR	2.2
1	C	296	GLY	2.2
1	A	435	GLN	2.2
1	C	463	THR	2.2
1	D	385	ASP	2.2
1	C	625	SER	2.2
1	C	17	ILE	2.2
1	D	185	PRO	2.2
2	G	365	VAL	2.2
1	B	680	GLN	2.2
1	D	607	LYS	2.2
2	H	191	LYS	2.2
1	C	156	LEU	2.1
1	C	362	PRO	2.1
1	B	179	CYS	2.1
1	C	575	LYS	2.1
1	B	473	ASN	2.1
1	A	465	SER	2.1
2	E	295	SER	2.1
1	D	384	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	12	GLN	2.1
1	C	657	PRO	2.1
1	D	260	ARG	2.1
1	C	667	GLU	2.1
1	B	357	SER	2.1
1	C	514	GLY	2.1
1	D	122	ASP	2.1
1	D	102	LEU	2.1
1	D	458	GLU	2.1
1	A	11	ASP	2.1
1	B	119	LEU	2.1
1	A	255	GLY	2.1
1	A	261	ILE	2.1
1	D	700	ASP	2.1
1	C	382	TYR	2.1
1	D	192	TYR	2.1
1	A	56	SER	2.1
1	D	120	LEU	2.1
1	A	72	ARG	2.1
1	C	703	ARG	2.1
2	H	19	PHE	2.1
1	D	435	GLN	2.1
1	C	95	GLY	2.1
1	D	426	PHE	2.1
1	D	566	PRO	2.1
1	C	440	LEU	2.1
1	B	267	PRO	2.1
1	C	706	SER	2.1
1	D	573	TYR	2.1
1	D	713	GLN	2.1
1	D	370	ALA	2.1
1	A	666	TYR	2.1
1	D	133	THR	2.1
1	C	435	GLN	2.1
1	D	574	ALA	2.1
1	D	570	GLU	2.1
1	C	264	LEU	2.1
1	D	555	SER	2.1
1	C	171	PHE	2.1
1	C	184	TYR	2.0
1	C	75	PRO	2.0
1	C	465	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	694	SER	2.0
2	G	55	VAL	2.0
1	C	666	TYR	2.0
1	A	392	ARG	2.0
1	B	530	ARG	2.0
1	D	466	ALA	2.0
1	C	260	ARG	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](#)

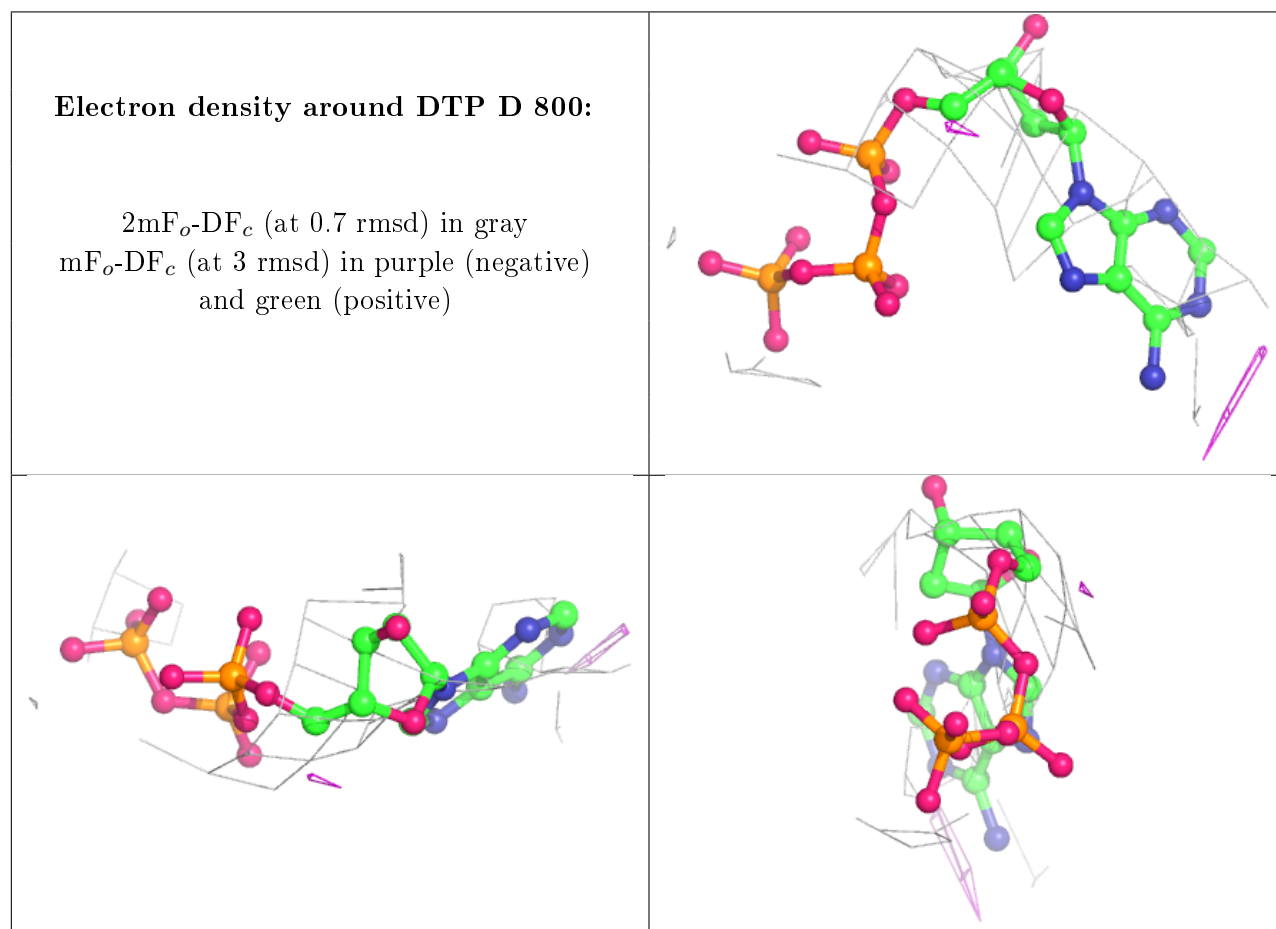
There are no carbohydrates in this entry.

## 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
3	DTP	D	800	30/30	0.31	0.53	318,318,318,318	0
3	DTP	D	900	30/30	0.57	0.50	308,308,308,308	0
3	DTP	C	900	30/30	0.60	0.40	284,284,284,284	0
3	DTP	B	900	30/30	0.67	0.41	232,232,232,232	0
3	DTP	A	800	30/30	0.70	0.59	306,306,306,306	0
3	DTP	C	800	30/30	0.71	0.65	326,326,326,326	0
3	DTP	B	800	30/30	0.79	0.50	279,279,279,279	0
3	DTP	A	900	30/30	0.80	0.37	267,267,267,267	0
4	FE	E	1004	1/1	0.95	0.23	133,133,133,133	0
4	FE	E	1003	1/1	0.96	0.26	168,168,168,168	0
4	FE	G	1003	1/1	0.98	0.29	89,89,89,89	0
4	FE	H	1002	1/1	0.99	0.32	114,114,114,114	0
4	FE	F	1002	1/1	0.99	0.20	125,125,125,125	0
4	FE	H	1001	1/1	0.99	0.26	110,110,110,110	0
4	FE	G	1004	1/1	0.99	0.34	122,122,122,122	0
4	FE	F	1001	1/1	0.99	0.20	94,94,94,94	0

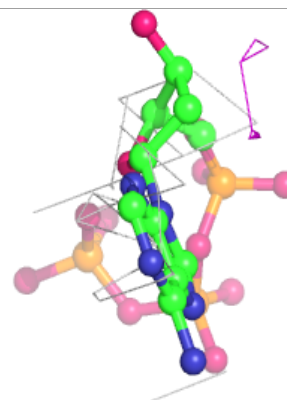
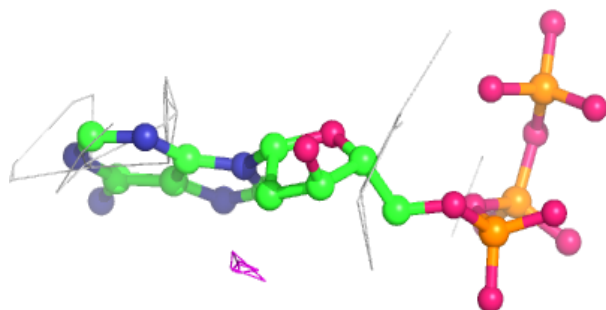
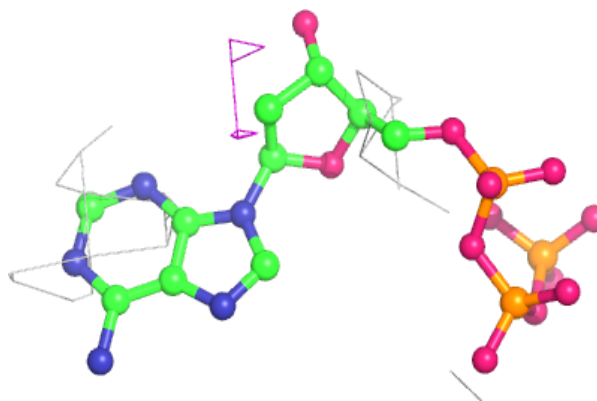
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



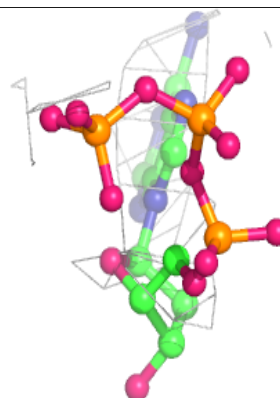
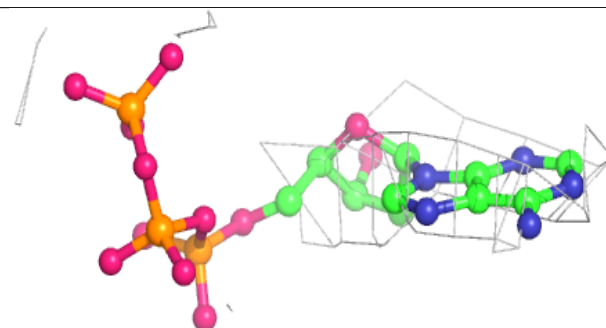
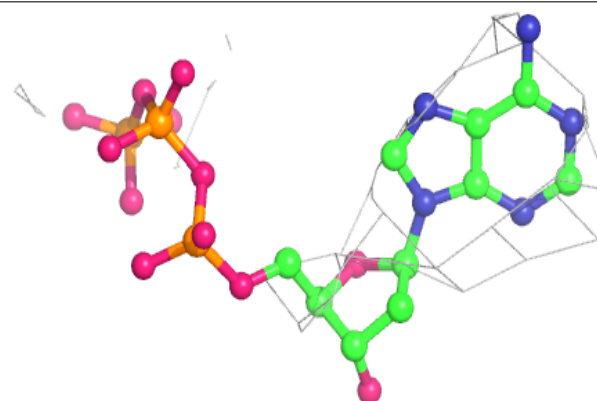


**Electron density around DTP D 900:**

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

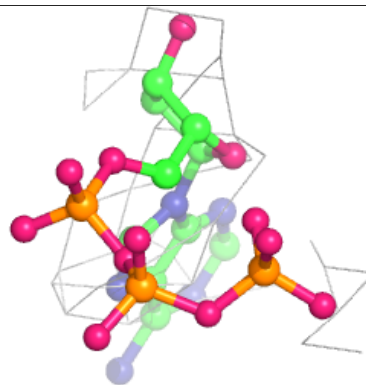
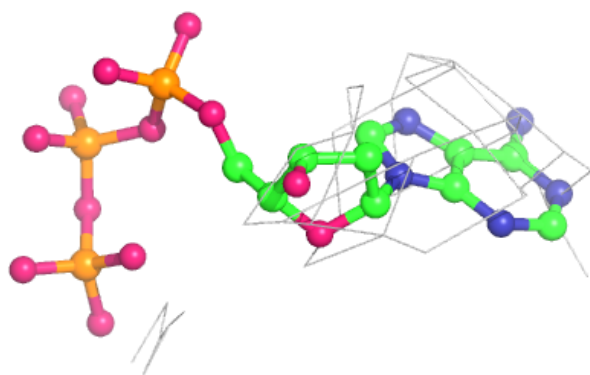
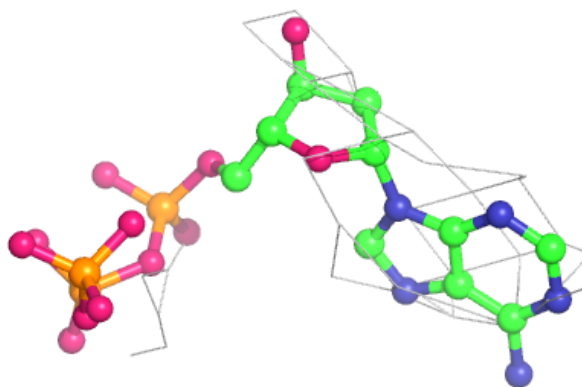
**Electron density around DTP C 900:**

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



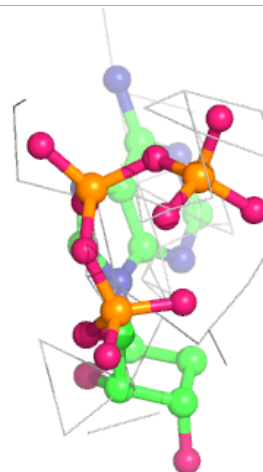
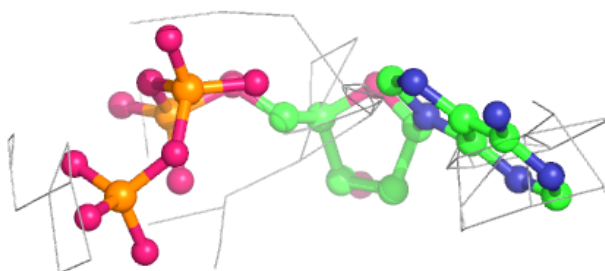
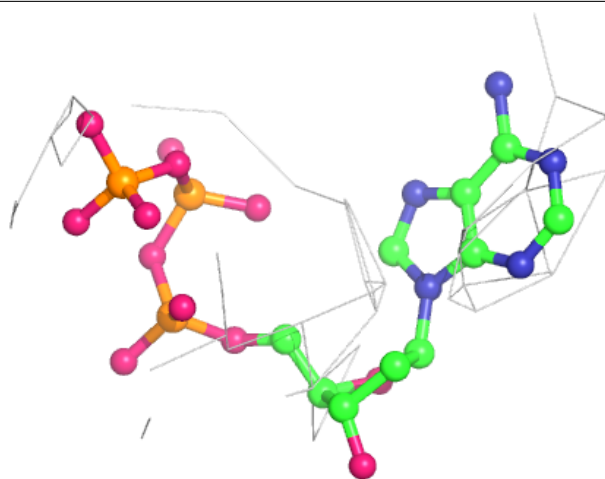
**Electron density around DTP B 900:**

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



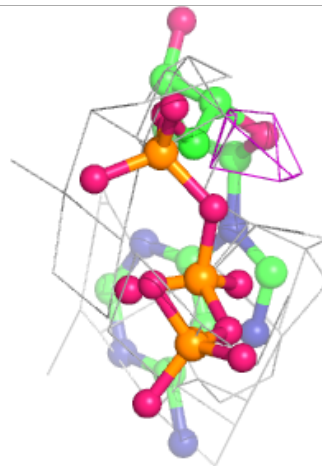
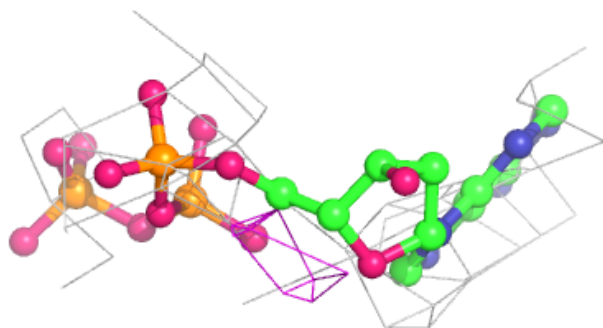
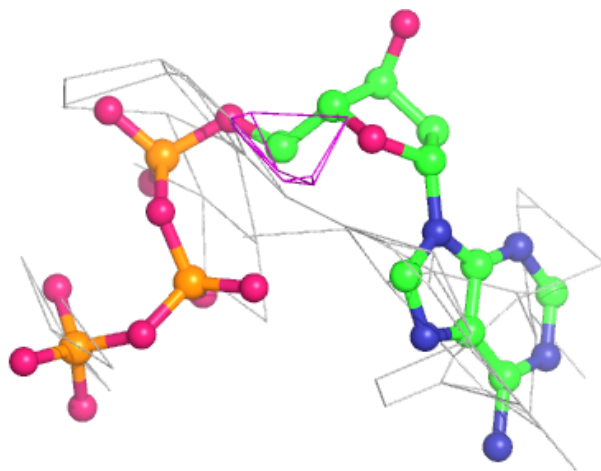
**Electron density around DTP A 800:**

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



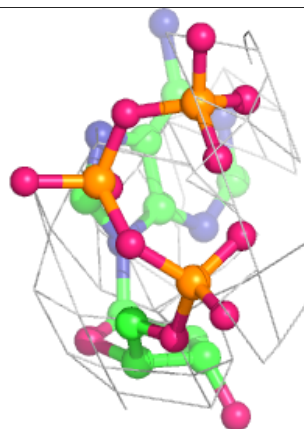
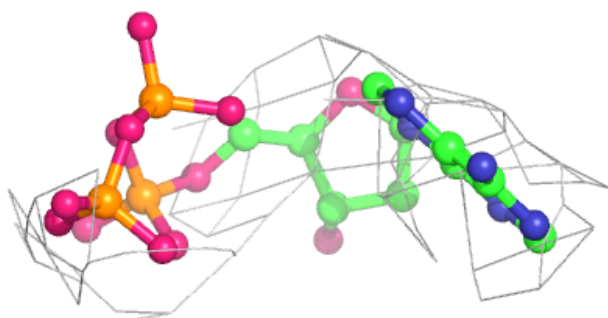
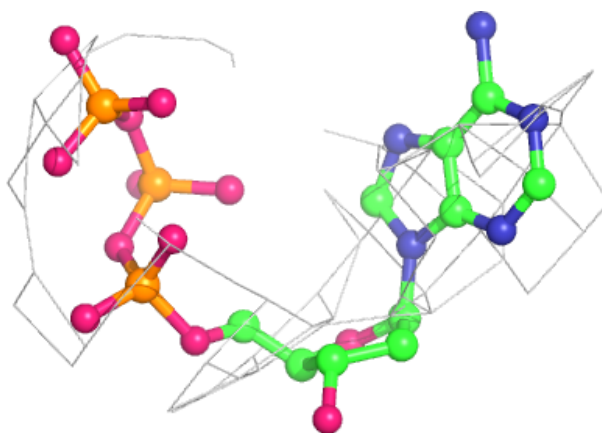
**Electron density around DTP C 800:**

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

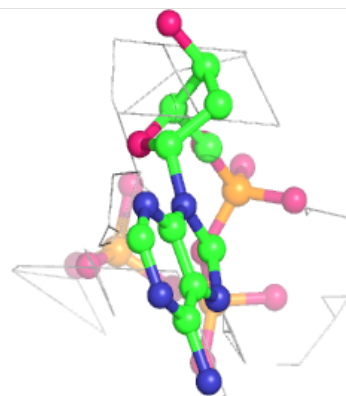
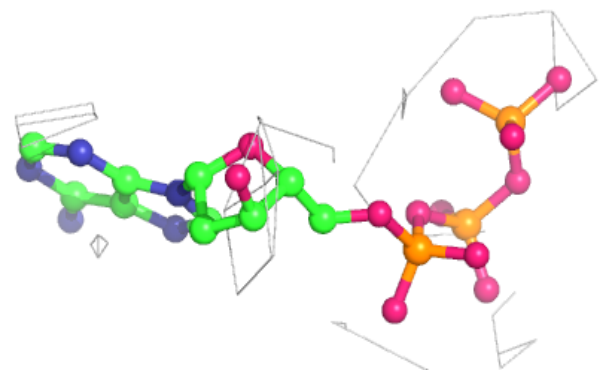
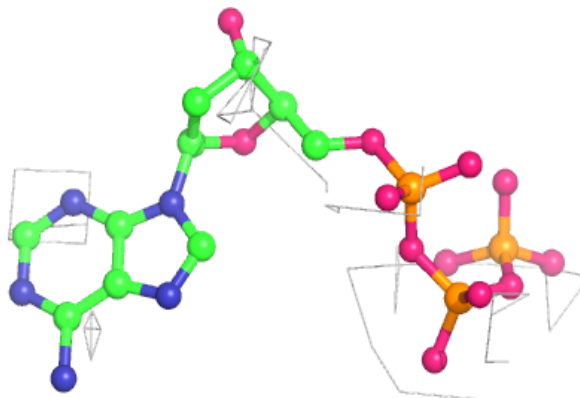


**Electron density around DTP B 800:**

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

**Electron density around DTP A 900:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.