



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:49 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

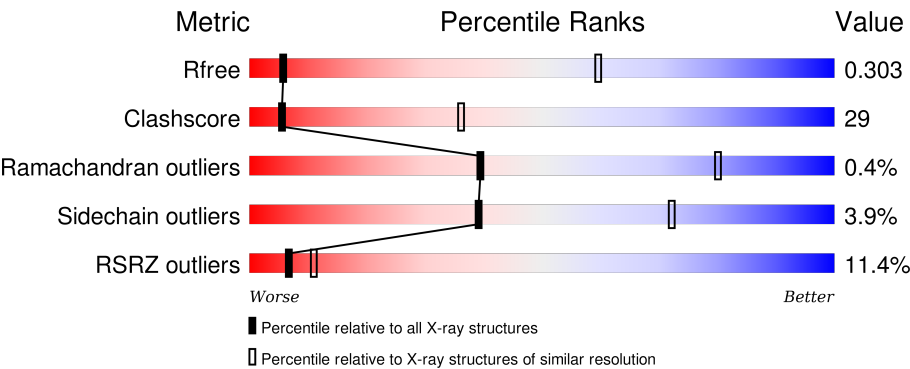
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1006 (7.66-3.64)
Clashscore	102246	1036 (7.60-3.70)
Ramachandran outliers	100387	1011 (7.60-3.66)
Sidechain outliers	100360	1001 (7.60-3.64)
RSRZ outliers	91569	1005 (7.66-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>8%</div><div>48%</div><div>45%</div><div>• •</div></div>
1	B	761	<div><div>8%</div><div>48%</div><div>46%</div><div>• •</div></div>
1	C	761	<div><div>22%</div><div>50%</div><div>44%</div><div>• •</div></div>
1	D	761	<div><div>24%</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>

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Mol	Chain	Length	Quality of chain
2	F	375	
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.

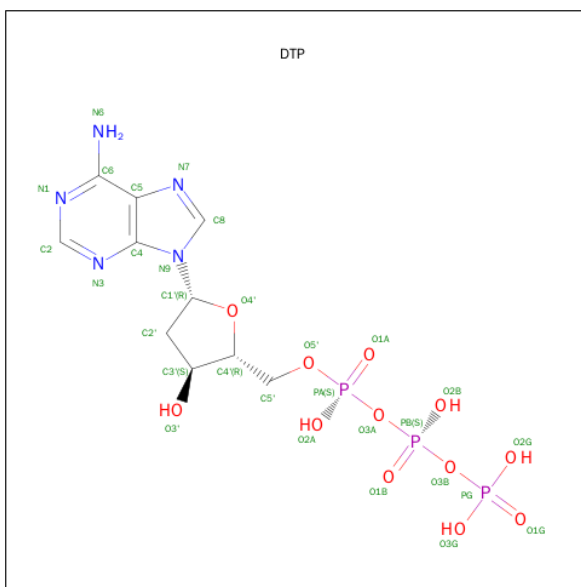
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

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 30	C 10	N 5	O 12	P 3	0	0
3	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	D	1	Total 30	C 10	N 5	O 12	P 3	0	0

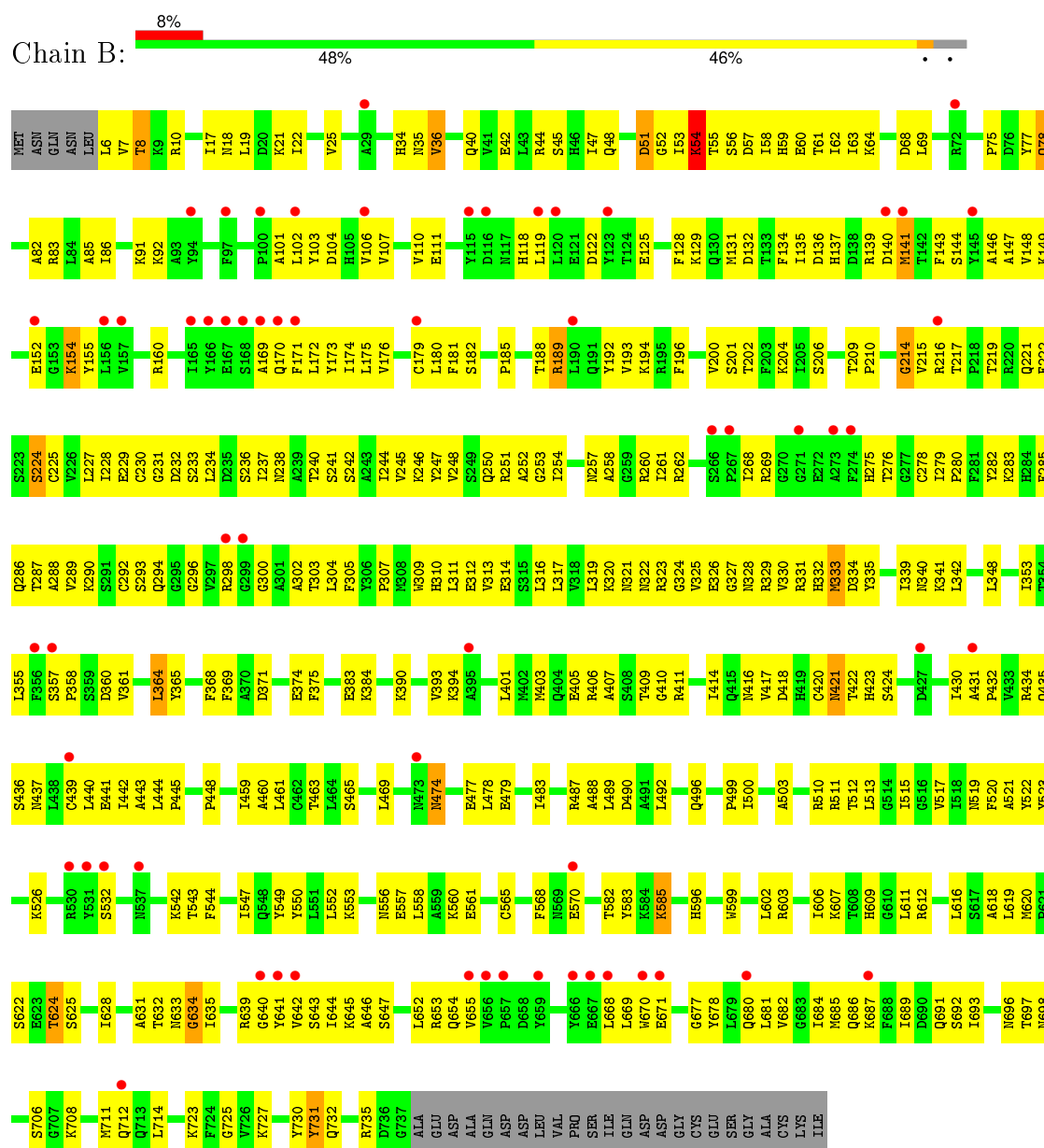
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

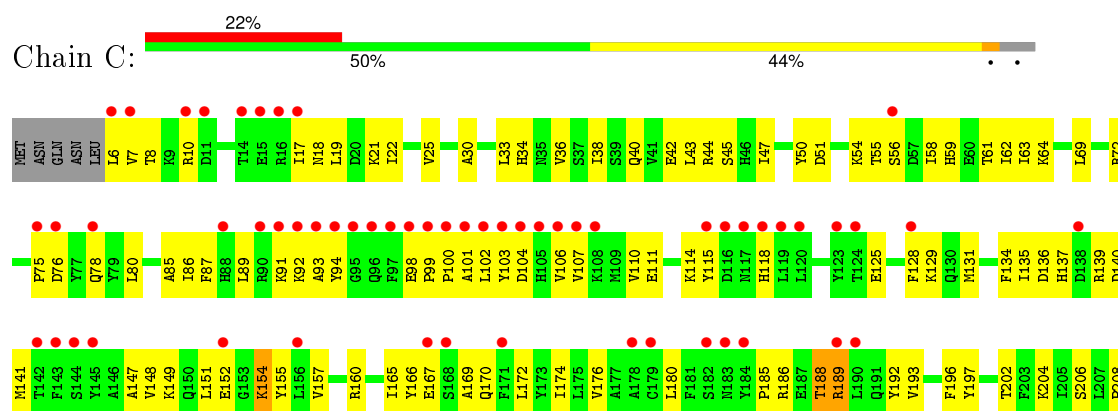
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

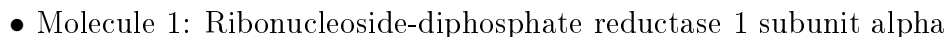
- [illegible]

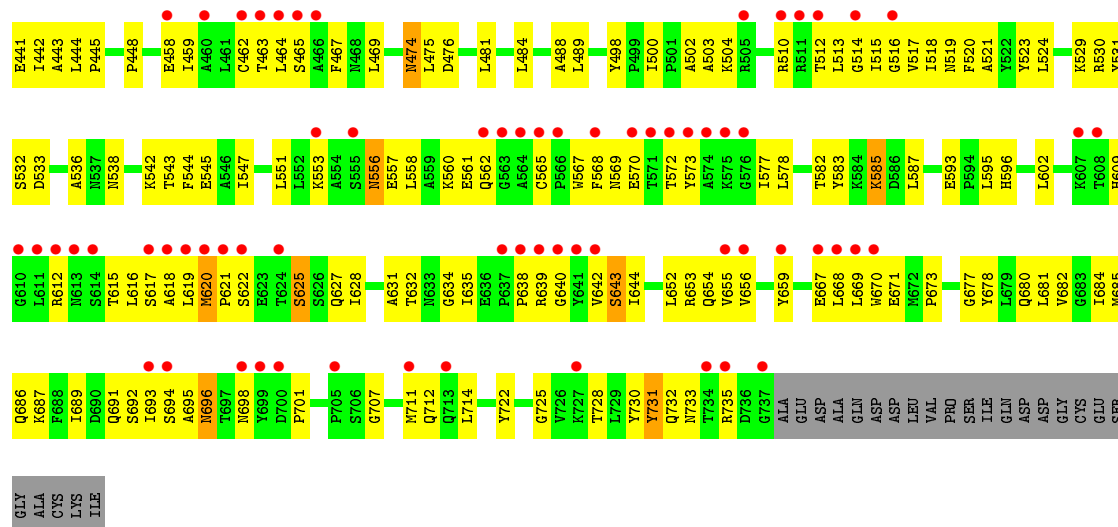
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



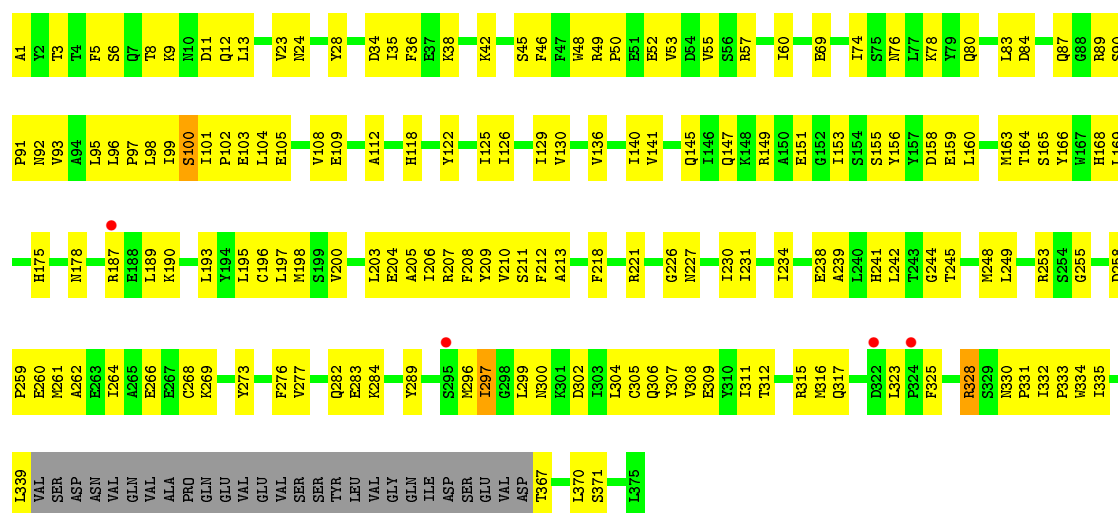
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



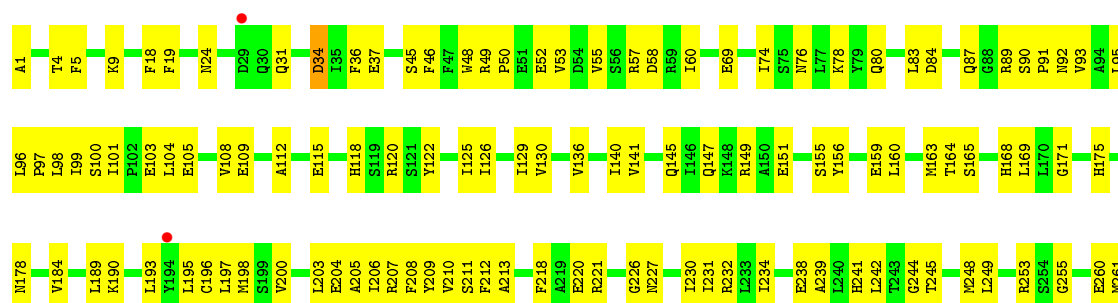


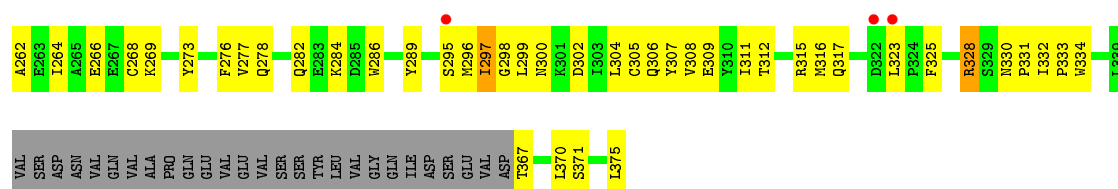


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

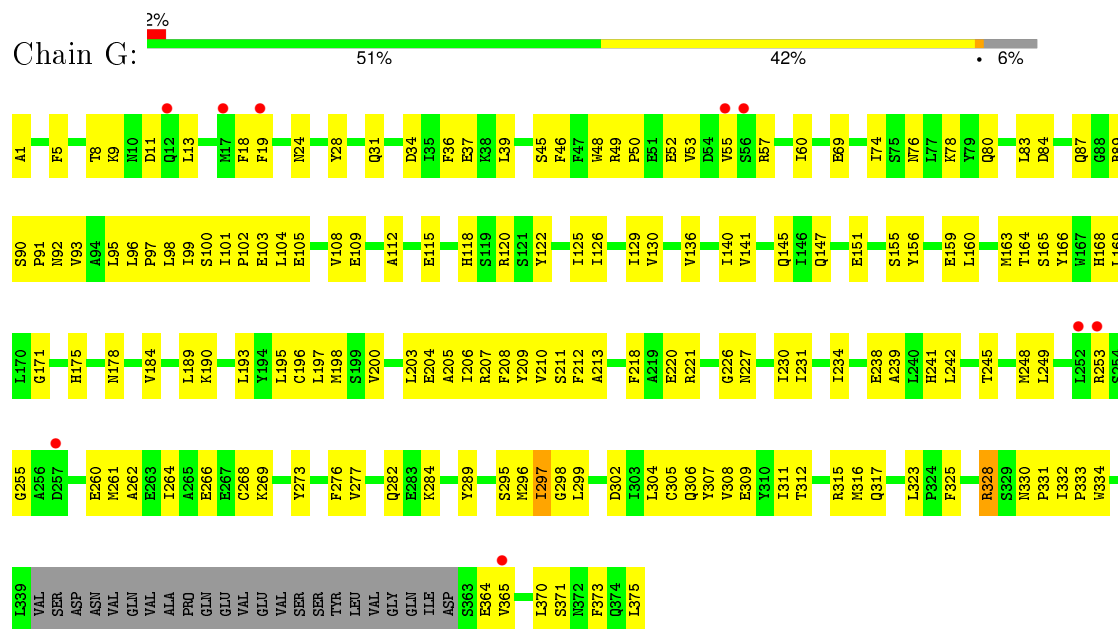


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

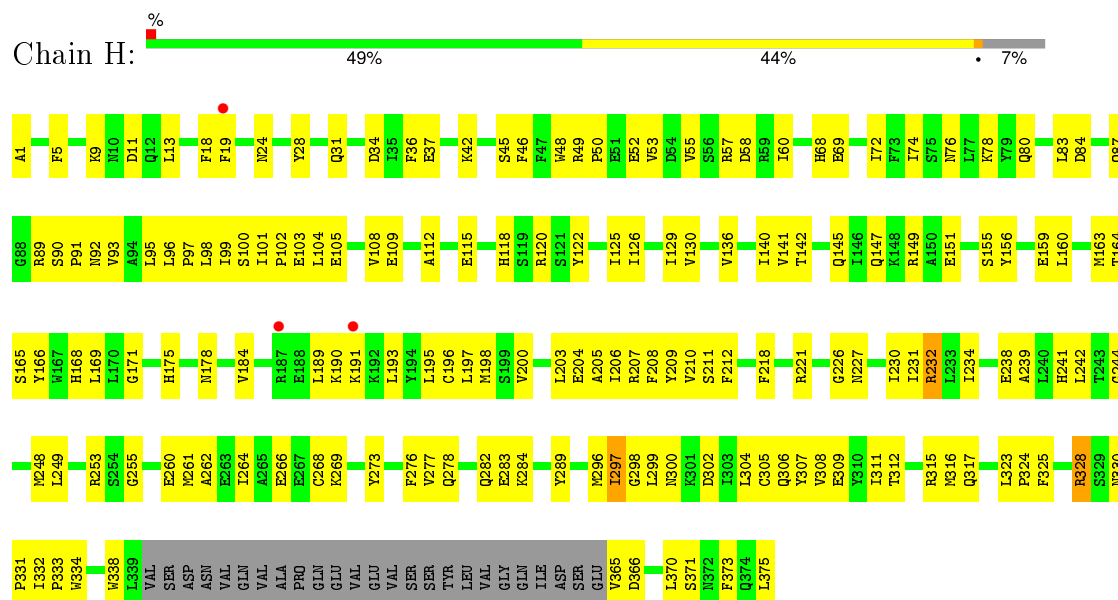




- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 5.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.303 0.257 , 0.303	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	194.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 178.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19134 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	35029	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:C:6:LEU:HD22	1:C:51:ASP:CB	1.81	1.10
1:B:185:PRO:HG2	1:B:188:THR:OG1	1.50	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:C:432:PRO:HG2	1:C:434:ARG:HD2	1.35	1.02
1:A:293:SER:HB3	1:A:298:ARG:O	1.57	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:6:LEU:HB2	1:B:52:GLY:H	1.26	0.99
1:B:155:TYR:CE1	1:B:209:THR:HG23	1.97	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:D:7:VAL:HG21	1:D:17:ILE:HG12	1.47	0.95
1:C:6:LEU:HD22	1:C:51:ASP:HB2	0.95	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:D:7:VAL:HG22	1:D:17:ILE:HG12	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:O	1:A:53:ILE:HG22	1.69	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:C:427:ASP:HB3	1:C:430:ILE:HD12	1.51	0.92
1:A:618:ALA:HB2	1:A:691:GLN:HB2	1.49	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:C:430:ILE:HG21	1:C:570:GLU:CB	2.00	0.91
1:A:297:VAL:HG12	1:A:298:ARG:HG3	1.49	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:D:7:VAL:CG2	1:D:17:ILE:CG1	2.49	0.89
1:C:42:GLU:OE1	2:G:298:GLY:HA2	1.71	0.89
1:D:290:LYS:CG	1:D:296:GLY:O	2.20	0.89
1:D:696:ASN:ND2	1:D:730:TYR:HB3	1.87	0.89
1:B:618:ALA:HB2	1:B:691:GLN:HB2	1.52	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:C:432:PRO:HG2	1:C:434:ARG:CD	2.04	0.87
1:A:439:CYS:SG	1:A:621:PRO:HD2	2.13	0.87
1:A:463:THR:HG23	1:A:492:LEU:HD23	1.53	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:618:ALA:HB2	1:B:691:GLN:CB	2.06	0.85
1:B:215:VAL:O	1:B:216:ARG:HG2	1.77	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:C:427:ASP:OD1	1:C:428:PRO:HD2	1.80	0.81
1:B:154:LYS:HD2	1:B:155:TYR:HE1	1.43	0.81
1:A:441:GLU:OE1	1:A:620:MET:HB2	1.80	0.81
1:D:40:GLN:OE1	2:E:334:TRP:CB	2.28	0.81
1:D:186:ARG:HH21	1:D:189:ARG:NH2	1.78	0.81
1:C:155:TYR:OH	1:C:624:THR:CG2	2.28	0.81
1:D:276:THR:CG2	3:D:900:DTP:H2	2.10	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: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:C:206:SER:HB2	1:C:466:ALA:HB3	0.80	0.80
1:A:730:TYR:O	1:A:731:TYR:O	1.99	0.80
1:D:293:SER:CB	1:D:298:ARG:O	2.30	0.79
1:B:418:ASP:O	1:B:422:THR:HG23	1.82	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
2:E:92:ASN:HA	2:E:96:LEU:HD23	1.63	0.79
1:D:6:LEU:CD2	1:D:14:THR:HG21	2.12	0.79
1:D:560:LYS:CD	1:D:609:HIS:NE2	2.46	0.79
1:A:325:VAL:HG22	1:A:327:GLY:H	1.48	0.79
1:A:544:PHE:HE2	1:A:685:MET:HG2	1.42	0.79
1:A:53:ILE:HD11	1:A:58:ILE:HD12	1.62	0.79
1:D:155:TYR:CE1	1:D:209:THR:HG23	2.18	0.79
1:B:432:PRO:HG2	1:B:434:ARG:HD2	1.65	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:D:619:LEU:HD12	1:D:693:ILE:HG12	1.66	0.77
1:B:155:TYR:CZ	1:B:209:THR:HG23	2.20	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:36:VAL:HG12	1:B:77:TYR:CE2	2.20	0.77
1:B:325:VAL:HG22	1:B:327:GLY:H	1.48	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
2:F:5:PHE:CE1	2:F:24:ASN:O	2.37	0.77
1:D:432:PRO:HG2	1:D:434:ARG:HD2	1.67	0.77
1:A:544:PHE:CE2	1:A:685:MET:CG	2.62	0.76
1:C:208:PRO:CA	1:C:464:LEU:HD11	2.15	0.76
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.67	0.76
1:D:45:SER:OG	1:D:61:THR:HG22	1.84	0.76
1:C:432:PRO:HG2	1:C:434:ARG:HH11	1.51	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
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
2:E:5:PHE:CE1	2:E:24:ASN:CB	2.69	0.76
1:C:51:ASP:OD1	1:C:51:ASP:O	2.04	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
2:E:5:PHE:CD1	2:E:24:ASN:CB	2.57	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:53:ILE:HG13	1:D:58:ILE:HD11	1.69	0.75
1:D:463:THR:HG22	1:D:489:LEU:HD22	1.68	0.75
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.69	0.75
1:D:249:SER:CB	1:D:292:CYS:SG	2.75	0.75
1:A:293:SER:CB	1:A:298:ARG:O	2.34	0.75
1:D:53:ILE:CG1	1:D:58:ILE:HD11	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:PHE:CZ	2:F:104:LEU:HD21	2.22	0.74
1:B:234:LEU:N	3:B:900:DTP:H3'	2.02	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:619:LEU:HD12	1:A:693:ILE:HG12	1.69	0.74
1:A:55:THR:C	1:A:58:ILE:HG12	2.07	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:D:7:VAL:HG22	1:D:17:ILE:CG1	2.17	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: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:C:465:SER:HB2	1:C:515:ILE:HG12	1.69	0.73
1:B:125:GLU:HG2	1:B:129:LYS:HE2	1.68	0.73
1:C:225:CYS:H	1:C:462:CYS:HB2	1.53	0.73
1:A:719:LEU:HD22	2:F:375:LEU:HD21	1.70	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:689:ILE:HG22	1:D:691:GLN:H	1.54	0.72
1:D:6:LEU:HA	1:D:14:THR:HG22	1.70	0.72
1:D:556:ASN:HD21	1:D:609:HIS:HB2	1.54	0.72
1:D:430:ILE:HG21	1:D:570:GLU:CG	2.19	0.72
1:C:45:SER:OG	1:C:61:THR:HG22	1.89	0.72
1:B:543:THR:O	1:B:547:ILE:HG13	1.90	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:D:40:GLN:OE1	2:E:334:TRP:HD1	1.69	0.72
1:D:678:TYR:OH	1:D:695:ALA:HB1	1.90	0.72
2:G:18:PHE:CZ	2:G:104:LEU:HD21	2.24	0.72
1:C:234:LEU:HB3	1:D:246:LYS:HZ3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.71	0.72
1:C:293:SER:HB2	1:C:296:GLY:HA2	1.72	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:D:268:ILE:HD11	1:D:275:HIS:HA	1.71	0.71
1:B:685:MET:O	1:B:689:ILE:HG12	1.90	0.71
2:E:69:GLU:HG2	2:E:296:MET:HG3	1.72	0.71
1:D:157:VAL:HG23	1:D:167:GLU:OE2	1.90	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:560:LYS:CD	1:D:609:HIS:CE1	2.72	0.71
1:D:430:ILE:CG2	1:D:570:GLU:HG2	2.20	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:D:514:GLY:CA	1:D:618:ALA:CB	2.66	0.70
1:D:464:LEU:HA	1:D:514:GLY:O	1.91	0.70
1:D:441:GLU:HG3	1:D:620:MET:HB3	1.72	0.70
1:C:297:VAL:HG12	1:C:297:VAL:O	1.92	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: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
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
2:H:18:PHE:CZ	2:H:104:LEU:HD21	2.27	0.70
1:A:185:PRO:HB2	1:A:187:GLU:HG2	1.74	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
3:A:800:DTP:H5'2	3:A:800:DTP:C8	2.22	0.69
1:D:551:LEU:C	1:D:616:LEU:HD13	2.12	0.69
1:A:407:ALA:HA	1:A:732:GLN:OE1	1.91	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:D:287:THR:O	1:D:291:SER:HB3	1.93	0.69
1:C:196:PHE:HD1	1:C:484:LEU:HB3	1.57	0.69
1:D:430:ILE:HG21	1:D:570:GLU:CB	2.23	0.69
1:A:317:LEU:HD23	1:A:401:LEU:HD23	1.73	0.69
2:G:90:SER:HB2	2:G:91:PRO:HD3	1.74	0.69
2:H:90:SER:HB2	2:H:91:PRO:HD3	1.74	0.69
2:H:218:PHE:CZ	2:H:296:MET:SD	2.85	0.69
1:C:186:ARG:HH21	1:C:189:ARG:HH22	1.41	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:H:311:ILE:HG23	2:H:312:THR:H	1.56	0.69
2:G:69:GLU:HG2	2:G:296:MET:HG3	1.72	0.69
1:C:370:ALA:HA	1:C:428:PRO:HB2	1.74	0.69
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.75	0.69
1:A:41:VAL:HG22	1:A:69:LEU:HD12	1.74	0.69
1:C:520:PHE:O	1:C:523:TYR:N	2.25	0.69
1:B:407:ALA:HA	1:B:732:GLN:OE1	1.93	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:H:221:ARG:HH12	2:H:296:MET:HG2	1.58	0.68
2:G:307:TYR:HA	2:G:331:PRO:HG3	1.75	0.68
1:D:40:GLN:O	1:D:44:ARG:HG2	1.92	0.68
1:B:19:LEU:HA	1:B:22:ILE:HD12	1.76	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
2:H:5:PHE:HE1	2:H:24:ASN:O	1.76	0.68
1:D:320:LYS:HB3	1:D:409:THR:HG21	1.76	0.68
1:C:10:ARG:HD2	1:C:91:LYS:HE2	1.75	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:D:301:ALA:O	1:D:438:LEU:CD1	2.42	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:A:55:THR:O	1:A:58:ILE:HG12	1.92	0.68
1:A:292:CYS:HA	1:B:276:THR:HG21	1.74	0.68
1:D:185:PRO:HB2	1:D:187:GLU:HG2	1.76	0.68
2:G:311:ILE:HG23	2:G:312:THR:H	1.57	0.67
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
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
2:F:5:PHE:HE1	2:F:24:ASN:O	1.77	0.67
1:C:234:LEU:HB3	1:D:246:LYS:NZ	2.08	0.67
1:A:521:ALA:HB3	1:A:632:THR:HG21	1.75	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: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:332:HIS:O	1:B:333:MET:HG2	1.95	0.67
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:B:307:PRO:HG2	1:B:310:HIS:HB2	1.77	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:58:ILE:HG21	3:B:800:DTP:H1'	1.77	0.66
1:B:585:LYS:HD3	1:B:585:LYS:H	1.60	0.66
1:D:618:ALA:O	1:D:620:MET:HE1	1.95	0.66
1:C:689:ILE:HG22	1:C:691:GLN:N	2.10	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
2:H:307:TYR:HA	2:H:331:PRO:HG3	1.76	0.66
1:B:294:GLN:O	1:B:296:GLY:N	2.25	0.66
1:B:321:ASN:ND2	1:B:323:ARG:O	2.28	0.66
1:D:560:LYS:CG	1:D:609:HIS:CD2	2.78	0.66
1:B:442:ILE:CD1	1:B:691:GLN:OE1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:PRO:HB2	1:C:434:ARG:CG	2.26	0.66
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:A:53:ILE:HD11	1:A:58:ILE:HD11	1.73	0.66
1:D:516:GLY:HA2	1:D:619:LEU:HD23	1.78	0.66
1:B:40:GLN:O	1:B:44:ARG:CG	2.42	0.66
3:B:800:DTP:H5'1	3:B:800:DTP:O2B	1.96	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
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:A:40:GLN:HE22	2:F:334:TRP:N	1.95	0.65
1:D:10:ARG:HD2	1:D:91:LYS:HE2	1.75	0.65
1:C:154:LYS:HG2	1:C:155:TYR:HD1	1.62	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: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:C:7:VAL:CG2	1:C:17:ILE:CG1	2.75	0.65
1:D:489:LEU:HB3	1:D:513:LEU:HD22	1.77	0.65
1:A:206:SER:OG	1:A:625:SER:HB3	1.96	0.65
1:C:208:PRO:HD3	1:C:464:LEU:CD1	2.26	0.65
1:D:560:LYS:HG2	1:D:609:HIS:CG	2.31	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:C:33:LEU:HD13	1:C:80:LEU:HB2	1.77	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:D:427:ASP:OD1	1:D:428:PRO:CD	2.40	0.65
1:C:320:LYS:HB3	1:C:409:THR:HG21	1.77	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:H:171:GLY:O	2:H:184:VAL:HG11	1.97	0.64
2:F:203:LEU:HG	2:F:207:ARG:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:ILE:CG2	1:D:570:GLU:CG	2.76	0.64
1:C:281:PHE:CZ	3:C:900:DTP:H2'1	2.31	0.64
1:A:585:LYS:H	1:A:585:LYS:HD3	1.61	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
2:E:307:TYR:O	2:E:311:ILE:HG22	1.98	0.64
1:B:206:SER:OG	1:B:625:SER:HB3	1.97	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
1:A:307:PRO:HG2	1:A:310:HIS:HB2	1.78	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:C:284:HIS:HA	1:D:287:THR:HB	1.79	0.64
1:A:260:ARG:NH1	1:A:448:PRO:HG3	2.13	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: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:B:34:HIS:O	1:B:35:ASN:HB3	1.98	0.63
1:D:233:SER:HA	3:D:900:DTP:C5'	2.29	0.63
1:B:618:ALA:CB	1:B:691:GLN:CB	2.77	0.63
1:B:294:GLN:C	1:B:296:GLY:H	2.02	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
1:B:712:GLN:HE22	2:H:370:LEU:HG	1.64	0.63
2:E:12:GLN:NE2	2:E:23:VAL:HG13	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ALA:HA	1:D:428:PRO:HB2	1.81	0.62
2:G:99:ILE:HD13	2:G:105:GLU:HA	1.81	0.62
1:C:215:VAL:O	1:C:216:ARG:CD	2.47	0.62
2:E:76:ASN:HD21	2:E:211:SER:HA	1.62	0.62
1:C:227:LEU:CB	1:C:435:GLN:NE2	2.59	0.62
1:A:151:LEU:HD23	1:A:155:TYR:CG	2.34	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
2:E:218:PHE:CZ	2:E:296:MET:SD	2.93	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: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:C:465:SER:O	1:C:516:GLY:N	2.23	0.62
1:A:723:LYS:HG3	2:F:375:LEU:OXT	2.00	0.62
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.81	0.62
1:D:249:SER:HB3	1:D:292:CYS:SG	2.39	0.62
1:A:463:THR:HG23	1:A:492:LEU:CD2	2.27	0.62
2:H:83:LEU:HD22	2:H:203:LEU:HD21	1.81	0.62
1:A:150:GLN:O	1:A:154:LYS:HG3	1.99	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
2:E:198:MET:SD	2:E:249:LEU:HD13	2.39	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
2:F:218:PHE:CZ	2:F:296:MET:SD	2.93	0.61
2:E:207:ARG:HH22	2:E:282:GLN:NE2	1.99	0.61
2:G:83:LEU:HD22	2:G:203:LEU:HD21	1.82	0.61
1:A:474:ASN:H	1:A:474:ASN:HD22	1.48	0.61
1:D:694:SER:O	1:D:696:ASN:ND2	2.33	0.61
1:C:125:GLU:HG2	1:C:129:LYS:HE2	1.82	0.61
1:C:246:LYS:HZ3	1:D:234:LEU:C	2.02	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
2:E:311:ILE:HG23	2:E:312:THR:N	2.16	0.61
2:H:203:LEU:HG	2:H:207:ARG:HD2	1.81	0.61
1:A:224:SER:O	1:A:252:ALA:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:TYR:HE1	1:C:578:LEU:HD23	1.65	0.61
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
1:D:189:ARG:HH11	1:D:189:ARG:CG	2.13	0.61
1:D:53:ILE:CD1	1:D:58:ILE:HD11	2.31	0.61
1:C:276:THR:O	1:D:294:GLN:HG3	2.00	0.61
2:H:49:ARG:O	2:H:52:GLU:HG2	2.01	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:B:221:GLN:NE2	1:B:250:GLN:HG2	2.16	0.61
1:A:215:VAL:O	1:A:216:ARG:CG	2.49	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:154:LYS:HA	1:A:160:ARG:HH22	1.64	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
2:H:74:ILE:HG13	2:H:78:LYS:HE3	1.81	0.61
1:D:669:LEU:HD11	1:D:698:ASN:ND2	2.15	0.61
1:A:221:GLN:NE2	1:A:250:GLN:HG2	2.16	0.61
1:B:18:ASN:O	3:B:800:DTP:H2	2.01	0.61
1:B:6:LEU:HD12	1:B:51:ASP:CB	2.30	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
2:F:118:HIS:CE1	2:F:234:ILE:HG23	2.35	0.61
1:B:319:LEU:O	1:B:329:ARG:HD2	2.00	0.61
1:D:15:GLU:HG2	3:D:800:DTP:N6	2.16	0.61
1:A:55:THR:HA	1:A:58:ILE:HG13	1.80	0.61
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: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
1:B:36:VAL:CG1	1:B:77:TYR:CE2	2.85	0.60
2:H:53:VAL:HG11	2:H:230:ILE:HG13	1.83	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
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:C:619:LEU:CD1	1:C:693:ILE:HD13	2.31	0.60
1:C:115:TYR:HA	1:C:216:ARG:O	2.02	0.60
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:SER:HB3	1:C:515:ILE:HG12	1.83	0.60
1:A:209:THR:N	1:A: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
1:B:209:THR:N	1:B:210:PRO:HD2	2.17	0.60
2:G:53:VAL:HG11	2:G:230:ILE:HG13	1.83	0.60
2:F:91:PRO:HB2	2:F:112:ALA:HB2	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
2:G:98:LEU:HD21	2:G:164:THR:HG23	1.83	0.60
1:A:68:ASP:HA	1:A:653:ARG:NH1	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
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
1:C:294:GLN:HB2	1:C:298:ARG:HD2	1.83	0.59
1:D:670:TRP:CZ2	1:D:735:ARG:HB2	2.37	0.59
2:H:99:ILE:HD11	2:H:108:VAL:HG21	1.84	0.59
1:C:128:PHE:HA	1:C:131:MET:HE3	1.84	0.59
2:E:53:VAL:HG11	2:E:230:ILE:HG13	1.84	0.59
2:E:98:LEU:HD21	2:E:164:THR:HG23	1.84	0.59
1:C:407:ALA:HA	1:C:732:GLN:OE1	2.02	0.59
1:B:320:LYS:O	1:B:321:ASN:C	2.41	0.59
1:B:185:PRO:CG	1:B:188:THR:OG1	2.39	0.59
1:D:53:ILE:HD11	1:D:58:ILE:HD11	1.83	0.59
2:H:18:PHE:O	2:H:19:PHE:HB2	2.02	0.59
2:E:23:VAL:HG22	2:E:100:SER:O	2.02	0.59
1:A:53:ILE:HD12	1:A:58:ILE:CD1	2.30	0.59
1:D:301:ALA:HB1	1:D:438:LEU:CD1	2.30	0.59
1:B:689:ILE:HG22	1:B:691:GLN:O	2.01	0.59
1:A:150:GLN:OE1	1:A:154:LYS:HE3	2.01	0.59
2:G:317:GLN:HB2	2:G:323:LEU:HD21	1.84	0.59
1:B:285:PHE:O	1:B:289:VAL:HG23	2.01	0.59
1:A:441:GLU:HG2	1:A:442:ILE:N	2.18	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: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
2:H:302:ASP:O	2:H:306:GLN:HG2	2.03	0.59
1:D:530:ARG:HH11	1:D:667:GLU:HB2	1.67	0.59
1:A:403:MET:HE2	1:A:714:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LYS:HD2	3:D:800:DTP:C2	2.32	0.59
1:C:513:LEU:HD11	1:C:613:ASN:HD21	1.65	0.59
2:E:99:ILE:HD13	2:E:105:GLU:HA	1.83	0.59
2:E:91:PRO:O	2:E:95:LEU:HB2	2.03	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:D:459:ILE:HB	1:D:503:ALA:HA	1.84	0.59
1:D:290:LYS:HE2	1:D:332:HIS:HB3	1.82	0.59
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.03	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: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
1:D:403:MET:HE2	1:D:714:LEU:HB3	1.85	0.59
2:H:57:ARG:HG2	2:H:60:ILE:HD11	1.84	0.59
2:H:92:ASN:O	2:H:96:LEU:HB2	2.03	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
1:D:55:THR:HG21	3:D:800:DTP:O1B	2.03	0.58
1:A:254:ILE:O	1:A:302:ALA:HB1	2.02	0.58
1:C:21:LYS:HB2	3:C:800:DTP:C2	2.32	0.58
1:C:189:ARG:O	1:C:193:VAL:HG23	2.03	0.58
1:D:407:ALA:HA	1:D:732:GLN:OE1	2.03	0.58
1:B:403:MET:HE2	1:B:714:LEU:HB3	1.85	0.58
1:B:8:THR:OG1	1:B:54:LYS:HA	2.03	0.58
1:B:276:THR:N	3:B:900:DTP:H2	2.16	0.58
2:E:221:ARG:HH12	2:E:296:MET:HG2	1.68	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
1:A:461:LEU:HD11	1:A:503:ALA:HB1	1.86	0.58
2:G:302:ASP:O	2:G:306:GLN:HG2	2.03	0.58
1:D:427:ASP:HB3	1:D:430:ILE:HG13	1.86	0.58
1:B:442:ILE:HG22	1:B:444:LEU:HG	1.85	0.58
1:B:215:VAL:O	1:B:216:ARG:CB	2.51	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:D:50:TYR:O	1:D:53:ILE:HG23	2.03	0.58
2:G:91:PRO:O	2:G:95:LEU:HB2	2.04	0.58
1:C:238:ASN:CG	1:D:246:LYS:HE2	2.23	0.58
2:F:311:ILE:HG23	2:F:312:THR:N	2.18	0.58
1:D:365:TYR:O	1:D:368:PHE:HB3	2.03	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:B:282:TYR:HA	1:B:285:PHE:HD2	1.69	0.58
1:C:465:SER:CB	1:C:515:ILE:HA	2.34	0.58
1:D:551:LEU:O	1:D:616:LEU:HD11	2.03	0.58
1:B:276:THR:H	3:B:900:DTP:H2	1.69	0.58
2:H:296:MET:O	2:H:299:LEU:O	2.22	0.58
1:D:196:PHE:HD1	1:D:484:LEU:HB3	1.68	0.58
2:E:101:ILE:HG13	2:E:104:LEU:HB3	1.85	0.58
1:C:459:ILE:HB	1:C:503:ALA:HA	1.86	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
1:C:622:SER:HB2	1:C:625:SER:CB	2.33	0.58
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.84	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:56:SER:O	1:B:60:GLU:HG2	2.04	0.58
2:F:92:ASN:O	2:F:96:LEU:HB2	2.04	0.58
2:F:99:ILE:HD11	2:F:108:VAL:HG21	1.86	0.58
1:D:62:ILE:HG13	1:D:63:ILE:N	2.19	0.58
2:H:198:MET:SD	2:H:249:LEU:HD13	2.44	0.58
1:B:42:GLU:OE1	2:H:298:GLY:HA2	2.03	0.58
1:A:10:ARG:HG3	1:A:91:LYS:HE2	1.85	0.57
1:A:62:ILE:HG13	1:A:63:ILE:N	2.18	0.57
2:E:198:MET:HG2	2:E:249:LEU:HD22	1.85	0.57
1:C:72:ARG:HG2	1:C:642:VAL:HG23	1.85	0.57
1:C:441:GLU:HA	1:C:692:SER:O	2.05	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
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:G:165:SER:O	2:G:169:LEU:HG	2.04	0.57
2:E:305:CYS:O	2:E:309:GLU:HG3	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:439:CYS:HB3	1:A:441:GLU:CD	2.23	0.57
1:D:18:ASN:HD22	1:D:21:LYS:HE3	1.69	0.57
1:A:254:ILE:O	1:A:302:ALA:CB	2.52	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:D:520:PHE:CB	1:D:635:ILE:HA	2.34	0.57
1:A:543:THR:O	1:A:547:ILE:HG13	2.04	0.57
2:G:101:ILE:HG13	2:G:104:LEU:HB3	1.86	0.57
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.87	0.57
2:F:57:ARG:HG2	2:F:60:ILE:HD11	1.87	0.57
1:D:227:LEU:HB3	1:D:435:GLN:NE2	2.20	0.57
1:C:619:LEU:HD13	1:C:693:ILE:HD13	1.86	0.57
1:A:44:ARG:NH1	1:A:69:LEU:CD2	2.57	0.57
1:B:258:ALA:HB1	1:B:261:ILE:HD12	1.86	0.57
2:H:305:CYS:O	2:H:309:GLU:HG3	2.05	0.57
1:D:465:SER:O	1:D:515:ILE:HA	2.05	0.57
1:B:101:ALA:HB3	1:B:104:ASP:OD2	2.04	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: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
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.87	0.57
2:G:207:ARG:HH22	2:G:282:GLN:NE2	2.03	0.57
1:D:128:PHE:HA	1:D:131:MET:HE3	1.86	0.57
2:G:160:LEU:HD21	2:G:193:LEU:HD22	1.87	0.57
1:A:101:ALA:HB3	1:A:104:ASP:OD2	2.05	0.57
2:E:3:THR:OG1	2:E:5:PHE:O	2.20	0.57
1:D:18:ASN:H	3:D:800:DTP:H2	1.68	0.57
1:D:441:GLU:HA	1:D:692:SER:O	2.05	0.57
1:B:439:CYS:O	1:B:440:LEU:HB2	2.03	0.57
1:B:369:PHE:O	1:B:421:ASN:CG	2.43	0.57
1:C:44:ARG:NE	1:C:44:ARG:HA	2.20	0.57
2:F:197:LEU:HB2	2:F:249:LEU:HD21	1.87	0.57
2:E:245:THR:HA	2:E:248:MET:HE3	1.86	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
2:E:296:MET:O	2:E:299:LEU:O	2.23	0.57
2:G:221:ARG:HH12	2:G:296:MET:HG2	1.69	0.57
1:A:234:LEU:HG	3:A:900:DTP:H2'2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LEU:HB3	2:G:371:SER:HA	1.85	0.57
1:A:439:CYS:CB	1:A:441:GLU:CD	2.74	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: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:D:209:THR:N	1:D:210:PRO:HD2	2.20	0.56
2:F:296:MET:O	2:F:299:LEU:O	2.23	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
1:D:341:LYS:HG2	1:D:722:TYR:OH	2.03	0.56
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.86	0.56
1:D:621:PRO:HD3	1:D:694:SER:CB	2.35	0.56
1:B:441:GLU:O	1:B:692:SER:O	2.24	0.56
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.86	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
1:B:317:LEU:O	1:B:405:GLU:HG3	2.06	0.56
2:G:305:CYS:O	2:G:309:GLU:HG3	2.05	0.56
2:H:160:LEU:HD21	2:H:193:LEU:HD22	1.87	0.56
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.87	0.56
1:A:173:TYR:CZ	1:A:201:SER:HA	2.40	0.56
1:C:93:ALA:HB1	1:C:166:TYR:O	2.05	0.56
1:A:21:LYS:O	1:A:25:VAL:HG23	2.05	0.56
2:G:92:ASN:O	2:G:96:LEU:HB2	2.05	0.56
2:F:311:ILE:HD11	2:F:315:ARG:HE	1.69	0.56
1:C:529:LYS:HB3	1:C:536:ALA:HB2	1.88	0.56
2:F:198:MET:HG2	2:F:249:LEU:HD22	1.87	0.56
1:B:62:ILE:HG13	1:B:63:ILE:N	2.19	0.56
2:H:317:GLN:HB2	2:H:323:LEU:HD21	1.87	0.56
1:C:639:ARG:HH22	1:C:733:ASN:HB3	1.71	0.56
1:A:19:LEU:HA	1:A:22:ILE:CD1	2.36	0.56
1:C:467:PHE:HB2	1:C:517:VAL:HG12	1.86	0.56
1:C:7:VAL:HG22	1:C:17:ILE:CG1	2.34	0.56
2:F:91:PRO:O	2:F:95:LEU:HB2	2.06	0.56
1:B:231:GLY:HA2	1:B:260:ARG:HD3	1.87	0.56
1:A:215:VAL:O	1:A:216:ARG:HG2	2.05	0.56
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.88	0.56
2:G:304:LEU:O	2:G:308:VAL:HG23	2.06	0.56
1:C:21:LYS:HD2	3:C:800:DTP:C6	2.35	0.56
1:A:320:LYS:HB3	1:A:409:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:GLN:HE21	2:E:23:VAL:HG13	1.69	0.56
1:C:530:ARG:NH1	1:C:667:GLU:HB2	2.20	0.56
2:H:255:GLY:CA	2:H:262:ALA:HB2	2.36	0.56
1:B:68:ASP:HA	1:B:653:ARG:NH1	2.21	0.56
1:D:39:SER:O	1:D:43:LEU:HG	2.06	0.56
2:E:91:PRO:HB2	2:E:112:ALA:HB2	1.87	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
1:A:217:THR:OG1	1:A:219:THR:HG22	2.06	0.56
1:A:439:CYS:SG	1:A:621:PRO:CD	2.92	0.56
1:D:430:ILE:CG2	1:D:570:GLU:CB	2.83	0.56
1:B:154:LYS:HA	1:B:160:ARG:NH2	2.16	0.56
1:C:154:LYS:HG2	1:C:155:TYR:CD1	2.41	0.56
1:B:229:GLU:HG3	1:B:257:ASN:ND2	2.20	0.56
1:A:215:VAL:O	1:A:216:ARG:CB	2.53	0.56
2:H:198:MET:HG2	2:H:249:LEU:HD22	1.87	0.56
1:B:106:VAL:O	1:B:110:VAL:HG23	2.05	0.56
1:D:639:ARG:HH22	1:D:733:ASN:HB3	1.71	0.56
1:B:173:TYR:CE2	1:B:201:SER:HA	2.41	0.56
1:C:154:LYS:HA	1:C:160:ARG:HH22	1.71	0.56
2:F:165:SER:O	2:F:169:LEU:HG	2.06	0.56
1:C:215:VAL:O	1:C:216:ARG:HG2	2.06	0.56
2:G:198:MET:SD	2:G:249:LEU:HD13	2.46	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
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:B:233:SER:C	3:B:900:DTP:H3'	2.26	0.55
2:E:49:ARG:HH12	2:F:45:SER:HB3	1.72	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
1:A:618:ALA:HA	1:A:689:ILE:CG2	2.36	0.55
1:D:18:ASN:H	3:D:800:DTP:C2	2.19	0.55
1:D:44:ARG:HE	1:D:44:ARG:HA	1.71	0.55
1:D:189:ARG:HH11	1:D:189:ARG:HG2	1.70	0.55
1:B:10:ARG:HE	1:B:91:LYS:NZ	2.03	0.55
1:A:670:TRP:CE2	1:A:735:ARG:HB2	2.41	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:C:719:LEU:HB3	2:G:373:PHE:CD2	2.40	0.55
2:E:92:ASN:O	2:E:96:LEU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:LEU:O	2:H:99:ILE:HG13	2.06	0.55
1:B:469:LEU:HD12	1:B:520:PHE:HA	1.87	0.55
2:F:330:ASN:HB3	2:F:333:PRO:HG3	1.88	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:D:530:ARG:NH1	1:D:667:GLU:HB2	2.22	0.55
1:B:463:THR:HG23	1:B:492:LEU:HD23	1.88	0.55
2:E:57:ARG:HG2	2:E:60:ILE:HD11	1.87	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
2:E:99:ILE:HD11	2:E:108:VAL:HG21	1.87	0.55
2:H:91:PRO:HB2	2:H:112:ALA:HB2	1.87	0.55
1:C:520:PHE:CB	1:C:635:ILE:HA	2.36	0.55
1:A:282:TYR:HA	1:A:285:PHE:HD2	1.71	0.55
1:D:530:ARG:HB2	1:D:533:ASP:OD2	2.07	0.55
1:D:106:VAL:O	1:D:110:VAL:HG23	2.06	0.55
1:B:173:TYR:CZ	1:B:201:SER:HA	2.42	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:98:LEU:HD21	2:H:164:THR:HG23	1.87	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
1:A:173:TYR:CE2	1:A:201:SER:HA	2.42	0.55
2:G:255:GLY:CA	2:G:262:ALA:HB2	2.37	0.55
1:B:254:ILE:O	1:B:302:ALA:HA	2.07	0.55
1:A:181:PHE:O	1:A:189:ARG:HD2	2.07	0.55
1:D:685:MET:O	1:D:689:ILE:HG12	2.07	0.55
1:A:185:PRO:HB2	1:A:187:GLU:CG	2.37	0.55
2:G:8:THR:HG22	2:G:9:LYS:N	2.22	0.55
1:A:278:CYS:HB3	1:A:282:TYR:CE1	2.41	0.55
2:G:49:ARG:HH12	2:H:45:SER:HB3	1.72	0.55
1:B:45:SER:OG	1:B:61:THR:HG22	2.06	0.55
1:B:6:LEU:O	1:B:53:ILE:HG22	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:C:106:VAL:O	1:C:110:VAL:HG23	2.07	0.55
1:B:102:LEU:HD23	1:B:128:PHE:O	2.07	0.55
1:D:40:GLN:O	1:D:44:ARG:N	2.38	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:O	1:B:618:ALA:O	2.24	0.55
1:B:403:MET:CE	1:B:714:LEU:HB3	2.36	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
1:A:242:SER:HB3	1:B:238:ASN:HB3	1.89	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:106:VAL:O	1:A:110:VAL:HG23	2.07	0.55
1:C:432:PRO:HG2	1:C:434:ARG:NH1	2.21	0.54
1:C:619:LEU:CD1	1:C:693:ILE:HG12	2.37	0.54
1:A:10:ARG:HH22	1:A:88:HIS:CE1	2.26	0.54
1:D:560:LYS:HD3	1:D:609:HIS:CD2	2.41	0.54
1:D:529:LYS:HB3	1:D:536:ALA:HB2	1.88	0.54
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.89	0.54
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.88	0.54
1:A:244:ILE:HG12	1:A:254:ILE:HG21	1.90	0.54
1:D:430:ILE:CD1	1:D:570:GLU:HA	2.37	0.54
1:B:21:LYS:O	1:B:25:VAL:HG23	2.07	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:B:403:MET:HB2	1:B:711:MET:HE1	1.89	0.54
1:D:678:TYR:OH	1:D:695:ALA:CB	2.56	0.54
2:H:306:GLN:HB3	2:H:328:ARG:NH1	2.22	0.54
1:D:368:PHE:CD2	1:D:369:PHE:CZ	2.95	0.54
1:B:647:SER:HB2	1:B:652:LEU:HD11	1.89	0.54
1:B:217:THR:OG1	1:B:219:THR:HG22	2.08	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
1:D:290:LYS:CE	1:D:332:HIS:HB3	2.37	0.54
1:C:685:MET:O	1:C:689:ILE:HG12	2.07	0.54
1:C:234:LEU:C	1:D:246:LYS:HZ3	2.11	0.54
2:H:206:ILE:HG12	2:H:315:ARG:HG3	1.90	0.54
2:E:160:LEU:HD21	2:E:193:LEU:HD22	1.87	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:A:238:ASN:HB3	1:B:242:SER:HB3	1.89	0.54
2:H:165:SER:O	2:H:169:LEU:HG	2.07	0.54
1:D:425:PRO:HG2	1:D:615:THR:HG22	1.88	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:B:304:LEU:HD23	1:B:305:PHE:N	2.23	0.54
1:A:254:ILE:O	1:A:302:ALA:HA	2.07	0.54
2:F:190:LYS:HB3	2:F:261:MET:SD	2.47	0.54
1:A:229:GLU:HG3	1:A:257:ASN:ND2	2.21	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
1:B:511:ARG:HH11	1:B:511:ARG:HG2	1.73	0.54
1:B:483:ILE:O	1:B:487:ARG:HB2	2.08	0.54
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.42	0.54
1:A:483:ILE:O	1:A:487:ARG:HB2	2.08	0.54
2:G:141:VAL:HG11	2:H:9:LYS:HA	1.90	0.54
1:C:208:PRO:CD	1:C:464:LEU:CD1	2.85	0.54
1:A:228:ILE:HG21	1:A:240:THR:HG23	1.90	0.54
1:D:233:SER:HA	3:D:900:DTP:O5'	2.08	0.54
1:A:231:GLY:HA2	1:A:260:ARG:HD3	1.90	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
2:G:306:GLN:HB3	2:G:328:ARG:NH1	2.23	0.54
1:A:321:ASN:ND2	1:A:323:ARG:O	2.41	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
1:D:545:GLU:OE1	1:D:595:LEU:HA	2.08	0.54
2:F:227:ASN:O	2:F:231:ILE:HG12	2.08	0.54
1:D:18:ASN:N	3:D:800:DTP:H2	2.22	0.54
1:D:151:LEU:HA	1:D:155:TYR:HB2	1.90	0.54
2:G:273:TYR:O	2:G:277:VAL:HG23	2.08	0.54
2:E:129:ILE:HG13	2:E:130:VAL:HG13	1.89	0.54
1:C:565:CYS:SG	1:C:568:PHE:HB2	2.47	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
2:E:36:PHE:CZ	2:E:104:LEU:HD13	2.43	0.53
2:H:197:LEU:HB2	2:H:249:LEU:HD21	1.89	0.53
1:D:642:VAL:HG22	1:D:655:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:330:ASN:HB3	2:G:333:PRO:HG3	1.89	0.53
1:C:92:LYS:HD3	1:C:165:ILE:HD12	1.88	0.53
2:E:141:VAL:HG11	2:F:9:LYS:HA	1.89	0.53
1:A:54:LYS:HB2	1:A:57:ASP:OD2	2.07	0.53
2:H:5:PHE:CD1	2:H:24:ASN:O	2.61	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
1:A:670:TRP:CH2	1:A:735:ARG:HB2	2.43	0.53
2:F:5:PHE:CD1	2:F:24:ASN:O	2.61	0.53
1:B:542:LYS:HG3	1:B:596:HIS:CD2	2.43	0.53
2:H:273:TYR:O	2:H:277:VAL:HG23	2.08	0.53
1:D:430:ILE:HG22	1:D:570:GLU:OE1	2.09	0.53
1:A:125:GLU:O	1:A:129:LYS:HG3	2.08	0.53
2:G:8:THR:CG2	2:G:9:LYS:N	2.72	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:701:PRO:O	1:D:707:GLY:HA2	2.08	0.53
1:C:613:ASN:CG	1:C:616:LEU:HD21	2.28	0.53
1:B:418:ASP:HA	1:B:421:ASN:HD22	1.73	0.53
2:G:169:LEU:HD22	2:H:166:TYR:CE2	2.43	0.53
1:A:102:LEU:O	1:A:106:VAL:HG23	2.08	0.53
1:D:226:VAL:HG21	1:D:247:TYR:CG	2.44	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:B:517:VAL:O	1:B:634:GLY:HA2	2.09	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:A:317:LEU:O	1:A:405:GLU:HG3	2.09	0.53
1:C:403:MET:HB2	1:C:711:MET:HE3	1.90	0.53
1:A:140:ASP:OD1	1:A:169:ALA:HB3	2.09	0.53
1:B:7:VAL:HG23	1:B:17:ILE:HG12	1.89	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
1:B:137:HIS:HA	1:B:170:GLN:HG3	1.89	0.53
2:G:196:CYS:O	2:G:200:VAL:HG23	2.07	0.53
1:C:474:ASN:OD1	1:C:476:ASP:HB2	2.09	0.53
1:C:430:ILE:CG2	1:C:570:GLU:OE1	2.57	0.53
1:D:364:LEU:HD23	1:D:378:LEU:CB	2.38	0.53
1:B:102:LEU:O	1:B:106:VAL:HG23	2.09	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:92:LYS:HD3	1:D:165:ILE:HD12	1.91	0.53
1:C:226:VAL:HG21	1:C:247:TYR:CG	2.44	0.53
1:C:87:PHE:CE1	3:C:800:DTP:O2A	2.62	0.52
1:B:293:SER:CB	1:B:298:ARG:O	2.53	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:A:242:SER:HA	1:B:238:ASN:OD1	2.09	0.52
1:C:642:VAL:HG22	1:C:655:VAL:HG22	1.91	0.52
1:A:102:LEU:HD23	1:A:128:PHE:O	2.08	0.52
2:H:227:ASN:O	2:H:231:ILE:HG12	2.09	0.52
1:A:152:GLU:O	1:A:158:GLN:NE2	2.42	0.52
1:B:140:ASP:OD1	1:B:169:ALA:HB3	2.09	0.52
1:A:18:ASN:N	3:A:800:DTP:H2	2.22	0.52
2:E:206:ILE:HG12	2:E:315:ARG:HG3	1.91	0.52
1:A:276:THR:HG21	1:B:292:CYS:HA	1.90	0.52
2:E:304:LEU:O	2:E:308:VAL:HG23	2.08	0.52
1:D:21:LYS:O	1:D:25:VAL:HG23	2.08	0.52
1:D:620:MET:HB2	1:D:621:PRO:HD2	1.90	0.52
1:D:464:LEU:HD13	1:D:620:MET:HG3	1.90	0.52
1:B:125:GLU:O	1:B:129:LYS:HG3	2.08	0.52
1:C:573:TYR:CE1	1:C:578:LEU:HD23	2.44	0.52
2:F:78:LYS:HE2	2:F:136:VAL:HG13	1.91	0.52
1:D:403:MET:HB2	1:D:711:MET:HE3	1.90	0.52
1:B:140:ASP:HA	1:B:143:PHE:CE2	2.43	0.52
1:D:519:ASN:HB2	1:D:631:ALA:HB1	1.90	0.52
1:C:38:ILE:O	1:C:42:GLU:HG3	2.09	0.52
1:B:618:ALA:CB	1:B:691:GLN:HB3	2.39	0.52
1:D:510:ARG:HG2	1:D:567:TRP:CE3	2.39	0.52
1:B:286:GLN:CD	1:B:332:HIS:HB2	2.29	0.52
2:H:89:ARG:O	2:H:93:VAL:HG23	2.09	0.52
1:B:82:ALA:O	1:B:86:ILE:HG12	2.09	0.52
1:D:316:LEU:HA	1:D:319:LEU:HG	1.92	0.52
2:G:175:HIS:CD2	2:H:178:ASN:HD21	2.28	0.52
1:C:432:PRO:CG	1:C:434:ARG:NH1	2.72	0.52
2:F:95:LEU:O	2:F:99:ILE:HG13	2.09	0.52
1:B:290:LYS:HG3	1:B:296:GLY:O	2.09	0.52
2:F:198:MET:SD	2:F:249:LEU:HD13	2.50	0.52
1:C:317:LEU:HD23	1:C:401:LEU:HD23	1.90	0.52
1:C:464:LEU:HD12	1:C:464:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HE	1:A:91:LYS:CE	2.22	0.52
1:D:189:ARG:O	1:D:193:VAL:CG2	2.49	0.52
1:B:224:SER:O	1:B:252:ALA:HA	2.10	0.52
2:G:206:ILE:HG12	2:G:315:ARG:HG3	1.92	0.52
1:D:638:PRO:O	1:D:668:LEU:HA	2.10	0.52
1:C:463:THR:CG2	1:C:489:LEU:HD22	2.35	0.52
2:E:197:LEU:HB2	2:E:249:LEU:HD21	1.90	0.52
2:G:163:MET:HB3	2:G:189:LEU:HD13	1.92	0.52
2:G:129:ILE:HG13	2:G:130:VAL:HG13	1.90	0.52
2:H:330:ASN:HB3	2:H:333:PRO:HG3	1.92	0.52
1:C:617:SER:OG	1:C:690:ASP:N	2.27	0.52
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.25	0.52
2:F:304:LEU:O	2:F:308:VAL:HG23	2.08	0.52
1:D:286:GLN:CD	1:D:332:HIS:HB2	2.29	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:C:206:SER:CA	1:C:466:ALA:HB3	2.38	0.52
1:B:303:THR:HG23	1:B:334:ASP:C	2.30	0.52
1:B:244:ILE:CG2	1:B:254:ILE:HG13	2.24	0.52
2:E:89:ARG:O	2:E:93:VAL:HG23	2.10	0.52
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.92	0.52
1:B:474:ASN:N	1:B:474:ASN:HD22	2.06	0.52
1:A:403:MET:HB2	1:A:711:MET:HE1	1.92	0.52
1:D:368:PHE:CZ	1:D:417:VAL:HG21	2.45	0.52
1:A:478:LEU:HB2	1:A:550:TYR:CD2	2.45	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: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:647:SER:HB2	1:A:652:LEU:HD11	1.92	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:C:638:PRO:O	1:C:668:LEU:HA	2.10	0.52
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.45	0.51
1:A:6:LEU:HB2	1:A:52:GLY:N	2.24	0.51
1:D:189:ARG:CG	1:D:189:ARG:NH1	2.72	0.51
1:C:364:LEU:HD23	1:C:378:LEU:CB	2.38	0.51
1:A:474:ASN:HD22	1:A:474:ASN:N	2.07	0.51
1:C:228:ILE:CG2	1:C:240:THR:HG23	2.40	0.51
1:C:131:MET:HA	1:C:134:PHE:CD2	2.44	0.51
1:A:279:ILE:HD12	1:A:319:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:HA	1:A:331:ARG:HE	1.75	0.51
1:A:517:VAL:O	1:A:634:GLY:HA2	2.10	0.51
1:C:371:ASP:HB3	1:C:374:GLU:HB3	1.93	0.51
1:C:19:LEU:HD12	2:G:295:SER:O	2.10	0.51
1:A:384:LYS:N	1:A:384:LYS:HD2	2.25	0.51
1:A:515:ILE:O	1:A:618:ALA:O	2.29	0.51
1:B:244:ILE:HG12	1:B:254: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:B:678:TYR:O	1:B:682:VAL:HG23	2.10	0.51
1:D:293:SER:HB2	1:D:298:ARG:O	2.07	0.51
1:A:622:SER:HB2	1:A:625:SER:HB2	1.92	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:B:305:PHE:CZ	1:B:436:SER:HB3	2.45	0.51
1:A:59:HIS:CD2	3:A:800:DTP:H4'	2.46	0.51
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.93	0.51
2:E:258:ASP:OD1	2:E:259:PRO:HD2	2.11	0.51
1:A:219:THR:HA	1:B:269:ARG:HH22	1.74	0.51
1:D:542:LYS:HG3	1:D:596:HIS:CD2	2.45	0.51
1:D:147:ALA:CB	1:D:628:ILE:HA	2.40	0.51
1:C:426:PHE:O	1:C:572:THR:HG23	2.10	0.51
1:C:686:GLN:HG2	1:C:725:GLY:O	2.11	0.51
1:C:180:LEU:HD13	1:C:488:ALA:HB1	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:137:HIS:HA	1:A:170:GLN:HG3	1.92	0.51
1:A:44:ARG:HG3	1:A:69:LEU:HD21	1.93	0.51
1:A:247:TYR:OH	1:A:461:LEU:HD21	2.10	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
2:H:145:GLN:HG2	2:H:289:TYR:CG	2.46	0.51
1:D:305:PHE:CZ	1:D:436:SER:HB3	2.45	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:544:PHE:CE2	1:B:685:MET:HG2	2.46	0.51
1:C:513:LEU:HD12	1:C:616:LEU:CD2	2.35	0.51
1:B:119:LEU:HD21	1:B:179:CYS:SG	2.50	0.51
1:C:543:THR:O	1:C:547:ILE:HG13	2.10	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:GLN:HG2	1:B:725:GLY:O	2.11	0.51
1:A:347:LEU:O	2:F:367:THR:HG21	2.11	0.51
1:B:384:LYS:N	1:B:384:LYS:HD2	2.24	0.51
2:G:227:ASN:O	2:G:231:ILE:HG12	2.10	0.51
1:A:442:ILE:CG2	1:A:444:LEU:HG	2.40	0.51
1:B:253:GLY:C	1:B:254:ILE:HD13	2.32	0.51
1:D:560:LYS:HD3	1:D:609:HIS:ND1	2.22	0.51
1:D:215:VAL:O	1:D:216:ARG:CB	2.58	0.51
1:C:151:LEU:HG	1:C:628:ILE:HD12	1.93	0.51
1:D:293:SER:HB3	1:D:298:ARG:O	2.09	0.51
2:F:36:PHE:CZ	2:F:104:LEU:HD13	2.45	0.51
2:E:311:ILE:HD11	2:E:315:ARG:HE	1.75	0.51
1:A:469:LEU:HB3	1:A:523:TYR:CD1	2.45	0.51
1:B:643:SER:C	1:B:644:ILE:HD12	2.32	0.51
1:A:421:ASN:HB3	1:A:428:PRO:HB3	1.93	0.51
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.92	0.51
1:B:553:LYS:O	1:B:557:GLU:HG2	2.10	0.51
1:A:8:THR:HG21	1:A:54:LYS:HG2	1.93	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: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:H:332:ILE:HB	2:H:334:TRP:NE1	2.26	0.51
1:D:131:MET:HA	1:D:134:PHE:CD2	2.45	0.51
1:A:606:ILE:HG23	1:A:611:LEU:HG	1.92	0.51
1:C:136:ASP:HB3	1:C:139:ARG:NE	2.25	0.51
1:B:247:TYR:OH	1:B:461:LEU:HD21	2.10	0.51
1:C:208:PRO:CD	1:C:464:LEU:HD11	2.41	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:A:19:LEU:CD1	2:F:295:SER:O	2.59	0.50
1:C:515:ILE:HD12	1:C:551:LEU:HD22	1.92	0.50
2:G:175:HIS:HD2	2:H:178:ASN:HD21	1.59	0.50
1:D:474:ASN:OD1	1:D:476:ASP:HB2	2.12	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:D:180:LEU:HD13	1:D:488:ALA:HB1	1.92	0.50
1:A:50:TYR:H	1:A:53:ILE:HG21	1.75	0.50
1:A:320:LYS:CD	1:A:411:ARG:HB2	2.40	0.50
1:D:148:VAL:HA	1:D:151:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:311:ILE:HD11	2:H:315:ARG:HE	1.76	0.50
2:F:74:ILE:O	2:F:78:LYS:HG3	2.11	0.50
1:A:276:THR:HB	3:A:900:DTP:H2	1.93	0.50
1:A:46:HIS:HE1	2:F:220:GLU:O	1.94	0.50
1:C:293:SER:CB	1:C:298:ARG:O	2.59	0.50
2:G:311:ILE:HD11	2:G:315:ARG:HE	1.75	0.50
1:C:286:GLN:CD	1:C:332:HIS:HB2	2.31	0.50
1:B:680:GLN:O	1:B:684:ILE:HG13	2.11	0.50
2:E:178:ASN:HD21	2:F:175:HIS:CD2	2.29	0.50
1:A:686:GLN:HG2	1:A:725:GLY:O	2.10	0.50
2:F:129:ILE:HG13	2:F:130:VAL:HG13	1.92	0.50
1:A:441:GLU:OE1	1:A:620:MET:CB	2.54	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
1:C:55:THR:HB	3:C:800:DTP:H8	1.92	0.50
1:C:313:VAL:HG13	1:C:314:GLU:N	2.26	0.50
1:A:196:PHE:O	1:A:200:VAL:HG22	2.11	0.50
2:H:163:MET:HB3	2:H:189:LEU:HD13	1.93	0.50
1:C:430:ILE:HG22	1:C:431:ALA:N	2.26	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
1:D:313:VAL:HG13	1:D:314:GLU:N	2.27	0.50
2:H:304:LEU:O	2:H:308:VAL:HG23	2.11	0.50
1:B:103:TYR:O	1:B:107:VAL:HG23	2.12	0.50
1:A:227:LEU:CA	1:A:435:GLN:NE2	2.73	0.50
1:B:53:ILE:HG23	1:B:53:ILE:O	2.11	0.50
2:G:36:PHE:CZ	2:G:104:LEU:HD13	2.47	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
1:A:618:ALA:HB2	1:A:691:GLN:CB	2.32	0.50
1:D:55:THR:OG1	3:D:800:DTP:H5'1	2.11	0.50
1:A:151:LEU:HD23	1:A:155:TYR:CD2	2.47	0.50
1:D:368:PHE:HD2	1:D:369:PHE:CZ	2.29	0.50
1:D:135:ILE:HD11	1:D:174:ILE:HG21	1.93	0.50
1:A:82:ALA:O	1:A:86:ILE:HG12	2.10	0.50
1:C:619:LEU:CD1	1:C:693:ILE:CD1	2.90	0.50
2:E:255:GLY:CA	2:E:258:ASP:O	2.57	0.50
1:B:469:LEU:HB3	1:B:523:TYR:CD1	2.46	0.50
1:A:680:GLN:O	1:A:684:ILE:HG13	2.11	0.50
1:C:656:VAL:HG23	1:C:659:TYR:HB2	1.94	0.50
1:C:303:THR:HG21	1:C:440:LEU:HD21	1.94	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
2:E:23:VAL:HG22	2:E:100:SER:C	2.32	0.50
1:A:153:GLY:O	1:A:160:ARG:NH1	2.45	0.50
2:G:160:LEU:HD21	2:G:193:LEU:CD2	2.41	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
1:B:35:ASN:O	1:B:35:ASN:CG	2.50	0.49
2:E:74:ILE:O	2:E:78:LYS:HG3	2.11	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:H:147:GLN:O	2:H:151:GLU:N	2.46	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
1:C:619:LEU:CD1	1:C:693:ILE:HG23	2.32	0.49
1:A:463:THR:CG2	1:A:492:LEU:CD2	2.78	0.49
1:D:33:LEU:HD22	1:D:76:ASP:HB3	1.93	0.49
1:A:224:SER:O	1:A:252:ALA:CA	2.60	0.49
2:H:78:LYS:HE2	2:H:136:VAL:HG13	1.93	0.49
1:C:348:LEU:O	2:G:371:SER:HB3	2.12	0.49
1:A:254:ILE:O	1:A:302:ALA:CA	2.60	0.49
1:D:514:GLY:HA2	1:D:618:ALA:HB2	1.91	0.49
1:C:276:THR:CB	3:C:900:DTP:H2	2.39	0.49
1:D:681:LEU:O	1:D:685:MET:HG3	2.13	0.49
1:A:247:TYR:CZ	1:A:461:LEU:HD21	2.47	0.49
1:D:227:LEU:HD23	1:D:435:GLN:HG3	1.93	0.49
1:D:519:ASN:HA	1:D:632:THR:H	1.77	0.49
1:A:103:TYR:O	1:A:107:VAL:HG23	2.13	0.49
1:A:227:LEU:CB	1:A:435:GLN:HE21	2.17	0.49
1:A:228:ILE:CG2	1:A:240:THR:HG23	2.42	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: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:A:669:LEU:HD11	1:A:698:ASN:ND2	2.28	0.49
1:A:40:GLN:HE22	2:F:334:TRP:H	1.60	0.49
1:D:54:LYS:O	1:D:58:ILE:HG12	2.13	0.49
1:D:114:LYS:HE2	1:D:166:TYR:CE2	2.47	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
2:G:332:ILE:HB	2:G:334:TRP:NE1	2.28	0.49
1:D:433:VAL:HG11	1:D:443:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PHE:O	1:B:200:VAL:HG22	2.12	0.49
1:B:478:LEU:HB2	1:B:550:TYR:CD2	2.47	0.49
1:C:469:LEU:HB3	1:C:523:TYR:CD1	2.47	0.49
1:B:696:ASN:N	1:B:696:ASN:HD22	2.11	0.49
1:A:552:LEU:HB3	1:A:602:LEU:HD21	1.93	0.49
1:C:342:LEU:HD21	1:C:379:TYR:CD2	2.47	0.49
1:C:154:LYS:CG	1:C:155:TYR:CD1	2.96	0.49
2:E:160:LEU:HD21	2:E:193:LEU:CD2	2.43	0.49
1:D:135:ILE:HA	1:D:197:TYR:CZ	2.47	0.49
1:C:583:TYR:HD2	1:C:587:LEU:HD12	1.77	0.49
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.48	0.49
1:B:520:PHE:CB	1:B:635:ILE:HA	2.43	0.49
1:A:520:PHE:CB	1:A:635:ILE:HA	2.43	0.49
1:D:368:PHE:HD2	1:D:369:PHE:CE1	2.31	0.49
1:A:238:ASN:OD1	1:B:242:SER:HA	2.12	0.49
1:B:107:VAL:O	1:B:111:GLU:HG3	2.11	0.49
1:C:542:LYS:HG3	1:C:596:HIS:CD2	2.46	0.49
1:B:214:GLY:O	1:B:215:VAL:C	2.50	0.49
1:B:134:PHE:HB3	1:B:194:LYS:HG3	1.95	0.49
1:A:119:LEU:HD21	1:A:179:CYS:SG	2.53	0.49
1:C:43:LEU:HD12	2:G:334:TRP:CD1	2.48	0.49
1:C:379:TYR:O	1:C:383:GLU:HG3	2.13	0.49
1:A:144:SER:O	1:A:148:VAL:HG23	2.12	0.49
2:G:155:SER:O	2:G:159:GLU:HG3	2.13	0.49
2:E:55:VAL:HG12	2:E:226:GLY:HA3	1.94	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
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:A:37:SER:HB3	1:A:40:GLN:HG2	1.93	0.49
2:H:147:GLN:NE2	2:H:147:GLN:HA	2.27	0.49
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.95	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:204:GLU:OE2	2:H:241:HIS:HB3	2.13	0.49
1:A:244:ILE:CG2	1:A:254:ILE:HG13	2.24	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
1:C:40:GLN:HG2	1:C:44:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:TYR:O	1:D:107:VAL:HG23	2.12	0.48
2:H:155:SER:O	2:H:159:GLU:HG3	2.13	0.48
1:B:361:VAL:O	1:B:364:LEU:HB2	2.13	0.48
1:D:379:TYR:O	1:D:383:GLU:HG3	2.12	0.48
1:A:151:LEU:CA	1:A:155:TYR:HB2	2.35	0.48
1:D:151:LEU:HG	1:D:628:ILE:HD12	1.94	0.48
2:H:160:LEU:HD21	2:H:193:LEU:CD2	2.42	0.48
1:D:248:VAL:HG11	1:D:289:VAL:HA	1.95	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
1:B:290:LYS:HE3	1:B:332:HIS:HB3	1.95	0.48
1:D:367:ALA:O	1:D:371:ASP:O	2.31	0.48
1:B:532:SER:HA	1:B:677:GLY:HA3	1.95	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:437:ASN:HB3	1:C:442:ILE:HB	1.93	0.48
1:D:692:SER:OG	1:D:728:THR:HG23	2.14	0.48
1:C:42:GLU:OE1	2:G:298:GLY:N	2.46	0.48
1:C:301:ALA:HB1	1:C:438:LEU:HD11	1.95	0.48
1:C:103:TYR:O	1:C:107:VAL:HG23	2.13	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: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:A:324:GLY:HA3	1:A:329:ARG:NH2	2.29	0.48
1:B:144:SER:O	1:B:148:VAL:HG23	2.14	0.48
1:D:583:TYR:HD2	1:D:587:LEU:HD12	1.77	0.48
1:A:645:LYS:NZ	1:A:645:LYS:HB2	2.29	0.48
1:A:312:GLU:O	1:A:316:LEU:HG	2.12	0.48
1:C:208:PRO:CB	1:C:464:LEU:CD1	2.60	0.48
1:B:441:GLU:HG2	1:B:442:ILE:N	2.29	0.48
2:G:74:ILE:O	2:G:78:LYS:HG3	2.14	0.48
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.95	0.48
1:B:430:ILE:HG21	1:B:570:GLU:HG2	1.94	0.48
1:C:148:VAL:HA	1:C:151:LEU:HD12	1.94	0.48
2:F:92:ASN:OD1	2:F:109:GLU:HG2	2.13	0.48
2:G:9:LYS:HD3	2:H:142:THR:HG23	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
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:245:THR:HA	2:F:248:MET:HE3	1.94	0.48
1:D:644:ILE:HA	1:D:652:LEU:O	2.14	0.48
1:D:572:THR:HB	1:D:577:ILE:HB	1.95	0.48
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.95	0.48
1:D:693:ILE:HG22	1:D:694:SER:N	2.28	0.48
1:C:86:ILE:HD11	1:C:148:VAL:HG22	1.95	0.48
2:G:92:ASN:OD1	2:G:109:GLU:HG2	2.14	0.48
1:A:696:ASN:HD22	1:A:696:ASN:N	2.11	0.48
1:C:294:GLN:CB	1:C:298:ARG:HD2	2.43	0.48
2:E:118:HIS:ND1	2:E:234:ILE:HG23	2.28	0.48
1:D:668:LEU:HB2	1:D:671:GLU:HG3	1.96	0.48
2:E:163:MET:HB3	2:E:189:LEU:HD13	1.95	0.48
1:A:383:GLU:O	1:A:390:LYS:HE2	2.14	0.48
2:G:204:GLU:OE2	2:G:241:HIS:HB3	2.14	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:A:182:SER:HA	1:A:189:ARG:HE	1.79	0.48
1:B:231:GLY:N	1:B:236:SER:OG	2.46	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:132:ASP:HA	1:A:135:ILE:HD12	1.96	0.48
1:B:312:GLU:O	1:B:316:LEU:HG	2.13	0.48
1:A:6:LEU:HB2	1:A:52:GLY:H	1.79	0.48
1:D:689:ILE:HG22	1:D:691:GLN:O	2.12	0.48
1:D:342:LEU:HD21	1:D:379:TYR:CD2	2.49	0.48
2:G:147:GLN:O	2:G:151:GLU:N	2.47	0.48
2:E:145:GLN:HG2	2:E:289:TYR:CG	2.49	0.48
1:B:19:LEU:HA	1:B:22:ILE:CD1	2.44	0.47
2:F:206:ILE:O	2:F:210:VAL:HG23	2.14	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
1:A:361:VAL:O	1:A:364:LEU:HB2	2.13	0.47
1:C:441:GLU:CA	1:C:692:SER:O	2.62	0.47
1:A:87:PHE:HE1	3:A:800:DTP:O2A	1.97	0.47
1:D:618:ALA:O	1:D:620:MET:HE3	2.12	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
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
1:C:437:ASN:O	1:C:440:LEU:HD22	2.15	0.47
1:A:107:VAL:O	1:A:111:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:204:GLU:HG2	2:G:238:GLU:OE2	2.14	0.47
2:F:55:VAL:HG12	2:F:226:GLY:HA3	1.97	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:H:102:PRO:HG2	2:H:103:GLU:OE1	2.14	0.47
2:F:145:GLN:HG2	2:F:289:TYR:CG	2.49	0.47
1:A:532:SER:HA	1:A:677:GLY:HA3	1.96	0.47
1:B:303:THR:HG23	1:B:334:ASP:O	2.14	0.47
1:D:561:GLU:HG2	1:D:562:GLN:HG3	1.96	0.47
1:C:186:ARG:HH21	1:C:189:ARG:NH2	2.08	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:C:668:LEU:HB2	1:C:671:GLU:HG3	1.96	0.47
1:A:490:ASP:CG	1:A:511:ARG:HH21	2.18	0.47
1:B:180:LEU:HD13	1:B:488:ALA:HB1	1.96	0.47
1:D:441:GLU:CA	1:D:692:SER:O	2.63	0.47
1:D:441:GLU:CB	1:D:619:LEU:O	2.59	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:C:287:THR:HB	1:D:284:HIS:ND1	2.30	0.47
1:A:231:GLY:N	1:A:236:SER:OG	2.45	0.47
1:B:181:PHE:O	1:B:189:ARG:HD2	2.15	0.47
1:A:644:ILE:HG13	1:A:653:ARG:HG2	1.95	0.47
1:C:403:MET:CE	1:C:714:LEU:HB3	2.45	0.47
1:C:285:PHE:O	1:C:289:VAL:HG23	2.15	0.47
1:C:309:TRP:O	1:C:355:LEU:HA	2.14	0.47
1:A:560:LYS:HG2	1:A:609:HIS:CB	2.44	0.47
1:C:619:LEU:CD1	1:C:693:ILE:CG1	2.93	0.47
1:D:15:GLU:HG3	1:D:16:ARG:N	2.28	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: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:A:320:LYS:HE3	1:A:411:ARG:HB3	1.96	0.47
1:C:681:LEU:O	1:C:685:MET:HG3	2.14	0.47
1:C:157:VAL:HG23	1:C:167:GLU:OE2	2.14	0.47
1:B:459:ILE:HB	1:B:503:ALA:CA	2.44	0.47
1:C:125:GLU:O	1:C:129:LYS:HG3	2.14	0.47
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.49	0.47
2:F:255:GLY:HA2	2:F:262:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ASN:CB	1:D:631:ALA:HB1	2.45	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
2:E:266:GLU:OE2	2:E:269:LYS:HD2	2.15	0.47
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.47
1:D:25:VAL:HG21	3:D:800:DTP:O3'	2.15	0.47
1:B:51:ASP:OD2	1:B:51:ASP:C	2.52	0.47
2:H:1:ALA:HB3	2:H:168:HIS:CA	2.42	0.47
1:C:567:TRP:O	1:C:569:ASN:N	2.48	0.47
1:B:309:TRP:O	1:B:355:LEU:HA	2.14	0.47
1:B:603:ARG:O	1:B:607:LYS:HB2	2.15	0.47
1:B:339:ILE:O	1:B:416:ASN:HA	2.15	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
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.50	0.47
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.95	0.47
1:B:10:ARG:HD3	1:B:55:THR:CG2	2.45	0.47
1:C:264:LEU:HD13	1:C:276:THR:O	2.15	0.47
1:C:234:LEU:HD22	1:D:246:LYS:HD3	1.96	0.47
2:H:205:ALA:HB1	2:H:315:ARG:HD2	1.97	0.47
2:G:206:ILE:O	2:G:210:VAL:HG23	2.15	0.47
1:A:431:ALA:HB1	1:A:445:PRO:CB	2.44	0.47
1:D:85:ALA:O	1:D:89:LEU:HG	2.15	0.47
2:G:48:TRP:CZ3	2:G:50:PRO:HG3	2.49	0.47
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.96	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
2:E:147:GLN:HA	2:E:147:GLN:NE2	2.30	0.46
1:A:42:GLU:O	2:F:297:ILE:CD1	2.63	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
1:B:294:GLN:C	1:B:296:GLY:N	2.69	0.46
2:H:118:HIS:ND1	2:H:234:ILE:HG23	2.30	0.46
1:B:463:THR:HG22	1:B:489:LEU:HD22	1.97	0.46
2:F:122:TYR:O	2:F:126:ILE:HG13	2.15	0.46
1:B:383:GLU:O	1:B:390:LYS:HE2	2.15	0.46
1:A:304:LEU:HB3	1:A:335:TYR:HD1	1.81	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
2:F:103:GLU:HG2	2:F:104:LEU:N	2.30	0.46
2:E:126:ILE:O	2:E:130:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASP:HA	1:B:143:PHE:CD2	2.51	0.46
1:C:617:SER:O	1:C:690:ASP:HB2	2.15	0.46
2:H:55:VAL:HG12	2:H:226:GLY:HA3	1.96	0.46
1:B:560:LYS:HG2	1:B:609:HIS:CB	2.45	0.46
1:A:180:LEU:HD13	1:A:488:ALA:HB1	1.97	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
1:D:55:THR:HG1	3:D:800:DTP:H5'1	1.80	0.46
1:D:176:VAL:HG22	1:D:215:VAL:HB	1.97	0.46
1:B:519:ASN:HA	1:B:632:THR:H	1.81	0.46
1:B:258:ALA:O	1:B:260:ARG:N	2.49	0.46
1:D:135:ILE:HG23	1:D:170:GLN:HB3	1.97	0.46
1:D:350:GLY:HA3	2:E:367:THR:HG21	1.98	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:A:394:LYS:NZ	1:A:394:LYS:HB2	2.30	0.46
1:A:253:GLY:O	1:A:254:ILE:HD13	2.16	0.46
2:F:1:ALA:HB3	2:F:168:HIS:CA	2.43	0.46
1:D:86:ILE:HD11	1:D:148:VAL:HG22	1.96	0.46
1:D:567:TRP:O	1:D:569:ASN:N	2.49	0.46
1:C:572:THR:HB	1:C:577:ILE:HB	1.97	0.46
1:D:185:PRO:HB2	1:D:187:GLU:CG	2.45	0.46
2:F:260:GLU:O	2:F:264:ILE:HG13	2.15	0.46
1:A:202:THR:OG1	1:A:204:LYS:HD3	2.15	0.46
1:B:320:LYS:CD	1:B:411:ARG:HB2	2.46	0.46
1:C:233:SER:HA	3:C:900:DTP:PA	2.56	0.46
1:D:6:LEU:O	1:D:14:THR:HG23	2.15	0.46
1:C:40:GLN:O	1:C:44:ARG:N	2.43	0.46
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.51	0.46
1:C:246:LYS:NZ	1:D:234:LEU:HB3	2.30	0.46
1:D:102:LEU:O	1:D:106:VAL:HG23	2.16	0.46
2:H:126:ILE:O	2:H:130:VAL:HG22	2.15	0.46
2:E:122:TYR:O	2:E:126:ILE:HG13	2.15	0.46
1:C:317:LEU:O	1:C:405:GLU:HG3	2.15	0.46
1:D:583:TYR:CB	1:D:687:LYS:HG3	2.46	0.46
2:F:239:ALA:O	2:F:242:LEU:HG	2.15	0.46
2:E:260:GLU:O	2:E:264:ILE:HG13	2.16	0.46
1:A:706:SER:HB2	1:A:708:LYS:CD	2.46	0.46
1:B:431:ALA:HB1	1:B:445:PRO:CB	2.46	0.46
2:E:204:GLU:OE2	2:E:241:HIS:HB3	2.16	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)
2:E:136:VAL:O	2:E:140:ILE:HG13	2.16	0.46
1:C:422:THR:O	1:C:582:THR:HB	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: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:B:172:LEU:O	1:B:176:VAL:HG23	2.16	0.46
1:A:353:ILE:HB	1:A:393:VAL:HG23	1.98	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
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
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
1:A:172:LEU:O	1:A:176:VAL:HG23	2.16	0.46
2:H:48:TRP:CZ3	2:H:50:PRO:HG3	2.51	0.46
1:C:692:SER:OG	1:C:728:THR:HG23	2.16	0.46
1:A:244:ILE:O	1:A:248:VAL:HG13	2.15	0.46
1:D:437:ASN:O	1:D:440:LEU:HD22	2.16	0.46
1:D:696:ASN:N	1:D:696:ASN:ND2	2.62	0.46
1:D:544:PHE:CE2	1:D:685:MET:HG2	2.51	0.46
2:E:255:GLY:HA2	2:E:262:ALA:HB2	1.97	0.46
1:C:520:PHE:O	1:C:523:TYR:CB	2.63	0.46
1:B:182:SER:HA	1:B:189:ARG:HE	1.80	0.46
1:C:137:HIS:HA	1:C:170:GLN:HG3	1.98	0.46
1:D:309:TRP:O	1:D:355:LEU:HA	2.15	0.46
1:C:339:ILE:HD12	1:C:414:ILE:HG23	1.98	0.46
1:B:706:SER:HB2	1:B:708:LYS:CD	2.45	0.46
1:A:357:SER:HB3	1:A:360:ASP:OD2	2.16	0.46
1:D:152:GLU:O	1:D:158:GLN:NE2	2.48	0.46
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:681:LEU:O	1:B:685:MET:HG3	2.16	0.45
1:A:41:VAL:HG22	1:A:69:LEU:CD1	2.44	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
1:D:217:THR:O	1:D:219:THR:N	2.49	0.45
2:G:118:HIS:ND1	2:G:234:ILE:HG23	2.31	0.45
1:B:511:ARG:NH1	1:B:511:ARG:HG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HG21	1:C:247:TYR:CD1	2.51	0.45
2:G:239:ALA:O	2:G:242:LEU:HG	2.16	0.45
2:H:276:PHE:HB3	2:H:316:MET:SD	2.56	0.45
2:E:46:PHE:O	2:E:48:TRP:HD1	1.99	0.45
1:A:365:TYR:O	1:A:368:PHE:HB3	2.16	0.45
2:H:260:GLU:O	2:H:264:ILE:HG13	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:A:59:HIS:NE2	3:A:800:DTP:H4'	2.30	0.45
1:C:59:HIS:CD2	3:C:800:DTP:H4'	2.50	0.45
1:B:418:ASP:HA	1:B:421:ASN:ND2	2.31	0.45
1:B:327:GLY:C	1:B:328:ASN:HD22	2.19	0.45
1:A:233:SER:OG	1:A:236:SER:HB2	2.15	0.45
1:B:619:LEU:CB	1:B:693:ILE:HG23	2.46	0.45
1:B:202:THR:OG1	1:B:204:LYS:HD3	2.17	0.45
2:F:266:GLU:OE2	2:F:269:LYS:HD2	2.17	0.45
1:D:320:LYS:HE2	1:D:333:MET:O	2.17	0.45
1:D:217:THR:O	1:D:218:PRO:C	2.55	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:D:137:HIS:HA	1:D:170:GLN:HG3	1.97	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
2:E:28:TYR:CD2	2:F:120:ARG:HA	2.51	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
2:E:103:GLU:HG2	2:E:104:LEU:N	2.31	0.45
1:A:106:VAL:HG21	1:A:128:PHE:CE1	2.52	0.45
1:C:242:SER:O	1:D:238:ASN:ND2	2.50	0.45
1:B:341:LYS:HE3	2:H:375:LEU:HB2	1.98	0.45
1:D:339:ILE:HD12	1:D:414:ILE:HG23	1.97	0.45
1:A:146:ALA:HB3	1:A:654:GLN:NE2	2.31	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
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:A:68:ASP:HA	1:A:653:ARG:HH12	1.78	0.45
2:H:266:GLU:OE2	2:H:269:LYS:HD2	2.16	0.45
1:A:430:ILE:HG21	1:A:570:GLU:HG2	1.98	0.45
1:C:613:ASN:HB2	1:C:616:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:HB3	1:C:139:ARG:HE	1.82	0.45
1:A:309:TRP:O	1:A:355:LEU:HA	2.17	0.45
2:F:204:GLU:HG2	2:F:238:GLU:OE2	2.16	0.45
1:A:43:LEU:CD2	2:F:298:GLY:HA3	2.45	0.45
2:H:92:ASN:OD1	2:H:109:GLU:HG2	2.17	0.45
1:C:544:PHE:CE2	1:C:685:MET:HG2	2.52	0.45
1:A:696:ASN:HD21	1:A:730:TYR:HB3	1.81	0.45
2:F:284:LYS:HE3	2:F:325:PHE:CE1	2.52	0.45
1:B:552:LEU:HD12	1:B:599:TRP:HZ3	1.82	0.45
2:E:34:ASP:O	2:E:38:LYS:HG3	2.17	0.45
1:A:512:THR:O	1:A:513:LEU:HD23	2.16	0.45
1:A:339:ILE:O	1:A:416:ASN:HA	2.16	0.45
1:B:342:LEU:HD23	1:B:375:PHE:HE2	1.81	0.45
2:E:239:ALA:O	2:E:242:LEU:HG	2.17	0.45
1:B:682:VAL:HA	1:B:685:MET:HE3	1.97	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
1:A:519:ASN:HA	1:A:632:THR:H	1.81	0.45
2:H:203:LEU:O	2:H:207:ARG:HB2	2.17	0.45
2:H:136:VAL:O	2:H:140:ILE:HG13	2.16	0.45
1:A:643:SER:C	1:A:644:ILE:HD12	2.37	0.45
2:G:284:LYS:HE3	2:G:325:PHE:CE1	2.52	0.45
1:C:135:ILE:HA	1:C:197:TYR:CE2	2.52	0.45
2:E:175:HIS:HD2	2:F:178:ASN:HD21	1.65	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: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
2:G:120:ARG:HA	2:H:28:TYR:CD2	2.52	0.45
1:C:98:GLU:HA	1:C:99:PRO:HD3	1.81	0.45
2:F:46:PHE:O	2:F:48:TRP:HD1	1.99	0.45
1:D:680:GLN:O	1:D:684:ILE:HG13	2.17	0.45
1:A:438:LEU:O	1:A:440:LEU:CD2	2.59	0.45
1:B:40:GLN:O	1:B:44:ARG:N	2.32	0.45
1:D:585:LYS:N	1:D:585:LYS:HD3	2.23	0.45
1:A:696:ASN:OD1	1:A:731:TYR:HB2	2.17	0.45
1:D:6:LEU:CA	1:D:14:THR:CG2	2.94	0.45
1:D:33:LEU:CD1	1:D:80:LEU:HB2	2.45	0.45
1:D:524:LEU:HD22	1:D:529:LYS:HB2	1.97	0.45
1:B:339:ILE:HG22	1:B:340:ASN:N	2.32	0.45
1:B:706:SER:HB2	1:B:708:LYS:HD2	1.99	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:59:HIS:CE1	3:A:800:DTP:O2A	2.71	0.44
1:A:134:PHE:HB3	1:A:194:LYS:HG3	1.99	0.44
2:H:103:GLU:HG2	2:H:104:LEU:N	2.32	0.44
2:G:136:VAL:O	2:G:140:ILE:HG13	2.17	0.44
2:H:365:VAL:HG12	2:H:366:ASP:N	2.30	0.44
1:D:254:ILE:HG22	1:D:255:GLY:N	2.32	0.44
1:A:140:ASP:HA	1:A:143:PHE:CD2	2.52	0.44
2:G:122:TYR:O	2:G:126:ILE:HG13	2.16	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:C:431:ALA:CB	1:C:445:PRO:HB3	2.32	0.44
1:A:682:VAL:HA	1:A:685:MET:HE3	1.98	0.44
1:B:55:THR:HA	1:B:58:ILE:HG12	1.98	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:C:240:THR:O	1:C:244:ILE:HG13	2.17	0.44
1:B:222:PHE:HD2	1:B:496:GLN:HB3	1.81	0.44
1:A:348:LEU:O	2:F:371:SER:HB3	2.17	0.44
1:C:500:ILE:HG22	1:C:502:ALA:H	1.83	0.44
1:D:585:LYS:CD	1:D:585:LYS:H	2.25	0.44
1:D:6:LEU:HB3	1:D:14:THR:CG2	2.47	0.44
1:C:167:GLU:OE2	1:C:216:ARG:NH2	2.47	0.44
2:H:284:LYS:HE3	2:H:325:PHE:CE1	2.52	0.44
1:B:63:ILE:HD13	1:B:85:ALA:HA	1.99	0.44
1:B:556:ASN:O	1:B:560:LYS:HG3	2.17	0.44
1:A:241:SER:O	1:A:245:VAL:HG23	2.18	0.44
1:D:538:ASN:HB3	1:D:593:GLU:OE1	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:188:THR:HB	1:B:192:TYR:HE2	1.82	0.44
1:D:694:SER:O	1:D:730:TYR:HB2	2.16	0.44
1:A:712:GLN:NE2	2:F:370:LEU:HG	2.21	0.44
1:A:327:GLY:C	1:A:328:ASN:HD22	2.20	0.44
1:D:348:LEU:HD22	2:E:370:LEU:O	2.18	0.44
1:A:697:THR:OG1	1:A:732:GLN:HG3	2.18	0.44
2:H:203:LEU:HA	2:H:207:ARG:HD2	1.98	0.44
2:E:284:LYS:HE3	2:E:325:PHE:CE1	2.52	0.44
1:B:479:GLU:O	1:B:483:ILE:HG13	2.18	0.44
2:F:48:TRP:CZ3	2:F:50:PRO:HG3	2.52	0.44
2:G:205:ALA:HB1	2:G:315:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:273:TYR:OH	2:H:324:PRO:HB3	2.17	0.44
1:D:226:VAL:HG21	1:D:247:TYR:CD1	2.53	0.44
1:C:307:PRO:HG2	1:C:310:HIS:HB2	2.00	0.44
2:F:204:GLU:OE2	2:F:241:HIS:HB3	2.18	0.44
1:D:75:PRO:O	1:D:78:GLN:HB2	2.18	0.44
1:A:685:MET:O	1:A:689:ILE:HG12	2.18	0.44
1:C:320:LYS:HE2	1:C:333:MET:O	2.17	0.44
1:C:254:ILE:HG22	1:C:255:GLY:N	2.32	0.44
2:G:309:GLU:HB3	2:G:325:PHE:HB3	1.99	0.44
1:B:670:TRP:CH2	1:B:735:ARG:HB2	2.53	0.44
1:D:307:PRO:HG2	1:D:310:HIS:HB2	2.00	0.44
1:A:339:ILE:HG22	1:A:340:ASN:N	2.32	0.44
1:B:320:LYS:HD2	1:B:411:ARG:HB2	2.00	0.44
1:A:46:HIS:CE1	2:F:220:GLU:O	2.71	0.44
1:C:553:LYS:HA	1:C:602:LEU:HD11	2.00	0.44
1:A:232:ASP:OD2	1:A:262:ARG:NH2	2.50	0.44
1:C:172:LEU:O	1:C:176:VAL:HG23	2.18	0.44
1:A:439:CYS:O	1:A:440:LEU:CB	2.58	0.44
1:D:441:GLU:CG	1:D:620:MET:HB3	2.46	0.44
1:C:155:TYR:OH	1:C:624:THR:HG21	2.14	0.44
2:E:206:ILE:O	2:E:210:VAL:HG23	2.17	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:A:706:SER:HB2	1:A:708:LYS:HD2	2.00	0.44
1:A:232:ASP:OD2	1:A:262:ARG:NE	2.49	0.44
2:H:149:ARG:HH21	2:H:283:GLU:CD	2.20	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
2:E:166:TYR:CE2	2:F:169:LEU:HD22	2.53	0.44
1:C:244:ILE:HG23	1:C:254:ILE:HG13	2.00	0.44
1:D:317:LEU:O	1:D:405:GLU:HG3	2.18	0.44
1:C:500:ILE:HD12	1:C:500:ILE:N	2.32	0.44
2:G:209:TYR:HA	2:G:212:PHE:CD2	2.53	0.44
1:C:538:ASN:HB3	1:C:593:GLU:OE1	2.17	0.44
2:G:266:GLU:OE2	2:G:269:LYS:HD2	2.17	0.44
1:A:510:ARG:HB3	1:A:510:ARG:HE	1.60	0.44
1:B:55:THR:HG23	1:B:56:SER:N	2.33	0.43
2:F:96:LEU:HB2	2:F:97:PRO:HD3	1.99	0.43
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:D:228:ILE:HG22	1:D:240:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:HD23	1:D:128:PHE:O	2.18	0.43
1:D:313:VAL:O	1:D:317:LEU:HB2	2.18	0.43
1:D:136:ASP:HB3	1:D:139:ARG:HE	1.82	0.43
1:D:248:VAL:C	1:D:250:GLN:H	2.22	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
1:C:640:GLY:HA2	1:C:668:LEU:HD22	2.00	0.43
2:H:209:TYR:HA	2:H:212:PHE:CD2	2.53	0.43
1:A:222:PHE:HD2	1:A:496:GLN:HB3	1.82	0.43
1:A:59:HIS:HA	1:A:62:ILE:HG12	1.99	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:96:LEU:CB	2:F:97:PRO:HD3	2.47	0.43
2:F:18:PHE:O	2:F:19:PHE:CB	2.66	0.43
2:H:206:ILE:O	2:H:210:VAL:HG23	2.18	0.43
1:B:697:THR:OG1	1:B:732:GLN:HG3	2.18	0.43
2:F:171:GLY:O	2:F:184:VAL:CG1	2.65	0.43
1:D:520:PHE:O	1:D:523:TYR:HB3	2.17	0.43
1:B:644:ILE:HA	1:B:652:LEU:O	2.18	0.43
2:H:46:PHE:O	2:H:48:TRP:HD1	2.01	0.43
1:C:75:PRO:O	1:C:78:GLN:HB2	2.18	0.43
1:B:668:LEU:HB2	1:B:671:GLU:HG3	2.00	0.43
1:B:152:GLU:HG2	1:B:152:GLU:O	2.17	0.43
1:A:439:CYS:HG	1:A:620:MET:HB2	1.83	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
1:B:244:ILE:O	1:B:248:VAL:HG22	2.17	0.43
2:G:96:LEU:HB2	2:G:97:PRO:HD3	2.00	0.43
1:A:131:MET:HA	1:A:134:PHE:CD2	2.53	0.43
1:B:189:ARG:O	1:B:193:VAL:HG23	2.18	0.43
2:E:309:GLU:HB3	2:E:325:PHE:HB3	2.00	0.43
2:H:309:GLU:HB3	2:H:325:PHE:HB3	2.00	0.43
1:B:106:VAL:HG21	1:B:128:PHE:CE1	2.53	0.43
1:A:549:TYR:CD1	1:A:602:LEU:HD22	2.54	0.43
2:H:239:ALA:O	2:H:242:LEU:HG	2.18	0.43
1:A:681:LEU:O	1:A:685:MET:HG3	2.18	0.43
2:E:92:ASN:OD1	2:E:109:GLU:HG2	2.18	0.43
1:B:179:CYS:HB2	1:B:215:VAL:HG12	2.00	0.43
2:H:221:ARG:NH1	2:H:296:MET:HG2	2.30	0.43
2:H:76:ASN:HD21	2:H:211:SER:CA	2.29	0.43
1:A:459:ILE:HB	1:A:503:ALA:CA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:MET:HA	1:B:134:PHE:CD2	2.54	0.43
1:B:132:ASP:HA	1:B:135:ILE:HD12	1.99	0.43
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:H:297:ILE:O	2:H:297:ILE:HG13	2.18	0.43
1:B:423:HIS:HB2	1:B:582:THR:O	2.18	0.43
1:D:678:TYR:CZ	1:D:695:ALA:HB1	2.54	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:A:730:TYR:O	1:A:731:TYR:C	2.57	0.43
2:E:166:TYR:CZ	2:F:169:LEU:HD13	2.53	0.43
1:D:320:LYS:HE2	1:D:334:ASP:HA	2.01	0.43
1:D:640:GLY:HA2	1:D:668:LEU:HD22	2.01	0.43
1:A:556:ASN:O	1:A:560:LYS:HG3	2.18	0.43
2:E:204:GLU:HG2	2:E:238:GLU:OE2	2.18	0.43
1:D:500:ILE:HD12	1:D:500:ILE:N	2.33	0.43
1:B:394:LYS:NZ	1:B:394:LYS:HB2	2.33	0.43
1:D:244:ILE:HG23	1:D:254:ILE:HG13	1.99	0.43
1:A:238:ASN:HB3	1:B:242:SER:CB	2.49	0.43
1:D:474:ASN:N	1:D:474:ASN:HD22	2.17	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: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
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
1:A:560:LYS:HG2	1:A:609:HIS:HB3	1.99	0.43
1:A:43:LEU:HD21	2:F:298:GLY:HA3	2.00	0.43
1:D:56:SER:O	1:D:59:HIS:HB2	2.18	0.43
2:G:178:ASN:HD21	2:H:175:HIS:HD2	1.65	0.43
1:B:353:ILE:HB	1:B:393:VAL:HG23	2.01	0.43
1:A:544:PHE:CZ	1:A:685:MET:CG	3.00	0.43
1:D:441:GLU:O	1:D:692:SER:O	2.36	0.43
1:B:8:THR:O	1:B:55:THR:HB	2.18	0.43
2:G:102:PRO:HG2	2:G:103:GLU:OE1	2.19	0.43
1:B:474:ASN:HD21	1:B:477:GLU:HG3	1.83	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:A:339:ILE:HD12	1:A:414:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LYS:HG3	1:B:330:VAL:HG22	2.01	0.43
2:E:149:ARG:HH21	2:E:283:GLU:CD	2.21	0.43
1:D:361:VAL:O	1:D:361:VAL:HG23	2.19	0.43
1:A:19:LEU:HD12	2:F:295:SER:O	2.18	0.43
2:F:118:HIS:ND1	2:F:234:ILE:HG23	2.32	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
2:F:115:GLU:OE1	2:F:115:GLU:HA	2.19	0.43
1:B:561:GLU:HG2	1:B:561:GLU:O	2.18	0.43
2:E:213:ALA:O	2:E:334:TRP:HH2	2.01	0.42
1:D:514:GLY:C	1:D:618:ALA:HB3	2.39	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
2:F:311:ILE:HD11	2:F:315:ARG:NE	2.33	0.42
1:A:474:ASN:HD21	1:A:477:GLU:HG3	1.84	0.42
2:G:46:PHE:O	2:G:48:TRP:HD1	2.01	0.42
1:C:553:LYS:O	1:C:557:GLU:HG2	2.19	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:D:430:ILE:HG21	1:D:570:GLU:HA	2.01	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: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
2:G:92:ASN:HB3	2:H:92:ASN:HB3	2.01	0.42
1:C:467:PHE:CE2	1:C:515:ILE:CG2	3.02	0.42
1:A:303:THR:HA	1:A:334:ASP:O	2.19	0.42
2:F:104:LEU:O	2:F:108:VAL:HG23	2.19	0.42
2:H:76:ASN:O	2:H:80:GLN:HG3	2.19	0.42
1:A:644:ILE:HA	1:A:652:LEU:O	2.18	0.42
1:A:479:GLU:O	1:A:483:ILE:HG13	2.19	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
1:C:532:SER:OG	1:C:673:PRO:HD2	2.20	0.42
1:A:37:SER:HB3	1:A:40:GLN:CG	2.49	0.42
2:E:92:ASN:HB3	2:F:92:ASN:HB3	2.00	0.42
1:B:490:ASP:CG	1:B:511:ARG:HH21	2.21	0.42
1:A:552:LEU:HD12	1:A:599:TRP:HZ3	1.84	0.42
1:A:353:ILE:N	1:A:393:VAL:O	2.51	0.42
2:G:28:TYR:CD2	2:H:120:ARG:HA	2.54	0.42
1:D:444:LEU:HA	1:D:445:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:LEU:HB3	1:C:693:ILE:HG23	2.01	0.42
1:C:320:LYS:HE2	1:C:334:ASP:HA	2.00	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
1:D:94:TYR:CG	1:D:100:PRO:HD3	2.54	0.42
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.00	0.42
2:G:178:ASN:HD21	2:H:175:HIS:CD2	2.37	0.42
1:A:284:HIS:CE1	1:B:288:ALA:HB2	2.54	0.42
1:A:618:ALA:HB2	1:A:691:GLN:CD	2.39	0.42
1:B:304:LEU:N	1:B:334:ASP:O	2.53	0.42
1:A:50:TYR:H	1:A:53:ILE:CG2	2.32	0.42
1:B:240:THR:O	1:B:244:ILE:HG13	2.19	0.42
1:B:54:LYS:HE2	1:B:57:ASP:OD2	2.20	0.42
2:G:96:LEU:CB	2:G:97:PRO:HD3	2.50	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
2:G:1:ALA:HB3	2:G:168:HIS:CA	2.41	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:213:ALA:O	2:G:334:TRP:HH2	2.03	0.42
1:C:94:TYR:CG	1:C:100:PRO:HD3	2.55	0.42
1:B:640:GLY:HA2	1:B:668:LEU:HD22	2.01	0.42
1:B:147:ALA:HB1	1:B:628:ILE:HA	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
2:E:96:LEU:HB2	2:E:97:PRO:HD3	2.00	0.42
1:B:478:LEU:HD13	1:B:547:ILE:HA	2.01	0.42
1:C:228:ILE:HG22	1:C:240:THR:HG23	2.01	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:D:553:LYS:HA	1:D:602:LEU:HD11	2.01	0.42
2:F:276:PHE:HB3	2:F:316:MET:SD	2.59	0.42
1:B:565:CYS:SG	1:B:568:PHE:HB2	2.59	0.42
2:E:5:PHE:CE1	2:E:24:ASN:CG	2.93	0.42
1:C:444:LEU:HA	1:C:445:PRO:HD3	1.90	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
2:E:96:LEU:HA	2:E:99:ILE:HD12	2.01	0.42
1:A:641:TYR:O	1:A:655:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:CG2	1:C:17:ILE:HG13	2.49	0.42
2:E:203:LEU:HA	2:E:207:ARG:HD2	2.02	0.42
2:E:76:ASN:HD21	2:E:211:SER:CA	2.31	0.42
1:A:179:CYS:HB2	1:A:215:VAL:HG12	2.00	0.42
2:E:102:PRO:HG2	2:E:103:GLU:OE1	2.19	0.42
1:C:617:SER:OG	1:C:690:ASP:OD2	2.38	0.42
2:E:42:LYS:HE3	2:E:46:PHE:CZ	2.55	0.42
1:B:139:ARG:NH1	1:B:202:THR:HG23	2.34	0.42
1:C:172:LEU:CD2	1:C:212:MET:HE2	2.49	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
2:F:213:ALA:O	2:F:334:TRP:HH2	2.03	0.42
1:C:467:PHE:O	1:C:518:ILE:N	2.37	0.42
1:D:543:THR:HG22	1:D:547:ILE:HD11	2.02	0.42
1:C:520:PHE:O	1:C:521:ALA:C	2.58	0.42
1:D:518:ILE:HD12	1:D:631:ALA:HB3	2.02	0.42
1:D:304:LEU:HD23	1:D:305:PHE:N	2.35	0.42
2:F:244:GLY:O	2:F:248:MET:HG3	2.20	0.42
1:D:310:HIS:O	1:D:355:LEU:HB3	2.18	0.42
2:H:191:LYS:HG3	2:H:264:ILE:HG23	2.02	0.42
1:C:140:ASP:OD1	1:C:169:ALA:HB3	2.20	0.42
1:D:467:PHE:CE1	1:D:481:LEU:HB3	2.54	0.42
2:E:335:ILE:O	2:E:339:LEU:HG	2.18	0.42
2:E:11:ASP:OD1	2:E:13:LEU:HB2	2.19	0.42
1:B:303:THR:CG2	1:B:334:ASP:O	2.67	0.42
1:C:436:SER:OG	1:C:440:LEU:HD13	2.20	0.42
1:B:228:ILE:CG2	1:B:240:THR:HG23	2.49	0.42
2:E:165:SER:HB3	2:F:165:SER:HB3	2.02	0.42
1:A:519:ASN:CB	1:A:631:ALA:HB1	2.50	0.42
1:B:317:LEU:HA	1:B:317:LEU:HD12	1.89	0.42
1:D:91:LYS:O	1:D:91:LYS:HG2	2.20	0.42
1:C:33:LEU:CD1	1:C:80:LEU:HB2	2.46	0.42
1:B:258:ALA:C	1:B:260:ARG:H	2.23	0.42
1:C:228:ILE:HG21	1:C:240:THR:HG23	2.00	0.42
1:D:367:ALA:C	1:D:369:PHE:N	2.73	0.42
1:C:723:LYS:HG3	2:G:375:LEU:OXT	2.19	0.42
2:E:125:ILE:O	2:E:129:ILE:HG12	2.20	0.42
2:E:187:ARG:NH1	2:E:260:GLU:HG3	2.35	0.42
1:B:406:ARG:O	1:B:410:GLY:HA2	2.20	0.42
2:F:149:ARG:HD2	2:F:286:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:LEU:HB2	2:H:97:PRO:HD3	2.01	0.42
1:A:173:TYR:HB3	1:A:197:TYR:HD1	1.84	0.42
1:C:248:VAL:C	1:C:250:GLN:H	2.23	0.42
1:B:560:LYS:HG2	1:B:609:HIS:HB3	2.01	0.42
1:B:136:ASP:OD2	1:B:139:ARG:HG3	2.18	0.42
1:A:75:PRO:O	1:A:78:GLN:HB2	2.19	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:498:TYR:CB	1:D:504:LYS:HB2	2.50	0.42
1:D:410:GLY:O	1:D:411:ARG:HD2	2.20	0.42
1:D:560:LYS:HD3	1:D:609:HIS:CG	2.55	0.41
2:H:96:LEU:CB	2:H:97:PRO:HD3	2.50	0.41
2:E:96:LEU:CB	2:E:97:PRO:HD3	2.50	0.41
1:B:519:ASN:CB	1:B:631:ALA:HB1	2.50	0.41
2:E:35:ILE:HG23	2:E:36:PHE:H	1.84	0.41
1:A:645:LYS:HG2	1:A:646:ALA:N	2.35	0.41
1:C:169:ALA:O	1:C:172:LEU:HB3	2.20	0.41
1:D:643:SER:O	1:D:653:ARG:HA	2.20	0.41
1:C:410:GLY:O	1:C:411:ARG:HD2	2.20	0.41
1:B:334:ASP:OD1	1:B:411:ARG:HB3	2.20	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:478:LEU:HD13	1:A:547:ILE:HA	2.02	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: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:A:463:THR:O	1:A:489:LEU:HD22	2.20	0.41
1:D:275:HIS:ND1	3:D:900:DTP:H1'	2.35	0.41
2:H:18:PHE:O	2:H:19:PHE:CB	2.66	0.41
2:F:76:ASN:O	2:F:80:GLN:HG3	2.20	0.41
2:G:76:ASN:O	2:G:80:GLN:HG3	2.20	0.41
2:G:171:GLY:O	2:G:184:VAL:CG1	2.66	0.41
2:E:300:ASN:OD1	2:E:302:ASP:HB2	2.21	0.41
1:B:686:GLN:NE2	1:B:727:LYS:HE3	2.35	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
2:E:209:TYR:HA	2:E:212:PHE:CD2	2.55	0.41
2:H:31:GLN:HG2	2:H:37:GLU:HB2	2.02	0.41
1:C:152:GLU:HG2	1:C:152:GLU:O	2.20	0.41
1:B:160:ARG:HA	1:B:160:ARG:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:LEU:HD12	1:B:693:ILE:CD1	2.51	0.41
1:D:521:ALA:HB3	1:D:632:THR:HG21	2.02	0.41
2:G:125:ILE:O	2:G:129:ILE:HG12	2.20	0.41
1:A:139:ARG:NH1	1:A:202:THR:HG23	2.36	0.41
1:C:202:THR:OG1	1:C:204:LYS:HD3	2.19	0.41
2:G:115:GLU:HA	2:G:115:GLU:OE1	2.21	0.41
1:A:313:VAL:HG13	1:A:314:GLU:N	2.36	0.41
1:D:437:ASN:OD1	1:D:441:GLU:OE1	2.39	0.41
1:D:169:ALA:O	1:D:172:LEU:HB3	2.21	0.41
1:B:442:ILE:CG2	1:B:444:LEU:HG	2.50	0.41
1:C:515:ILE:HD12	1:C:551:LEU:CD2	2.50	0.41
2:G:203:LEU:O	2:G:207:ARG:HB2	2.19	0.41
1:C:246:LYS:HZ3	1:D:234:LEU:HB3	1.85	0.41
1:C:425:PRO:CG	1:C:615:THR:HG22	2.50	0.41
1:B:549:TYR:CD1	1:B:602:LEU:HD22	2.55	0.41
1:D:224:SER:O	1:D:252:ALA:HA	2.20	0.41
1:B:353:ILE:N	1:B:393:VAL:O	2.52	0.41
2:E:276:PHE:HB3	2:E:316:MET:SD	2.60	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:C:304:LEU:HD23	1:C:305:PHE:N	2.36	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
1:C:227:LEU:HB3	1:C:435:GLN:HE21	1.72	0.41
1:B:641:TYR:O	1:B:655:VAL:HA	2.21	0.41
1:A:258:ALA:C	1:A:260:ARG:H	2.22	0.41
1:D:463:THR:CG2	1:D:489:LEU:HD22	2.46	0.41
2:G:9:LYS:CA	2:H:141:VAL:HG11	2.45	0.41
1:D:367:ALA:HB1	1:D:375:PHE:HB2	2.02	0.41
1:B:644:ILE:HD12	1:B:644:ILE:N	2.36	0.41
1:C:313:VAL:O	1:C:317:LEU:HB2	2.19	0.41
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.21	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
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
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.49	0.41
2:E:244:GLY:O	2:E:248:MET:HG3	2.21	0.41
1:C:224:SER:O	1:C:252:ALA:HA	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:O	1:A:92:LYS:HG2	2.20	0.41
1:D:437:ASN:OD1	1:D:442:ILE:HG12	2.21	0.41
1:A:45:SER:O	1:A:46:HIS:C	2.59	0.41
1:C:465:SER:CB	1:C:514:GLY:O	2.61	0.41
2:H:36:PHE:HZ	2:H:248:MET:HG2	1.85	0.41
2:F:205:ALA:HB1	2:F:315:ARG:HD2	2.03	0.41
2:H:278:GLN:O	2:H:282:GLN:HG3	2.21	0.41
1:B:68:ASP:HA	1:B:653:ARG:HH12	1.85	0.41
1:A:686:GLN:CD	1:A:727:LYS:HG3	2.41	0.41
1:B:645:LYS:HG2	1:B:646:ALA:N	2.36	0.41
1:C:645:LYS:HG2	1:C:646:ALA:N	2.36	0.41
1:A:77:TYR:CD1	1:A:80:LEU:HD23	2.55	0.41
1:C:498:TYR:CB	1:C:504:LYS:HB2	2.51	0.41
2:F:31:GLN:HG2	2:F:37:GLU:HB2	2.02	0.41
2:F:34:ASP:N	2:F:34:ASP:OD1	2.54	0.41
1:A:619:LEU:HD12	1:A:693:ILE:CD1	2.50	0.41
1:A:437:ASN:ND2	1:A:439:CYS:H	2.18	0.41
1:C:437:ASN:OD1	1:C:441:GLU:OE1	2.39	0.41
2:H:332:ILE:HG22	2:H:334:TRP:HE1	1.84	0.41
1:B:441:GLU:O	1:B:692:SER:N	2.54	0.41
2:H:69:GLU:HG2	2:H:296:MET:HG3	2.03	0.41
1:C:260:ARG:HH11	1:C:448:PRO:HG3	1.86	0.41
1:C:102:LEU:HD23	1:C:128:PHE:O	2.21	0.41
1:B:619:LEU:HD12	1:B:693:ILE:CG1	2.51	0.41
1:C:639:ARG:NH2	1:C:733:ASN:HB3	2.33	0.41
2:H:125:ILE:O	2:H:129:ILE:HG12	2.20	0.41
1:A:541:HIS:O	1:A:545:GLU:HB2	2.21	0.41
1:B:357:SER:O	1:B:358:PRO:C	2.58	0.41
1:A:425:PRO:HB3	1:A:573:TYR:CE2	2.55	0.41
2:H:11:ASP:OD1	2:H:13:LEU:HB2	2.20	0.41
1:C:34:HIS:O	1:C:36:VAL:HG13	2.21	0.41
1:A:406:ARG:O	1:A:410:GLY:HA2	2.21	0.41
1:D:18:ASN:N	3:D:800:DTP:C2	2.82	0.41
1:B:53:ILE:O	1:B:54:LYS:O	2.39	0.41
1:A:39:SER:O	1:A:40:GLN:C	2.58	0.41
2:E:153:ILE:HD13	2:E:203:LEU:CD1	2.51	0.41
2:F:278:GLN:O	2:F:282:GLN:HG3	2.21	0.41
2:E:76:ASN:O	2:E:80:GLN:HG3	2.21	0.41
1:D:524:LEU:HD12	1:D:531:TYR:CE1	2.56	0.41
1:C:524:LEU:HD12	1:C:531:TYR:CE1	2.55	0.41
1:C:474:ASN:N	1:C:474:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:ASN:HD21	2:F:175:HIS:HD2	1.67	0.41
1:D:583:TYR:CG	1:D:687:LYS:HG3	2.56	0.41
1:D:553:LYS:O	1:D:557:GLU:HG2	2.20	0.41
1:B:232:ASP:OD2	1:B:262:ARG:NH2	2.53	0.41
1:B:583:TYR:CB	1:B:687:LYS:HG3	2.51	0.41
1:A:443:ALA:O	1:A:444:LEU:HD23	2.21	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
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:640:GLY:CA	1:C:668:LEU:HD22	2.51	0.40
1:A:136:ASP:OD2	1:A:139:ARG:HG3	2.20	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
2:G:364:GLU:HG3	2:G:365:VAL:N	2.36	0.40
1:D:55:THR:OG1	3:D:800:DTP:C5'	2.68	0.40
1:A:244:ILE:O	1:A:248:VAL:HG22	2.21	0.40
1:D:441:GLU:CG	1:D:619:LEU:O	2.70	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
2:G:36:PHE:O	2:G:39:LEU:HB2	2.22	0.40
2:H:244:GLY:O	2:H:248:MET:HG3	2.21	0.40
2:G:76:ASN:HD21	2:G:211:SER:CA	2.29	0.40
1:B:174:ILE:HG23	1:B:175:LEU:N	2.36	0.40
1:A:238:ASN:HD21	1:B:246:LYS:HG2	1.86	0.40
1:C:583:TYR:CG	1:C:687:LYS:HG3	2.57	0.40
2:H:42:LYS:HE3	2:H:46:PHE:CZ	2.56	0.40
1:C:101:ALA:HB3	1:C:104:ASP:OD2	2.20	0.40
2:H:232:ARG:HD2	2:H:338:TRP:HE3	1.87	0.40
2:H:171:GLY:O	2:H:184:VAL:CG1	2.65	0.40
1:D:367:ALA:O	1:D:369:PHE:N	2.54	0.40
2:E:317:GLN:O	2:E:317:GLN:HG2	2.21	0.40
2:E:158:ASP:OD1	2:F:4:THR:HG23	2.21	0.40
1:B:313:VAL:HG13	1:B:314:GLU:N	2.37	0.40
1:C:678:TYR:O	1:C:682:VAL:HG23	2.21	0.40
1:D:354:THR:HG21	1:D:390:LYS:HD3	2.03	0.40
1:C:643:SER:O	1:C:653:ARG:HA	2.21	0.40
1:A:228:ILE:N	1:A:435:GLN:HE22	2.19	0.40
1:A:7:VAL:O	1:A:14:THR:HA	2.21	0.40
1:D:430:ILE:HG21	1:D:570:GLU:CA	2.51	0.40
1:B:155:TYR:N	1:B:155:TYR:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:SER:OG	1:D:673:PRO:HD2	2.20	0.40
1:A:45:SER:HG	1:A:61:THR:HG22	1.86	0.40
2:G:93:VAL:HG13	2:H:97:PRO:HG3	2.04	0.40
1:A:122:ASP:O	1:A:189:ARG:NH2	2.54	0.40
2:G:104:LEU:O	2:G:108:VAL:HG23	2.21	0.40
2:H:300:ASN:OD1	2:H:302:ASP:HB2	2.21	0.40
1:D:519:ASN:OD1	1:D:632:THR:HG23	2.21	0.40
1:C:696:ASN:ND2	1:C:730:TYR:HB3	2.36	0.40
2:E:6:SER:H	2:E:24:ASN:HB3	1.85	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
1:A:283:LYS:HG3	1:A:330:VAL:HG22	2.04	0.40
2:H:68:HIS:O	2:H:72:ILE:HG13	2.21	0.40
2:H:115:GLU:OE1	2:H:115:GLU:HA	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%)	26	71
1	B	730/761 (96%)	684 (94%)	41 (6%)	5 (1%)	26	71
1	C	730/761 (96%)	686 (94%)	41 (6%)	3 (0%)	39	80
1	D	730/761 (96%)	685 (94%)	42 (6%)	3 (0%)	39	80
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%)	39 80

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%)	29 66
1	B	627/651 (96%)	600 (96%)	27 (4%)	35 70
1	C	627/651 (96%)	602 (96%)	25 (4%)	38 71
1	D	627/651 (96%)	596 (95%)	31 (5%)	31 67
2	E	315/340 (93%)	309 (98%)	6 (2%)	65 86
2	F	315/340 (93%)	306 (97%)	9 (3%)	50 78
2	G	319/340 (94%)	312 (98%)	7 (2%)	60 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	317/340 (93%)	308 (97%)	9 (3%)	51 78
All	All	3774/3964 (95%)	3628 (96%)	146 (4%)	39 72

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	A	800	-	24,32,32	1.62	5 (20%)	32,50,50	1.84	7 (21%)
3	DTP	A	900	-	24,32,32	1.61	5 (20%)	32,50,50	1.96	6 (18%)
3	DTP	B	800	-	24,32,32	1.62	5 (20%)	32,50,50	1.93	6 (18%)
3	DTP	B	900	-	24,32,32	1.63	6 (25%)	32,50,50	1.94	7 (21%)
3	DTP	C	800	-	24,32,32	1.61	5 (20%)	32,50,50	1.96	7 (21%)
3	DTP	C	900	-	24,32,32	1.61	5 (20%)	32,50,50	1.93	7 (21%)
3	DTP	D	800	-	24,32,32	1.65	5 (20%)	32,50,50	1.99	7 (21%)
3	DTP	D	900	-	24,32,32	1.67	6 (25%)	32,50,50	1.94	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	A	800	-	-	0/18/34/34	0/3/3/3
3	DTP	A	900	-	-	0/18/34/34	0/3/3/3
3	DTP	B	800	-	-	0/18/34/34	0/3/3/3
3	DTP	B	900	-	-	0/18/34/34	0/3/3/3
3	DTP	C	800	-	-	0/18/34/34	0/3/3/3
3	DTP	C	900	-	-	0/18/34/34	0/3/3/3
3	DTP	D	800	-	-	0/18/34/34	0/3/3/3
3	DTP	D	900	-	-	0/18/34/34	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	800	DTP	O3'-C3'	-3.75	1.34	1.43
3	D	900	DTP	O3'-C3'	-3.71	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	DTP	O3'-C3'	-3.69	1.35	1.43
3	B	900	DTP	O3'-C3'	-3.69	1.35	1.43
3	C	800	DTP	O3'-C3'	-3.69	1.35	1.43
3	A	800	DTP	O3'-C3'	-3.68	1.35	1.43
3	A	900	DTP	O3'-C3'	-3.67	1.35	1.43
3	C	900	DTP	O3'-C3'	-3.65	1.35	1.43
3	B	800	DTP	C5'-C4'	-2.94	1.42	1.51
3	A	800	DTP	C5'-C4'	-2.88	1.42	1.51
3	D	800	DTP	C5'-C4'	-2.88	1.42	1.51
3	D	900	DTP	C5'-C4'	-2.86	1.42	1.51
3	A	900	DTP	C5'-C4'	-2.82	1.42	1.51
3	C	800	DTP	C5'-C4'	-2.76	1.42	1.51
3	C	900	DTP	C5'-C4'	-2.74	1.42	1.51
3	B	900	DTP	C5'-C4'	-2.69	1.42	1.51
3	A	800	DTP	O5'-C5'	-2.69	1.33	1.44
3	D	900	DTP	O5'-C5'	-2.65	1.33	1.44
3	B	800	DTP	O5'-C5'	-2.65	1.34	1.44
3	D	800	DTP	O5'-C5'	-2.63	1.34	1.44
3	B	900	DTP	O5'-C5'	-2.60	1.34	1.44
3	A	900	DTP	O5'-C5'	-2.59	1.34	1.44
3	C	900	DTP	O5'-C5'	-2.58	1.34	1.44
3	D	900	DTP	C2'-C3'	-2.56	1.45	1.52
3	C	900	DTP	C2'-C3'	-2.54	1.46	1.52
3	D	800	DTP	C2'-C3'	-2.54	1.46	1.52
3	C	800	DTP	O5'-C5'	-2.52	1.34	1.44
3	B	800	DTP	C2'-C3'	-2.49	1.46	1.52
3	A	900	DTP	C2'-C3'	-2.49	1.46	1.52
3	B	900	DTP	C2'-C3'	-2.45	1.46	1.52
3	C	800	DTP	C2'-C3'	-2.45	1.46	1.52
3	A	800	DTP	C2'-C3'	-2.39	1.46	1.52
3	D	900	DTP	C3'-C4'	-2.29	1.46	1.53
3	B	900	DTP	C3'-C4'	-2.11	1.47	1.53
3	A	900	DTP	C6-N6	3.85	1.46	1.34
3	B	800	DTP	C6-N6	3.90	1.47	1.34
3	D	900	DTP	C6-N6	3.91	1.47	1.34
3	C	800	DTP	C6-N6	3.92	1.47	1.34
3	D	800	DTP	C6-N6	3.93	1.47	1.34
3	C	900	DTP	C6-N6	3.94	1.47	1.34
3	B	900	DTP	C6-N6	3.95	1.47	1.34
3	A	800	DTP	C6-N6	3.96	1.47	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	DTP	N3-C2-N1	-7.25	123.34	128.89
3	C	800	DTP	N3-C2-N1	-7.19	123.39	128.89
3	B	900	DTP	N3-C2-N1	-7.10	123.46	128.89
3	B	800	DTP	N3-C2-N1	-7.09	123.47	128.89
3	D	800	DTP	N3-C2-N1	-7.06	123.49	128.89
3	C	900	DTP	N3-C2-N1	-6.98	123.55	128.89
3	A	800	DTP	N3-C2-N1	-6.88	123.63	128.89
3	D	900	DTP	N3-C2-N1	-6.37	124.01	128.89
3	D	900	DTP	PA-O3A-PB	-4.27	120.73	132.73
3	D	800	DTP	PA-O3A-PB	-4.22	120.89	132.73
3	A	900	DTP	PA-O3A-PB	-4.15	121.06	132.73
3	C	900	DTP	PA-O3A-PB	-4.09	121.25	132.73
3	A	800	DTP	PA-O3A-PB	-3.82	122.01	132.73
3	B	900	DTP	PB-O3B-PG	-3.81	119.88	132.67
3	C	800	DTP	PB-O3B-PG	-3.67	120.38	132.67
3	C	800	DTP	PA-O3A-PB	-3.63	122.54	132.73
3	C	900	DTP	PB-O3B-PG	-3.40	121.25	132.67
3	A	900	DTP	PB-O3B-PG	-3.28	121.69	132.67
3	B	900	DTP	PA-O3A-PB	-3.08	124.08	132.73
3	D	900	DTP	PB-O3B-PG	-3.04	122.47	132.67
3	D	800	DTP	PB-O3B-PG	-3.04	122.48	132.67
3	B	800	DTP	C4-C5-N7	-2.70	107.00	109.48
3	B	800	DTP	PA-O3A-PB	-2.57	125.51	132.73
3	A	800	DTP	PB-O3B-PG	-2.57	124.06	132.67
3	D	900	DTP	C4-C5-N7	-2.47	107.21	109.48
3	B	800	DTP	PB-O3B-PG	-2.44	124.50	132.67
3	D	800	DTP	C4-C5-N7	-2.34	107.32	109.48
3	C	900	DTP	C4-C5-N7	-2.32	107.34	109.48
3	A	900	DTP	C4-C5-N7	-2.31	107.35	109.48
3	C	800	DTP	C4-C5-N7	-2.27	107.39	109.48
3	A	800	DTP	C4-C5-N7	-2.26	107.40	109.48
3	D	900	DTP	C1'-N9-C4	-2.25	123.34	127.16
3	B	900	DTP	C4-C5-N7	-2.16	107.49	109.48
3	B	900	DTP	O3A-PA-O5'	2.08	108.47	102.94
3	D	900	DTP	O3A-PA-O5'	2.13	108.58	102.94
3	D	900	DTP	O5'-C5'-C4'	2.18	117.14	109.12
3	A	900	DTP	O5'-C5'-C4'	2.24	117.37	109.12
3	D	800	DTP	O3A-PA-O5'	2.24	108.88	102.94
3	D	800	DTP	O5'-C5'-C4'	2.25	117.40	109.12
3	C	900	DTP	O5'-C5'-C4'	2.30	117.59	109.12
3	C	800	DTP	O5'-C5'-C4'	2.36	117.81	109.12
3	C	900	DTP	O3A-PA-O5'	2.38	109.25	102.94
3	A	800	DTP	O5'-C5'-C4'	2.38	117.90	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	DTP	O3A-PA-O5'	2.41	109.33	102.94
3	A	800	DTP	O3A-PA-O5'	2.43	109.39	102.94
3	B	900	DTP	O5'-C5'-C4'	2.50	118.33	109.12
3	B	800	DTP	O3A-PA-O5'	2.78	110.32	102.94
3	A	800	DTP	O4'-C1'-N9	3.43	113.65	107.72
3	B	900	DTP	O4'-C1'-N9	3.59	113.94	107.72
3	C	800	DTP	O4'-C1'-N9	3.72	114.17	107.72
3	A	900	DTP	O4'-C1'-N9	3.75	114.20	107.72
3	C	900	DTP	O4'-C1'-N9	3.90	114.47	107.72
3	D	800	DTP	O4'-C1'-N9	4.23	115.04	107.72
3	D	900	DTP	O4'-C1'-N9	4.30	115.17	107.72
3	B	800	DTP	O4'-C1'-N9	4.47	115.45	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 70 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	732/761 (96%)	0.53	61 (8%) 14 17	157, 231, 260, 283	0
1	B	732/761 (96%)	0.59	62 (8%) 13 16	161, 232, 262, 279	0
1	C	732/761 (96%)	1.08	167 (22%) 1 5	197, 289, 342, 359	0
1	D	732/761 (96%)	1.24	184 (25%) 1 4	194, 290, 343, 359	0
2	E	348/375 (92%)	0.05	4 (1%) 82 77	145, 207, 237, 289	0
2	F	348/375 (92%)	-0.00	5 (1%) 78 71	147, 206, 235, 285	0
2	G	352/375 (93%)	0.21	9 (2%) 59 54	147, 207, 237, 293	0
2	H	350/375 (93%)	0.12	3 (0%) 85 81	141, 203, 235, 286	0
All	All	4326/4544 (95%)	0.61	495 (11%) 7 11	141, 235, 312, 359	0

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	611	LEU	10.9
1	D	613	ASN	7.5
1	D	267	PRO	7.3
1	B	167	GLU	7.2
1	D	564	ALA	7.2
1	D	614	SER	6.9
1	C	100	PRO	6.6
1	D	462	CYS	6.6
1	D	360	ASP	6.6
1	C	15	GLU	6.4
1	D	641	TYR	6.3
1	C	621	PRO	6.3
1	D	383	GLU	6.2
1	C	266	SER	6.0
1	D	390	LYS	6.0
1	D	357	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	167	GLU	5.8
1	D	266	SER	5.8
1	D	174	ILE	5.8
1	D	389	ARG	5.6
1	D	181	PHE	5.6
1	D	178	ALA	5.6
1	C	14	THR	5.5
1	D	392	ARG	5.4
1	D	224	SER	5.3
1	D	179	CYS	5.3
1	D	612	ARG	5.1
1	D	223	SER	5.1
1	A	14	THR	5.0
1	B	168	SER	4.9
1	D	621	PRO	4.9
1	A	271	GLY	4.9
1	D	56	SER	4.8
1	B	171	PHE	4.8
1	C	432	PRO	4.8
1	D	253	GLY	4.8
1	C	259	GLY	4.8
1	D	565	CYS	4.8
1	D	640	GLY	4.8
1	B	166	TYR	4.7
1	C	390	LYS	4.7
1	D	225	CYS	4.7
1	D	737	GLY	4.6
1	B	667	GLU	4.5
1	D	510	ARG	4.5
1	D	698	ASN	4.5
1	C	388	ILE	4.5
1	C	263	ALA	4.5
1	D	187	GLU	4.5
1	D	188	THR	4.5
1	D	119	LEU	4.4
1	C	439	CYS	4.4
1	C	622	SER	4.4
1	D	463	THR	4.4
1	B	165	ILE	4.4
1	C	119	LEU	4.3
1	C	216	ARG	4.3
1	C	120	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	105	HIS	4.3
1	A	272	GLU	4.3
1	D	106	VAL	4.3
1	C	145	TYR	4.2
1	D	610	GLY	4.2
1	D	356	PHE	4.2
1	C	692	SER	4.1
1	D	72	ARG	4.1
1	C	143	PHE	4.1
1	C	458	GLU	4.1
1	D	140	ASP	4.1
1	C	620	MET	4.1
1	D	130	GLN	4.1
1	D	11	ASP	4.0
1	D	655	VAL	4.0
1	C	389	ARG	4.0
1	D	262	ARG	3.9
1	B	97	PHE	3.9
1	C	104	ASP	3.9
1	C	92	LYS	3.9
1	D	252	ALA	3.9
1	C	123	TYR	3.9
1	C	93	ALA	3.9
1	D	135	ILE	3.9
1	C	99	PRO	3.9
1	D	255	GLY	3.8
1	C	446	THR	3.8
1	D	425	PRO	3.8
1	A	16	ARG	3.8
1	C	98	GLU	3.8
1	A	641	TYR	3.8
1	D	439	CYS	3.8
1	C	167	GLU	3.8
1	D	638	PRO	3.8
1	C	16	ARG	3.8
1	C	107	VAL	3.7
1	D	637	PRO	3.7
1	C	392	ARG	3.7
1	D	137	HIS	3.7
1	D	177	ALA	3.7
1	C	727	LYS	3.7
1	D	571	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	3.7
1	C	436	SER	3.7
2	F	322	ASP	3.6
1	D	263	ALA	3.6
1	B	666	TYR	3.6
1	C	299	GLY	3.6
1	D	208	PRO	3.6
1	C	190	LEU	3.5
1	C	694	SER	3.5
1	C	437	ASN	3.5
1	C	106	VAL	3.5
1	D	182	SER	3.5
1	C	737	GLY	3.5
1	D	620	MET	3.5
1	D	75	PRO	3.5
1	D	699	TYR	3.5
1	B	72	ARG	3.4
1	B	298	ARG	3.4
1	C	88	HIS	3.4
1	D	265	GLY	3.4
1	D	388	ILE	3.4
1	C	101	ALA	3.4
1	D	309	TRP	3.4
1	B	641	TYR	3.4
1	D	105	HIS	3.4
1	C	391	GLN	3.4
1	C	108	LYS	3.4
1	C	730	TYR	3.4
1	A	622	SER	3.4
1	A	94	TYR	3.3
1	C	360	ASP	3.3
1	C	728	THR	3.3
1	D	354	THR	3.3
1	A	15	GLU	3.3
1	C	96	GLN	3.3
1	C	301	ALA	3.3
1	B	273	ALA	3.3
1	C	262	ARG	3.3
1	C	731	TYR	3.3
1	B	640	GLY	3.3
1	D	563	GLY	3.3
1	B	216	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	576	GLY	3.3
1	A	270	GLY	3.3
1	D	359	SER	3.3
1	B	190	LEU	3.3
1	D	622	SER	3.2
1	C	303	THR	3.2
1	A	96	GLN	3.2
1	C	97	PHE	3.2
1	D	465	SER	3.2
1	D	141	MET	3.2
1	B	157	VAL	3.2
1	A	165	ILE	3.2
1	A	95	GLY	3.2
1	D	136	ASP	3.2
1	B	668	LEU	3.2
1	D	210	PRO	3.2
1	B	120	LEU	3.2
1	C	352	ASP	3.2
1	C	225	CYS	3.2
1	D	300	GLY	3.2
1	C	358	PRO	3.2
1	C	624	THR	3.1
1	C	103	TYR	3.1
1	D	165	ILE	3.1
1	B	427	ASP	3.1
1	D	170	GLN	3.1
1	C	265	GLY	3.1
1	C	428	PRO	3.1
1	C	10	ARG	3.1
1	D	54	LYS	3.1
1	D	308	MET	3.1
1	C	462	CYS	3.1
1	C	295	GLY	3.1
1	A	88	HIS	3.1
1	B	116	ASP	3.1
1	D	88	HIS	3.0
1	C	215	VAL	3.0
1	C	655	VAL	3.0
1	C	116	ASP	3.0
1	D	572	THR	3.0
1	C	267	PRO	3.0
2	G	257	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	223	SER	3.0
1	C	179	CYS	3.0
1	C	421	ASN	3.0
1	B	687	LYS	3.0
1	D	511	ARG	3.0
1	A	667	GLU	3.0
1	C	11	ASP	3.0
2	F	295	SER	3.0
1	C	573	TYR	3.0
2	G	19	PHE	3.0
1	C	94	TYR	3.0
1	A	269	ARG	3.0
1	C	178	ALA	3.0
1	D	123	TYR	3.0
1	C	189	ARG	3.0
1	D	139	ARG	3.0
1	D	380	THR	2.9
1	D	301	ALA	2.9
1	A	614	SER	2.9
1	C	359	SER	2.9
1	B	671	GLU	2.9
1	A	166	TYR	2.9
1	B	115	TYR	2.9
1	C	102	LEU	2.9
1	D	99	PRO	2.9
1	D	642	VAL	2.9
1	C	128	PHE	2.9
1	C	429	ALA	2.9
1	A	58	ILE	2.9
1	C	357	SER	2.9
1	C	438	LEU	2.9
1	D	379	TYR	2.8
1	C	702	SER	2.8
2	E	322	ASP	2.8
1	B	145	TYR	2.8
1	C	671	GLU	2.8
1	A	17	ILE	2.8
1	D	437	ASN	2.8
1	D	12	GLY	2.8
1	D	639	ARG	2.8
1	A	570	GLU	2.8
1	B	156	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	700	ASP	2.8
1	C	370	ALA	2.8
1	B	141	MET	2.8
1	C	356	PHE	2.8
1	D	668	LEU	2.8
1	A	659	TYR	2.8
1	D	131	MET	2.8
1	D	271	GLY	2.8
1	A	516	GLY	2.8
1	C	7	VAL	2.8
1	C	510	ARG	2.8
1	A	144	SER	2.7
1	B	94	TYR	2.7
1	D	57	ASP	2.7
1	A	426	PHE	2.7
1	B	439	CYS	2.7
1	B	659	TYR	2.7
1	C	445	PRO	2.7
1	C	144	SER	2.7
1	B	140	ASP	2.7
1	C	379	TYR	2.7
1	D	656	VAL	2.7
1	A	273	ALA	2.7
1	D	259	GLY	2.7
1	C	323	ARG	2.7
1	C	56	SER	2.7
2	G	252	LEU	2.7
1	A	93	ALA	2.7
1	D	327	GLY	2.7
1	C	217	THR	2.7
1	B	152	GLU	2.7
1	D	15	GLU	2.7
1	C	90	ARG	2.7
1	D	667	GLU	2.7
1	B	271	GLY	2.7
1	D	261	ILE	2.7
1	C	383	GLU	2.7
1	C	733	ASN	2.7
1	C	710	PRO	2.7
1	A	268	ILE	2.6
1	B	655	VAL	2.6
1	C	413	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	699	TYR	2.6
1	C	732	GLN	2.6
1	D	8	THR	2.6
1	D	183	ASN	2.6
1	D	94	TYR	2.6
2	G	17	MET	2.6
1	A	145	TYR	2.6
1	D	562	GLN	2.6
1	D	274	PHE	2.6
1	A	360	ASP	2.6
1	B	170	GLN	2.6
1	C	138	ASP	2.6
1	B	395	ALA	2.6
1	D	168	SER	2.6
1	D	619	LEU	2.6
1	C	277	GLY	2.6
1	C	431	ALA	2.6
1	C	586	ASP	2.6
1	B	656	VAL	2.6
1	D	55	THR	2.6
1	D	516	GLY	2.6
1	B	431	ALA	2.6
1	D	734	THR	2.6
1	B	670	TRP	2.6
1	C	670	TRP	2.6
1	D	128	PHE	2.6
1	D	275	HIS	2.6
1	B	274	PHE	2.5
1	A	466	ALA	2.5
2	G	56	SER	2.5
1	A	6	LEU	2.5
1	D	427	ASP	2.5
1	C	385	ASP	2.5
1	D	184	TYR	2.5
1	C	76	ASP	2.5
1	D	391	GLN	2.5
1	A	206	SER	2.5
1	D	353	ILE	2.5
1	C	78	GLN	2.5
1	D	10	ARG	2.5
1	A	208	PRO	2.5
1	D	171	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	514	GLY	2.5
1	C	182	SER	2.5
1	A	35	ASN	2.5
1	C	576	GLY	2.5
1	D	568	PHE	2.5
1	B	531	TYR	2.5
1	A	259	GLY	2.5
1	D	464	LEU	2.5
1	A	356	PHE	2.5
1	C	322	ASN	2.5
1	D	97	PHE	2.5
1	D	624	THR	2.5
1	D	659	TYR	2.5
1	C	296	GLY	2.5
1	D	157	VAL	2.5
1	D	197	TYR	2.5
2	H	187	ARG	2.5
1	C	183	ASN	2.4
1	D	618	ALA	2.4
1	A	621	PRO	2.4
1	D	505	ARG	2.4
1	C	184	TYR	2.4
1	C	659	TYR	2.4
1	C	142	THR	2.4
1	C	734	THR	2.4
1	D	193	VAL	2.4
1	A	62	ILE	2.4
1	D	705	PRO	2.4
1	C	441	GLU	2.4
1	D	299	GLY	2.4
1	C	273	ALA	2.4
1	B	123	TYR	2.4
1	C	382	TYR	2.4
1	D	166	TYR	2.4
1	A	655	VAL	2.4
1	D	617	SER	2.4
1	C	411	ARG	2.4
1	D	358	PRO	2.4
1	C	509	GLY	2.4
1	D	574	ALA	2.4
1	C	156	LEU	2.4
1	D	102	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	434	ARG	2.4
1	C	575	LYS	2.4
1	D	100	PRO	2.4
1	C	447	LYS	2.4
1	A	257	ASN	2.4
1	D	175	LEU	2.4
1	D	573	TYR	2.3
1	A	92	LYS	2.3
1	C	709	VAL	2.3
1	C	168	SER	2.3
1	C	463	THR	2.3
1	D	122	ASP	2.3
1	C	312	GLU	2.3
1	C	17	ILE	2.3
1	D	83	ARG	2.3
1	D	434	ARG	2.3
1	D	120	LEU	2.3
2	G	365	VAL	2.3
1	A	11	ASP	2.3
1	A	261	ILE	2.3
1	D	458	GLU	2.3
1	C	224	SER	2.3
1	D	385	ASP	2.3
1	D	735	ARG	2.3
1	B	532	SER	2.3
1	D	14	THR	2.3
1	C	440	LEU	2.3
1	D	370	ALA	2.3
1	B	119	LEU	2.3
1	C	91	LYS	2.3
1	D	192	TYR	2.3
1	A	666	TYR	2.3
1	C	614	SER	2.3
1	C	657	PRO	2.3
1	A	56	SER	2.3
1	C	505	ARG	2.3
1	A	255	GLY	2.3
2	E	324	PRO	2.3
1	C	387	SER	2.3
1	C	625	SER	2.3
1	A	425	PRO	2.3
1	B	657	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	295	SER	2.3
1	C	514	GLY	2.3
1	D	460	ALA	2.3
1	A	465	SER	2.3
1	B	680	GLN	2.3
1	D	133	THR	2.2
1	D	466	ALA	2.2
1	C	667	GLU	2.2
1	C	264	LEU	2.2
2	H	19	PHE	2.2
1	B	473	ASN	2.2
1	D	607	LYS	2.2
1	D	426	PHE	2.2
1	C	666	TYR	2.2
1	D	260	ARG	2.2
1	D	185	PRO	2.2
1	A	435	GLN	2.2
1	B	179	CYS	2.2
2	H	191	LYS	2.2
1	C	152	GLU	2.2
1	B	357	SER	2.2
2	F	194	TYR	2.2
1	B	712	GLN	2.2
1	C	599	TRP	2.2
1	C	706	SER	2.2
2	G	12	GLN	2.2
1	C	117	ASN	2.2
1	D	384	LYS	2.2
1	D	669	LEU	2.2
1	B	100	PRO	2.2
1	A	72	ARG	2.2
1	C	95	GLY	2.2
1	B	299	GLY	2.2
1	D	694	SER	2.2
1	D	381	LYS	2.2
1	D	700	ASP	2.2
1	C	362	PRO	2.2
1	A	392	ARG	2.2
1	A	610	GLY	2.2
1	C	75	PRO	2.2
2	G	55	VAL	2.2
1	D	670	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	713	GLN	2.2
1	B	570	GLU	2.2
1	D	273	ALA	2.2
1	D	435	GLN	2.1
2	F	29	ASP	2.1
1	C	465	SER	2.1
1	D	566	PRO	2.1
1	B	267	PRO	2.1
1	C	466	ALA	2.1
1	C	171	PHE	2.1
1	C	580	ILE	2.1
1	D	727	LYS	2.1
1	C	6	LEU	2.1
1	C	703	ARG	2.1
1	A	704	PHE	2.1
1	B	169	ALA	2.1
1	D	711	MET	2.1
1	A	97	PHE	2.1
1	D	608	THR	2.1
1	C	300	GLY	2.1
1	C	415	GLN	2.1
1	C	450	ASN	2.1
1	D	268	ILE	2.1
1	D	555	SER	2.1
1	C	435	GLN	2.1
1	A	431	ALA	2.1
1	B	29	ALA	2.1
1	B	106	VAL	2.1
1	D	570	GLU	2.1
2	F	323	LEU	2.1
1	C	260	ARG	2.1
1	A	59	HIS	2.1
1	D	121	GLU	2.1
1	B	530	ARG	2.1
1	D	206	SER	2.1
1	D	323	ARG	2.1
2	G	253	ARG	2.1
1	A	36	VAL	2.1
1	A	361	VAL	2.1
1	B	537	ASN	2.1
1	B	642	VAL	2.1
1	B	266	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	432	PRO	2.0
1	D	575	LYS	2.0
1	B	356	PHE	2.0
1	C	115	TYR	2.0
1	D	118	HIS	2.0
1	D	116	ASP	2.0
1	D	553	LYS	2.0
2	E	187	ARG	2.0
1	A	49	PHE	2.0
1	C	118	HIS	2.0
1	C	124	THR	2.0
1	D	512	THR	2.0
1	C	574	ALA	2.0
1	B	102	LEU	2.0
1	D	693	ILE	2.0
1	A	462	CYS	2.0
1	A	624	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DTP	B	800	30/30	0.79	0.50	0.49	279,279,279,279	0
4	FE	E	1003	1/1	0.96	0.26	0.21	168,168,168,168	0
4	FE	G	1004	1/1	0.99	0.34	0.11	122,122,122,122	0
3	DTP	C	800	30/30	0.70	0.65	-0.05	326,326,326,326	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DTP	B	900	30/30	0.67	0.41	-0.18	232,232,232,232	0
3	DTP	C	900	30/30	0.59	0.41	-0.18	284,284,284,284	0
3	DTP	D	800	30/30	0.31	0.53	-0.19	318,318,318,318	0
3	DTP	A	800	30/30	0.70	0.59	-0.25	306,306,306,306	0
3	DTP	D	900	30/30	0.57	0.51	-0.26	308,308,308,308	0
4	FE	E	1004	1/1	0.95	0.23	-0.36	133,133,133,133	0
4	FE	H	1002	1/1	0.99	0.32	-0.43	114,114,114,114	0
4	FE	G	1003	1/1	0.98	0.29	-0.44	89,89,89,89	0
3	DTP	A	900	30/30	0.80	0.37	-0.58	267,267,267,267	0
4	FE	F	1001	1/1	0.99	0.21	-2.04	94,94,94,94	0
4	FE	H	1001	1/1	0.99	0.27	-2.21	110,110,110,110	0
4	FE	F	1002	1/1	0.99	0.21	-2.29	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.