



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:50 AM UTC

PDB ID : 6N61 / pdb_00006n61
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA and Capistruin
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.
Deposited on : 2018-11-24
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

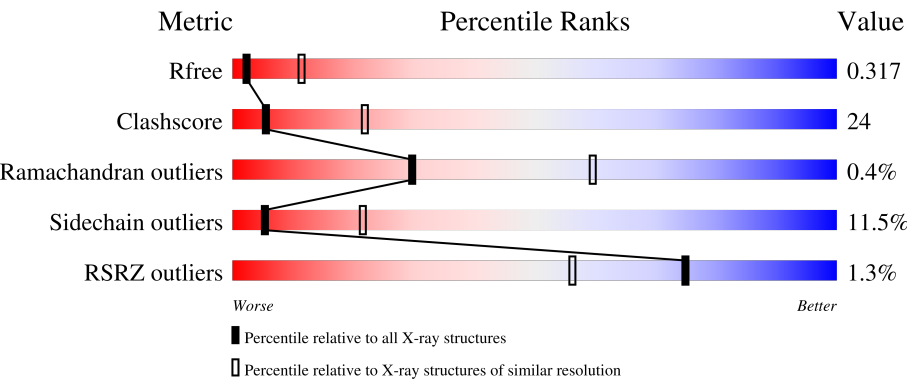
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	239	3% 54% 36% 5% 5%
1	B	239	4% 48% 35% 8% 9%
2	C	1342	% 54% 40% 6% •
3	D	1409	% 46% 36% 6% 12%
4	E	90	% 48% 38% • 12%

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Mol	Chain	Length	Quality of chain
5	F	613	
6	N	29	
7	T	24	
8	I	19	

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
12	EPE	D	1504	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28613 atoms, of which 23 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1709	1067	300	336	6			
1	B	217	Total	C	N	O	S	0	0	0
			1658	1035	290	327	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z4
A	236	VAL	-	expression tag	UNP P0A7Z4
A	237	LEU	-	expression tag	UNP P0A7Z4
A	238	PHE	-	expression tag	UNP P0A7Z4
A	239	GLN	-	expression tag	UNP P0A7Z4
B	235	GLU	-	expression tag	UNP P0A7Z4
B	236	VAL	-	expression tag	UNP P0A7Z4
B	237	LEU	-	expression tag	UNP P0A7Z4
B	238	PHE	-	expression tag	UNP P0A7Z4
B	239	GLN	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1332	Total	C	N	O	S	0	0	0
			10489	6581	1829	2036	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1239	Total	C	N	O	S	0	0	0
			9649	6061	1733	1807	48			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T7
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	395	Total	C	N	O	S	0	0	0
			3197	1993	578	603	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9

- Molecule 6 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

- Molecule 7 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

- Molecule 8 is a protein called Capistrain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	17	Total	C	N	O	0	0	0
			126	80	24	22			

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			10	2	6	2		

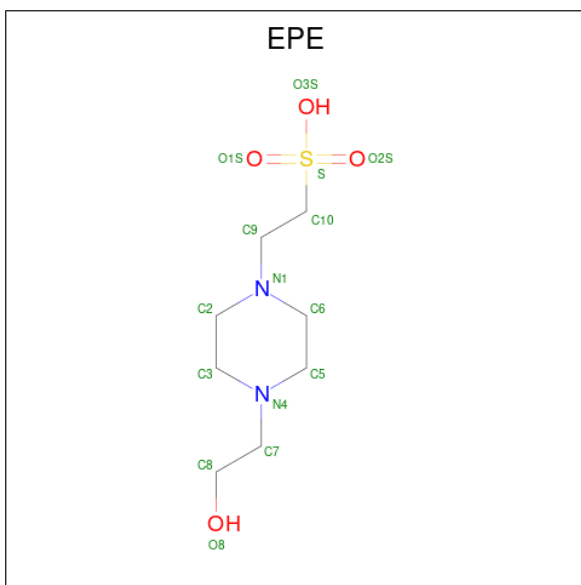
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	H	N	O	S	
			32	8	17	2	4	1	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	O		
			1	1	0	0
13	B	2	Total	O		
			2	2	0	0
13	C	13	Total	O		
			13	13	0	0
13	D	3	Total	O		
			3	3	0	0
13	E	1	Total	O		
			1	1	0	0
13	F	5	Total	O		
			5	5	0	0
13	T	1	Total	O		
			1	1	0	0

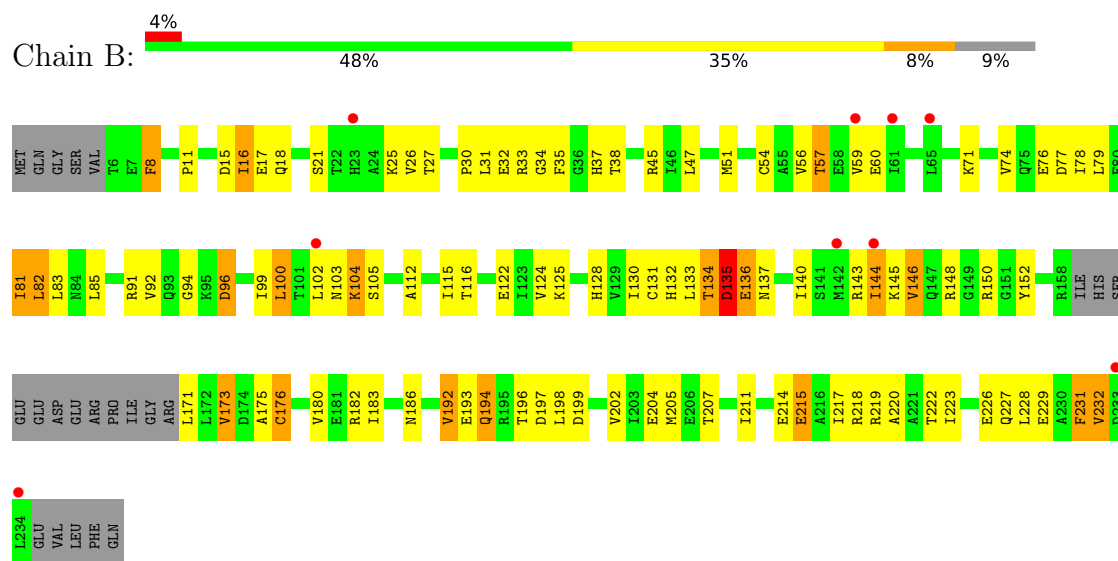
3 Residue-property plots [i](#)

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

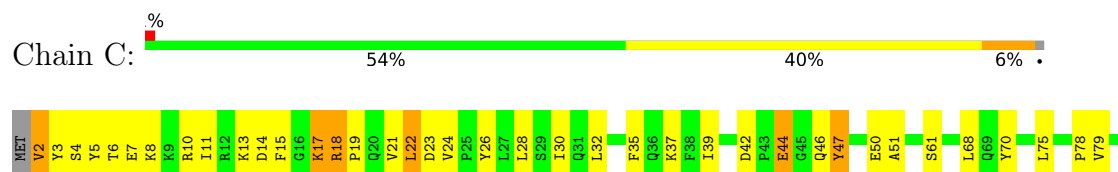
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

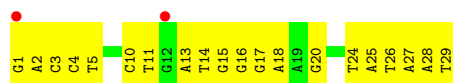








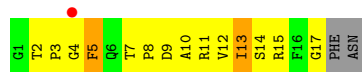
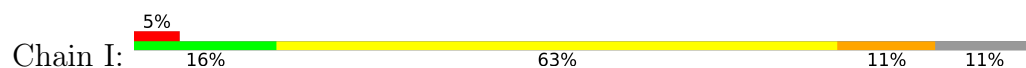
● Molecule 6: non-template strand DNA



● Molecule 7: template strand DNA



● Molecule 8: Capistruin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.89Å 172.89Å 385.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.25 49.45 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.45-3.25) 99.3 (49.45-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.273 , 0.316 0.276 , 0.317	Depositor DCC
R_{free} test set	1980 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28613	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, ZN, EPE

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	0.13	0/1729	0.37	0/2349
1	B	0.11	0/1677	0.40	0/2274
2	C	0.13	0/10654	0.34	0/14375
3	D	0.13	0/9794	0.36	1/13212 (0.0%)
4	E	0.11	0/629	0.32	0/847
5	F	0.12	0/3239	0.33	0/4352
6	N	0.24	0/666	0.39	0/1026
7	T	0.26	0/552	0.41	1/849 (0.1%)
8	I	0.28	0/129	0.53	0/173
All	All	0.14	0/29069	0.36	2/39457 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	C	0	4
3	D	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1244	GLN	N-CA-C	8.11	123.21	113.16
7	T	11	DA	C4'-C3'-O3'	-5.64	101.54	110.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ASP	Peptide
1	B	231	PHE	Peptide
2	C	1340	GLU	Peptide
2	C	198	ILE	Peptide
2	C	234	ASP	Peptide
2	C	985	GLU	Peptide
3	D	1023	HIS	Peptide
3	D	357	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1709	0	1700	69	0
1	B	1658	0	1669	87	0
2	C	10489	0	10490	475	0
3	D	9649	0	9859	548	0
4	E	627	0	634	34	0
5	F	3197	0	3251	152	0
6	N	595	0	329	35	0
7	T	492	0	269	36	0
8	I	126	0	123	22	0
9	C	4	6	6	1	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
12	D	15	17	17	7	0
13	A	1	0	0	1	0
13	B	2	0	0	0	0
13	C	13	0	0	2	0
13	D	3	0	0	3	0
13	E	1	0	0	0	0
13	F	5	0	0	0	0
13	T	1	0	0	1	0
All	All	28590	23	28347	1348	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 24.

All (1348) 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)
7:T:10:DC:H2''	7:T:11:DA:H5'	1.27	1.11
1:A:26:VAL:HG23	1:A:203:ILE:HG13	1.37	1.07
2:C:746:ALA:HB1	2:C:747:GLY:HA3	1.33	1.06
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.40	1.02
1:B:192:VAL:HG21	1:B:198:LEU:HD22	1.46	0.96
7:T:10:DC:H2'	7:T:11:DA:C8	2.03	0.94
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.48	0.93
3:D:161:THR:HG22	3:D:164:GLN:HE21	1.29	0.92
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.51	0.92
5:F:277:MET:HG3	5:F:362:ASN:HD22	1.30	0.92
3:D:615:LYS:HE2	4:E:7:GLN:HB3	1.52	0.91
1:B:47:LEU:HD21	1:B:220:ALA:HB2	1.49	0.91
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.52	0.90
3:D:860:ARG:HD2	3:D:861:ASN:HD22	1.35	0.90
2:C:246:LEU:HD12	2:C:246:LEU:H	1.37	0.90
1:B:54:CYS:SG	1:B:148:ARG:NH1	2.46	0.88
3:D:1155:ILE:HG12	3:D:1210:ILE:HD11	1.52	0.88
5:F:401:PHE:HA	5:F:404:LEU:HD12	1.55	0.87
7:T:10:DC:H5'	7:T:10:DC:C6	2.08	0.87
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.55	0.87
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.56	0.87
2:C:251:ALA:HB2	2:C:269:ILE:HD12	1.56	0.86
3:D:822:MET:HE2	3:D:822:MET:HA	1.57	0.86
2:C:1151:LEU:HD22	2:C:1198:LEU:HD23	1.58	0.86
2:C:368:ARG:NE	13:C:1502:HOH:O	2.08	0.85
2:C:1298:VAL:HA	2:C:1301:ARG:HD2	1.58	0.85
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.39	0.85
8:I:4:GLY:HA3	8:I:15:ARG:N	1.90	0.85
2:C:111:GLU:N	13:C:1501:HOH:O	2.08	0.85
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.59	0.84
3:D:846:GLU:HB2	13:D:1601:HOH:O	1.76	0.84
7:T:10:DC:H2''	7:T:11:DA:C5'	2.07	0.84
2:C:1109:ILE:HD11	3:D:740:LEU:HD12	1.60	0.84
7:T:9:DC:H2''	7:T:10:DC:C5'	2.08	0.84
2:C:1161:LEU:HD12	2:C:1169:VAL:HG22	1.59	0.83
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.42	0.83
1:A:56:VAL:HG22	1:A:146:VAL:HG22	1.62	0.82
3:D:282:LEU:HD21	5:F:410:ILE:HD12	1.61	0.82
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.61	0.82
2:C:550:VAL:HG23	3:D:780:ARG:HG3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.60	0.82
3:D:490:ILE:HG13	3:D:491:LEU:HD23	1.61	0.82
3:D:1179:PRO:HG2	3:D:1184:ASP:HA	1.61	0.82
5:F:492:ASP:HA	5:F:495:ARG:HE	1.44	0.81
2:C:118:LYS:NZ	2:C:487:LEU:O	2.12	0.81
2:C:199:ASP:O	2:C:201:ARG:N	2.11	0.81
6:N:13:DA:H61	7:T:12:DT:H3	1.29	0.81
2:C:847:PRO:HB3	2:C:1047:LEU:HD11	1.61	0.81
1:A:91:ARG:HB2	1:A:210:THR:HG23	1.60	0.81
3:D:781:LYS:HB3	8:I:5:PHE:HE1	1.46	0.81
3:D:502:PRO:HB3	3:D:506:VAL:HB	1.63	0.81
5:F:284:GLU:OE2	5:F:359:LYS:NZ	2.13	0.81
7:T:10:DC:C2'	7:T:11:DA:H5'	2.09	0.80
3:D:559:ALA:O	3:D:560:ASN:ND2	2.14	0.80
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.47	0.80
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.62	0.80
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.63	0.80
2:C:232:ILE:HD12	2:C:237:LEU:HD22	1.64	0.79
2:C:400:VAL:HG12	2:C:584:TYR:HB3	1.62	0.79
3:D:491:LEU:HA	3:D:498:PRO:HA	1.62	0.79
3:D:888:CYS:SG	3:D:890:THR:OG1	2.41	0.79
1:A:95:LYS:O	1:A:148:ARG:NH2	2.14	0.79
3:D:157:GLN:N	3:D:157:GLN:OE1	2.15	0.79
3:D:1282:TYR:O	3:D:1285:VAL:HG12	1.83	0.78
2:C:1109:ILE:HD12	3:D:763:PHE:HB3	1.64	0.78
8:I:7:THR:O	8:I:14:SER:N	2.15	0.78
3:D:230:SER:OG	3:D:232:ASN:ND2	2.17	0.78
2:C:231:GLU:OE1	2:C:332:ARG:NH2	2.16	0.78
3:D:525:MET:O	3:D:548:VAL:HG13	1.84	0.77
3:D:591:ILE:HG23	3:D:604:MET:HE2	1.66	0.77
2:C:609:ILE:HD13	2:C:609:ILE:H	1.50	0.76
3:D:1184:ASP:N	3:D:1185:PRO:HD3	1.99	0.76
3:D:1344:LEU:O	3:D:1346:GLY:N	2.18	0.76
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.68	0.76
2:C:582:ASN:HD21	2:C:586:PHE:H	1.31	0.76
7:T:10:DC:H5'	7:T:10:DC:H6	1.50	0.76
3:D:1179:PRO:HD2	3:D:1184:ASP:HB3	1.67	0.76
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.67	0.76
5:F:572:THR:HG22	5:F:575:GLU:HB2	1.67	0.76
5:F:583:THR:HG22	5:F:584:ARG:H	1.50	0.76
1:A:215:GLU:OE1	1:A:219:ARG:NH1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1155:ILE:CG1	3:D:1210:ILE:HD11	2.16	0.75
1:A:13:LEU:HD23	1:A:13:LEU:H	1.52	0.75
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.68	0.75
3:D:1243:LEU:HD13	3:D:1243:LEU:O	1.87	0.75
5:F:115:GLY:O	5:F:119:ILE:HG12	1.87	0.74
2:C:199:ASP:C	2:C:201:ARG:H	1.95	0.74
5:F:277:MET:CG	5:F:362:ASN:HD22	2.01	0.74
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.69	0.74
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.70	0.74
3:D:1283:SER:O	3:D:1287:ILE:HG23	1.88	0.74
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.21	0.74
2:C:1164:PHE:CB	2:C:1168:GLU:HB2	2.18	0.73
3:D:1172:LYS:HB3	3:D:1191:PRO:HA	1.69	0.73
3:D:20:ILE:HD13	3:D:1344:LEU:HD21	1.68	0.73
3:D:797:THR:O	3:D:801:VAL:HG13	1.87	0.73
5:F:360:ASP:HA	5:F:363:ARG:HD3	1.70	0.73
1:B:228:LEU:O	1:B:231:PHE:HB2	1.88	0.73
3:D:1252:HIS:O	3:D:1255:VAL:HG12	1.88	0.73
7:T:6:DT:H5''	13:T:101:HOH:O	1.88	0.73
1:A:162:GLU:O	1:A:164:ASP:N	2.21	0.73
2:C:198:ILE:O	2:C:199:ASP:O	2.05	0.73
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.71	0.73
3:D:1368:ASP:HA	3:D:1371:ARG:HH11	1.54	0.73
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.71	0.72
3:D:1210:ILE:HD13	3:D:1210:ILE:H	1.53	0.72
2:C:886:LYS:HB3	2:C:916:SER:O	1.89	0.72
5:F:515:GLU:HG2	5:F:516:ASP:H	1.54	0.72
2:C:528:ARG:NH2	2:C:576:SER:O	2.22	0.72
2:C:720:ARG:HH21	2:C:741:MET:HA	1.54	0.72
5:F:127:ILE:O	5:F:130:VAL:HG22	1.89	0.72
3:D:504:GLN:OE1	3:D:731:ARG:NH1	2.23	0.72
3:D:1012:ALA:HB3	3:D:1015:GLU:HG3	1.70	0.72
7:T:9:DC:H2''	7:T:10:DC:H5''	1.69	0.72
1:B:74:VAL:HG12	1:B:76:GLU:H	1.55	0.72
5:F:597:LYS:HG2	5:F:603:ARG:HH12	1.55	0.72
5:F:493:LYS:O	5:F:496:LYS:HG2	1.89	0.71
5:F:396:ASN:C	5:F:397:ARG:HD2	2.15	0.71
3:D:76:LYS:O	3:D:77:ARG:HG2	1.90	0.71
3:D:781:LYS:HB3	8:I:5:PHE:CE1	2.24	0.71
6:N:14:DT:H2'	6:N:15:DG:N7	2.05	0.71
7:T:14:DA:H2''	7:T:15:DG:H5'	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:832:LYS:HE2	3:D:1242:ARG:HG2	1.72	0.71
2:C:533:LEU:HD21	2:C:540:ARG:HG3	1.71	0.71
3:D:186:GLN:O	3:D:190:LYS:HG3	1.91	0.71
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.71	0.70
2:C:1146:GLN:HG2	2:C:1161:LEU:HD23	1.72	0.70
4:E:25:ARG:HD2	4:E:64:LEU:HD13	1.72	0.70
5:F:346:GLN:NE2	5:F:350:GLU:OE2	2.21	0.70
5:F:396:ASN:O	5:F:397:ARG:HD2	1.90	0.70
3:D:364:HIS:HB2	3:D:485:MET:HE3	1.73	0.70
3:D:768:ASN:H	3:D:768:ASN:HD22	1.36	0.70
3:D:935:PHE:HB2	8:I:13:ILE:HD11	1.71	0.70
3:D:292:VAL:O	3:D:296:LYS:HG2	1.92	0.70
2:C:18:ARG:HH12	2:C:621:SER:H	1.39	0.70
2:C:582:ASN:ND2	2:C:586:PHE:H	1.89	0.70
3:D:325:LYS:HE3	3:D:330:MET:HG2	1.72	0.70
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.40	0.70
3:D:549:LYS:HG2	3:D:571:ASP:HA	1.74	0.70
2:C:270:THR:O	2:C:274:ILE:HD12	1.91	0.70
3:D:596:LEU:H	12:D:1504:EPE:H71	1.56	0.70
2:C:960:LEU:HB3	2:C:1025:PHE:HE1	1.57	0.70
3:D:785:ASP:OD1	3:D:789:LYS:NZ	2.24	0.70
6:N:24:DT:H4'	6:N:25:DA:OP2	1.92	0.70
2:C:521:LEU:HB2	2:C:794:LEU:HD21	1.74	0.70
5:F:530:LEU:HD23	5:F:530:LEU:H	1.57	0.69
3:D:220:ARG:NH1	3:D:224:LEU:HD11	2.07	0.69
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.74	0.69
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.57	0.69
5:F:290:LEU:HB3	5:F:333:VAL:CG2	2.21	0.69
1:B:136:GLU:HG2	1:B:137:ASN:OD1	1.93	0.69
3:D:596:LEU:HD22	12:D:1504:EPE:O8	1.93	0.69
8:I:8:PRO:HA	8:I:13:ILE:HA	1.75	0.69
2:C:299:LYS:HE3	2:C:334:GLU:HG3	1.75	0.69
2:C:1005:GLU:O	2:C:1006:GLU:HB3	1.93	0.69
3:D:128:LEU:HB2	3:D:130:MET:HG2	1.75	0.69
7:T:9:DC:C2'	7:T:10:DC:H5''	2.22	0.69
2:C:1299:ASN:O	2:C:1303:LYS:HG2	1.91	0.69
3:D:161:THR:HG22	3:D:164:GLN:NE2	2.07	0.69
3:D:658:GLU:O	3:D:661:VAL:HG22	1.93	0.69
5:F:394:TYR:O	5:F:397:ARG:HD3	1.92	0.69
3:D:129:ASP:OD2	3:D:220:ARG:NH2	2.27	0.68
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:THR:HG23	2:C:133:ASN:H	1.59	0.68
2:C:237:LEU:HD23	2:C:237:LEU:H	1.58	0.68
3:D:756:GLU:O	3:D:758:PRO:HD3	1.94	0.68
3:D:1002:VAL:HB	3:D:1019:ASN:HB3	1.75	0.68
3:D:264:ASP:HB3	3:D:324:LEU:HB2	1.76	0.68
3:D:556:GLU:O	3:D:564:VAL:HG22	1.94	0.68
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.07	0.68
3:D:514:THR:HG21	3:D:596:LEU:CB	2.24	0.68
5:F:123:ILE:HG12	5:F:375:ALA:HB3	1.76	0.68
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.75	0.67
1:B:192:VAL:HG12	1:B:193:GLU:H	1.59	0.67
2:C:841:ARG:CZ	3:D:257:GLY:HA3	2.24	0.67
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	1.76	0.67
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.22	0.67
2:C:241:LEU:CD1	2:C:246:LEU:HD11	2.24	0.67
2:C:1101:LEU:HD13	3:D:504:GLN:HB3	1.76	0.67
2:C:2:VAL:HG12	2:C:3:TYR:H	1.59	0.67
3:D:709:ARG:HD2	3:D:710:ASP:OD2	1.94	0.67
3:D:950:ILE:HG13	3:D:1020:TRP:HH2	1.60	0.67
5:F:547:VAL:HG21	5:F:607:LEU:HD11	1.77	0.67
2:C:227:LYS:H	2:C:227:LYS:HD3	1.59	0.66
2:C:736:VAL:HG22	2:C:747:GLY:O	1.95	0.66
3:D:615:LYS:HE3	4:E:8:ASP:OD1	1.95	0.66
2:C:5:TYR:O	2:C:8:LYS:HG2	1.95	0.66
3:D:415:VAL:HG23	3:D:416:ILE:HD12	1.76	0.66
2:C:30:ILE:HD12	2:C:30:ILE:H	1.61	0.66
2:C:37:LYS:HD2	2:C:47:TYR:CD1	2.30	0.66
2:C:107:ARG:O	2:C:112:GLY:HA2	1.95	0.66
2:C:548:ARG:NH2	2:C:567:PRO:O	2.28	0.66
2:C:1060:ILE:HD11	2:C:1076:ILE:HD11	1.75	0.66
3:D:1238:GLN:HB3	3:D:1242:ARG:HH21	1.61	0.66
3:D:337:ARG:HE	3:D:341:ASN:HD22	1.44	0.66
3:D:1023:HIS:CD2	3:D:1024:THR:HA	2.30	0.66
2:C:1082:ILE:H	2:C:1082:ILE:HD12	1.60	0.66
2:C:1105:SER:HB2	3:D:731:ARG:HG3	1.76	0.66
2:C:1124:ILE:HG21	2:C:1180:MET:HE3	1.76	0.66
3:D:279:LEU:HD11	3:D:296:LYS:HD3	1.78	0.66
5:F:406:GLN:O	5:F:410:ILE:HG12	1.96	0.66
2:C:736:VAL:HG23	2:C:741:MET:HE2	1.76	0.66
2:C:888:THR:HG23	2:C:914:LYS:HB3	1.78	0.66
2:C:1296:ASP:OD1	3:D:345:LYS:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:362:ARG:H	3:D:365:GLN:HE21	1.42	0.66
5:F:554:ARG:HG3	5:F:580:PHE:HE2	1.61	0.66
2:C:131:THR:HG22	2:C:135:THR:H	1.61	0.65
3:D:1344:LEU:O	3:D:1349:GLU:HG3	1.95	0.65
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.77	0.65
3:D:957:SER:OG	3:D:1009:GLU:O	2.11	0.65
5:F:573:LEU:H	5:F:573:LEU:HD23	1.61	0.65
2:C:400:VAL:HG11	2:C:452:ARG:HH11	1.61	0.65
2:C:1341:ASP:OD1	2:C:1341:ASP:N	2.16	0.65
3:D:42:GLU:OE2	5:F:451:ARG:NE	2.21	0.65
5:F:532:LEU:HD12	5:F:532:LEU:H	1.62	0.65
3:D:1327:GLU:HG3	3:D:1330:ARG:HB3	1.79	0.65
5:F:280:VAL:HG13	5:F:344:LEU:HD11	1.79	0.65
7:T:12:DT:H2''	7:T:13:DC:C5	2.32	0.65
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.79	0.65
3:D:984:LEU:HD22	3:D:993:GLU:HG3	1.79	0.65
2:C:230:PHE:O	2:C:333:ILE:HB	1.96	0.65
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.30	0.65
2:C:164:THR:HG22	2:C:165:HIS:ND1	2.12	0.65
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.79	0.65
3:D:950:ILE:HG13	3:D:1020:TRP:CH2	2.32	0.65
1:A:97:GLU:OE1	1:A:147:GLN:NE2	2.28	0.65
2:C:1223:ARG:NH2	3:D:721:SER:OG	2.29	0.65
8:I:13:ILE:H	8:I:13:ILE:HD12	1.61	0.65
3:D:681:LYS:O	3:D:685:ILE:HG23	1.96	0.65
7:T:9:DC:H1'	7:T:10:DC:H5''	1.79	0.65
2:C:838:CYS:HB2	2:C:918:LEU:HB2	1.80	0.64
3:D:478:LEU:HG	4:E:47:THR:HG23	1.79	0.64
3:D:1177:ILE:HG22	3:D:1179:PRO:HD3	1.78	0.64
3:D:357:VAL:HG13	3:D:461:PHE:CE2	2.32	0.64
3:D:1167:LYS:HG2	3:D:1174:ARG:HD2	1.79	0.64
3:D:196:GLN:OE1	3:D:196:GLN:N	2.30	0.64
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.62	0.64
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.80	0.64
2:C:206:ALA:O	2:C:209:ILE:HG22	1.97	0.64
3:D:709:ARG:N	3:D:712:GLN:O	2.26	0.64
7:T:10:DC:H2'	7:T:11:DA:N9	2.12	0.64
1:B:82:LEU:HD23	1:B:173:VAL:HG22	1.78	0.64
3:D:514:THR:OG1	3:D:595:ALA:O	2.15	0.64
3:D:1172:LYS:HB3	3:D:1191:PRO:CA	2.28	0.64
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.78	0.64
2:C:985:GLU:HB2	2:C:989:LEU:HB2	1.80	0.64
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.80	0.64
3:D:664:ILE:HG23	3:D:681:LYS:HD3	1.80	0.64
3:D:1172:LYS:CB	3:D:1191:PRO:HA	2.28	0.64
3:D:1189:MET:C	3:D:1190:ILE:HD12	2.23	0.64
1:B:194:GLN:HE21	1:B:194:GLN:HA	1.62	0.64
3:D:1361:THR:HG23	4:E:21:LEU:HD21	1.79	0.64
1:A:29:GLU:HG3	1:A:200:LYS:HB2	1.80	0.63
5:F:497:VAL:O	5:F:500:ILE:HG22	1.98	0.63
5:F:516:ASP:OD1	5:F:516:ASP:N	2.30	0.63
6:N:1:DG:H2"	6:N:2:DA:C8	2.32	0.63
1:B:78:ILE:HA	1:B:81:ILE:HD12	1.81	0.63
3:D:597:GLY:H	12:D:1504:EPE:H51	1.64	0.63
5:F:597:LYS:HG2	5:F:603:ARG:NH1	2.12	0.63
2:C:995:ASP:OD1	2:C:995:ASP:N	2.32	0.63
3:D:246:PRO:HB2	3:D:249:LEU:HD23	1.80	0.63
3:D:1162:ILE:O	3:D:1178:THR:HB	1.98	0.63
2:C:135:THR:HG21	2:C:515:MET:HE2	1.80	0.63
2:C:593:LYS:NZ	2:C:594:VAL:O	2.30	0.63
3:D:361:LEU:HD13	3:D:366:CYS:HA	1.80	0.63
3:D:528:THR:HG22	3:D:532:GLU:OE2	1.99	0.63
1:B:57:THR:HA	1:B:175:ALA:HB2	1.79	0.63
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.80	0.63
2:C:1042:LEU:HB3	2:C:1046:VAL:HG13	1.79	0.63
3:D:71:LEU:HB2	3:D:90:VAL:HG21	1.81	0.63
3:D:45:ASN:O	3:D:46:TYR:HD1	1.80	0.63
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.80	0.63
3:D:520:ALA:HB3	3:D:546:ALA:HA	1.81	0.63
6:N:16:DG:N2	7:T:10:DC:O2	2.32	0.63
1:A:83:LEU:HD23	2:C:694:ARG:NH2	2.14	0.62
2:C:906:PHE:HZ	5:F:604:SER:HB2	1.62	0.62
5:F:125:ASP:O	5:F:129:GLN:HG3	1.99	0.62
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.82	0.62
2:C:268:ARG:NH2	2:C:269:ILE:O	2.32	0.62
3:D:700:ASN:O	3:D:704:GLU:HB2	1.98	0.62
1:B:34:GLY:N	1:B:199:ASP:OD2	2.32	0.62
2:C:894:GLN:OE1	2:C:894:GLN:N	2.33	0.62
3:D:211:GLU:O	3:D:214:ARG:N	2.27	0.62
2:C:106:GLU:HB2	2:C:114:VAL:HG22	1.80	0.62
2:C:237:LEU:H	2:C:237:LEU:CD2	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:493:LYS:O	5:F:497:VAL:HG23	2.00	0.62
7:T:10:DC:H2''	7:T:11:DA:O4'	2.00	0.62
1:B:25:LYS:HG2	1:B:204:GLU:HG3	1.82	0.61
3:D:848:VAL:HB	3:D:858:VAL:HG12	1.81	0.61
3:D:936:HIS:HA	8:I:12:VAL:HG12	1.81	0.61
4:E:26:ARG:NE	4:E:53:GLU:OE1	2.23	0.61
3:D:271:ARG:O	3:D:275:ARG:HG3	2.00	0.61
5:F:426:LYS:NZ	6:N:28:DA:OP1	2.27	0.61
8:I:7:THR:OG1	8:I:8:PRO:HD2	2.00	0.61
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.81	0.61
2:C:1070:HIS:O	2:C:1108:ASN:ND2	2.34	0.61
2:C:548:ARG:HE	2:C:569:ILE:HD12	1.65	0.61
2:C:877:VAL:HG21	2:C:883:LEU:HD21	1.82	0.61
2:C:1252:SER:HB2	2:C:1255:THR:O	2.00	0.61
2:C:1060:ILE:HD11	2:C:1076:ILE:CD1	2.30	0.61
3:D:514:THR:HG21	3:D:596:LEU:HG	1.83	0.61
3:D:984:LEU:HB2	3:D:993:GLU:HB2	1.83	0.61
8:I:7:THR:CG2	8:I:17:GLY:CA	2.79	0.61
2:C:960:LEU:HB3	2:C:1025:PHE:CE1	2.35	0.61
3:D:78:LEU:HD11	3:D:81:ARG:HD3	1.81	0.61
1:B:99:ILE:HB	1:B:145:LYS:HG2	1.83	0.61
2:C:195:PHE:CD1	2:C:203:LYS:HG2	2.34	0.61
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.31	0.61
2:C:1062:PRO:HG3	2:C:1078:LYS:HA	1.82	0.60
4:E:7:GLN:O	4:E:11:GLU:HG2	2.01	0.60
5:F:479:THR:HG23	5:F:480:PRO:HD2	1.83	0.60
1:A:51:MET:HB2	1:A:179:PRO:HD2	1.82	0.60
1:B:131:CYS:SG	1:B:132:HIS:N	2.73	0.60
3:D:1135:THR:N	3:D:1136:GLY:HA2	2.15	0.60
3:D:1218:HIS:O	3:D:1222:ARG:HG3	2.01	0.60
1:B:47:LEU:HD12	1:B:183:ILE:CD1	2.32	0.60
2:C:237:LEU:CD1	2:C:292:ILE:HD12	2.30	0.60
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.84	0.60
2:C:1073:LYS:HG3	3:D:462:ASP:HB2	1.81	0.60
2:C:624:ASP:CB	2:C:625:GLU:HG2	2.31	0.60
2:C:979:LEU:HD13	2:C:1011:LEU:HD11	1.83	0.60
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.34	0.60
3:D:1022:PRO:HG2	3:D:1023:HIS:ND1	2.15	0.60
3:D:1146:GLU:OE2	3:D:1310:THR:HG22	2.00	0.60
1:A:74:VAL:HG22	1:A:76:GLU:H	1.66	0.60
2:C:1142:ARG:HH22	2:C:1165:SER:C	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:650:LYS:HE2	3:D:654:ILE:CD1	2.31	0.60
3:D:1179:PRO:HB2	3:D:1184:ASP:OD2	2.02	0.60
5:F:561:MET:HG3	5:F:571:TYR:CD1	2.37	0.60
2:C:364:VAL:HG13	2:C:376:PRO:HG3	1.83	0.60
2:C:1027:LYS:HG3	2:C:1028:LYS:N	2.17	0.60
3:D:78:LEU:CD1	3:D:81:ARG:HD3	2.31	0.60
3:D:396:ALA:O	3:D:400:MET:HG3	2.01	0.60
5:F:130:VAL:O	5:F:134:VAL:HG23	2.01	0.60
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.23	0.60
5:F:530:LEU:HD12	5:F:532:LEU:HD13	1.84	0.60
2:C:365:GLU:OE1	2:C:368:ARG:NH2	2.35	0.60
3:D:390:LEU:O	3:D:400:MET:HE1	2.02	0.60
3:D:1314:LEU:HD11	3:D:1330:ARG:HH22	1.66	0.60
2:C:494:ASN:HD22	2:C:496:LYS:H	1.47	0.59
5:F:601:PRO:O	5:F:602:SER:OG	2.16	0.59
1:B:102:LEU:HD23	1:B:115:ILE:HG23	1.84	0.59
3:D:405:GLU:O	3:D:408:VAL:HG12	2.02	0.59
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.84	0.59
3:D:656:GLU:O	3:D:660:GLU:HG3	2.02	0.59
3:D:1005:LYS:HB3	3:D:1009:GLU:HG3	1.84	0.59
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.83	0.59
2:C:836:LEU:HD21	2:C:1054:LEU:HD13	1.83	0.59
1:B:54:CYS:SG	1:B:92:VAL:HB	2.41	0.59
2:C:308:GLU:OE2	2:C:309:LEU:N	2.36	0.59
5:F:571:TYR:HB3	5:F:575:GLU:HB3	1.84	0.59
2:C:448:LEU:HB2	2:C:553:THR:HB	1.84	0.59
3:D:885:VAL:HG22	3:D:899:TYR:HA	1.85	0.59
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.85	0.59
3:D:1347:LEU:HD23	3:D:1358:PRO:HD2	1.84	0.59
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.85	0.59
2:C:1262:LYS:H	2:C:1262:LYS:HD2	1.67	0.59
6:N:15:DG:H8	6:N:15:DG:P	2.25	0.59
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.85	0.59
3:D:961:SER:HB2	3:D:981:GLU:HB3	1.83	0.59
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.85	0.59
5:F:437:GLN:HG3	5:F:438:ALA:N	2.16	0.59
5:F:316:PHE:HZ	5:F:333:VAL:HG13	1.68	0.58
8:I:9:ASP:OD1	8:I:10:ALA:N	2.34	0.58
5:F:127:ILE:HA	5:F:130:VAL:HG13	1.84	0.58
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.84	0.58
3:D:131:PRO:O	3:D:135:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:273:MET:HE3	5:F:365:MET:HE1	1.85	0.58
3:D:265:LEU:HD21	3:D:327:LEU:HG	1.85	0.58
3:D:220:ARG:HH11	3:D:224:LEU:HD11	1.69	0.58
3:D:600:ALA:HB1	3:D:603:LYS:HG2	1.86	0.58
1:B:16:ILE:HD13	1:B:17:GLU:N	2.18	0.58
2:C:906:PHE:CZ	5:F:604:SER:HB2	2.38	0.58
2:C:1104:PRO:HG2	3:D:725:MET:SD	2.44	0.58
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.85	0.58
3:D:647:PRO:HG3	3:D:697:MET:CB	2.33	0.58
3:D:901:ARG:NH1	3:D:906:GLY:O	2.37	0.58
1:B:8:PHE:HE1	1:B:32:GLU:HG3	1.69	0.58
2:C:303:ASP:HB3	2:C:306:THR:HG23	1.85	0.58
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.85	0.58
1:A:165:GLU:O	1:A:165:GLU:HG3	2.02	0.58
2:C:810:TYR:HE2	2:C:1078:LYS:HE3	1.69	0.58
2:C:812:PHE:HB3	3:D:357:VAL:HG11	1.86	0.58
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.85	0.58
5:F:452:ILE:HB	5:F:457:ILE:HD11	1.85	0.58
2:C:1268:GLN:HE22	3:D:352:ARG:NE	2.02	0.57
3:D:1368:ASP:HA	3:D:1371:ARG:NH1	2.19	0.57
1:B:100:LEU:HD12	1:B:100:LEU:H	1.69	0.57
3:D:96:LYS:H	3:D:96:LYS:HD2	1.68	0.57
3:D:362:ARG:H	3:D:365:GLN:NE2	2.02	0.57
3:D:814:CYS:SG	3:D:816:THR:HG22	2.45	0.57
3:D:935:PHE:HB2	8:I:13:ILE:CD1	2.34	0.57
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.39	0.57
2:C:742:TYR:O	2:C:974:ARG:NH2	2.38	0.57
2:C:1244:HIS:NE2	3:D:352:ARG:NH2	2.52	0.57
2:C:684:ASN:O	2:C:687:ARG:HG2	2.03	0.57
3:D:679:TYR:OH	3:D:754:ILE:HG23	2.05	0.57
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.85	0.57
2:C:35:PHE:O	2:C:39:ILE:HG22	2.05	0.57
2:C:191:LYS:NZ	2:C:191:LYS:HB3	2.20	0.57
7:T:10:DC:C6	7:T:10:DC:C5'	2.85	0.57
2:C:1282:GLY:O	3:D:483:LEU:HD13	2.05	0.57
3:D:644:MET:O	3:D:764:ARG:NH2	2.38	0.57
3:D:418:GLU:OE1	4:E:2:ALA:N	2.38	0.57
3:D:901:ARG:O	3:D:1251:LYS:NZ	2.38	0.57
6:N:25:DA:H8	6:N:25:DA:H5''	1.69	0.57
3:D:615:LYS:HG2	4:E:5:THR:HG21	1.87	0.57
3:D:847:ASP:N	13:D:1601:HOH:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.87	0.56
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	1.86	0.56
3:D:232:ASN:HD22	3:D:232:ASN:N	2.01	0.56
3:D:1250:ASP:O	3:D:1254:GLU:HG3	2.04	0.56
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.86	0.56
2:C:91:THR:HB	2:C:138:ILE:O	2.05	0.56
2:C:246:LEU:H	2:C:246:LEU:CD1	2.12	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.39	0.56
3:D:342:LEU:HD13	3:D:1352:ILE:HG23	1.87	0.56
3:D:482:ALA:O	4:E:16:ARG:NH1	2.34	0.56
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.87	0.56
5:F:357:GLN:O	5:F:361:ILE:HG13	2.05	0.56
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.87	0.56
3:D:877:VAL:HG13	3:D:877:VAL:O	2.05	0.56
5:F:385:ARG:HB2	6:N:29:DT:O2	2.05	0.56
2:C:235:ASN:OD1	2:C:236:LYS:N	2.38	0.56
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.88	0.56
2:C:13:LYS:HE3	2:C:15:PHE:CZ	2.41	0.56
3:D:1243:LEU:CD1	8:I:3:PRO:HD3	2.35	0.56
5:F:503:GLU:OE1	5:F:504:PRO:HD2	2.06	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.87	0.56
6:N:4:DC:H2'	6:N:5:DT:H71	1.88	0.56
7:T:12:DT:H2''	7:T:13:DC:C6	2.41	0.56
2:C:231:GLU:HB2	2:C:331:LYS:HG2	1.88	0.56
2:C:364:VAL:HG13	2:C:376:PRO:CG	2.36	0.56
2:C:847:PRO:CB	2:C:1047:LEU:HD11	2.36	0.56
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	1.88	0.56
5:F:511:ILE:HG13	5:F:512:GLY:H	1.71	0.56
2:C:976:ARG:O	2:C:980:VAL:HG23	2.06	0.55
3:D:1155:ILE:C	3:D:1156:LEU:HD22	2.31	0.55
3:D:1159:ILE:HG21	3:D:1179:PRO:HG3	1.88	0.55
5:F:515:GLU:HG2	5:F:516:ASP:N	2.19	0.55
2:C:1006:GLU:O	2:C:1006:GLU:HG3	2.04	0.55
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.88	0.55
3:D:334:LYS:HA	3:D:339:ARG:HD2	1.89	0.55
3:D:736:GLN:O	3:D:740:LEU:HD22	2.06	0.55
3:D:1165:PHE:HE2	3:D:1200:GLU:HG3	1.71	0.55
5:F:108:VAL:HG11	5:F:381:GLU:HB3	1.88	0.55
5:F:474:MET:HG3	5:F:478:PRO:HA	1.87	0.55
1:B:15:ASP:OD1	1:B:16:ILE:N	2.40	0.55
3:D:689:ALA:O	3:D:693:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HG3	1:B:232:VAL:HA	1.87	0.55
2:C:850:ILE:HG22	2:C:850:ILE:O	2.06	0.55
2:C:1101:LEU:O	3:D:731:ARG:HG2	2.07	0.55
3:D:826:ILE:HG21	3:D:992:LYS:HA	1.88	0.55
2:C:234:ASP:O	2:C:235:ASN:HB2	2.06	0.55
3:D:963:VAL:HG23	3:D:975:ILE:HG23	1.89	0.55
3:D:1357:ILE:HD12	3:D:1357:ILE:O	2.07	0.55
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.89	0.55
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.89	0.55
3:D:201:LEU:HB3	3:D:217:LEU:HD11	1.89	0.55
3:D:686:TRP:CD2	3:D:758:PRO:HG2	2.41	0.55
6:N:13:DA:H2''	6:N:14:DT:C6	2.42	0.55
2:C:103:VAL:HA	2:C:116:ASP:O	2.07	0.55
2:C:398:SER:OG	2:C:399:ALA:N	2.40	0.55
3:D:759:ILE:HD12	3:D:771:GLN:HB3	1.89	0.55
5:F:388:ILE:H	5:F:388:ILE:HD12	1.72	0.55
2:C:980:VAL:O	2:C:980:VAL:HG12	2.07	0.54
3:D:572:THR:OG1	3:D:573:THR:N	2.38	0.54
3:D:26:SER:HB3	3:D:236:TRP:CE2	2.42	0.54
3:D:211:GLU:C	3:D:214:ARG:H	2.15	0.54
3:D:600:ALA:CB	3:D:603:LYS:HG2	2.36	0.54
5:F:124:GLU:O	5:F:127:ILE:HG13	2.07	0.54
6:N:27:DA:H2''	6:N:28:DA:H5'	1.89	0.54
2:C:79:VAL:HG21	5:F:476:ARG:HH11	1.72	0.54
2:C:402:ARG:HG2	2:C:416:GLY:H	1.72	0.54
2:C:1080:ASN:HD21	2:C:1084:ASP:HB2	1.72	0.54
3:D:264:ASP:HB3	3:D:324:LEU:CB	2.37	0.54
3:D:1349:GLU:OE2	3:D:1349:GLU:N	2.35	0.54
2:C:400:VAL:HG11	2:C:452:ARG:NH1	2.22	0.54
2:C:598:VAL:HA	2:C:627:GLY:O	2.07	0.54
3:D:497:GLU:OE2	3:D:1247:LYS:NZ	2.22	0.54
2:C:746:ALA:CB	2:C:747:GLY:HA3	2.13	0.54
1:A:94:GLY:N	1:A:120:ASP:OD2	2.36	0.54
3:D:1273:ASP:N	3:D:1273:ASP:OD1	2.41	0.54
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.88	0.54
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.90	0.54
2:C:10:ARG:HE	2:C:1181:PRO:HG2	1.73	0.54
2:C:635:THR:HG23	2:C:644:LEU:HD22	1.90	0.54
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.90	0.54
3:D:269:TYR:O	3:D:273:ILE:HG13	2.07	0.54
5:F:123:ILE:HG12	5:F:375:ALA:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:ASP:O	3:D:175:GLU:HG2	2.07	0.54
3:D:198:CYS:HB2	3:D:224:LEU:HD13	1.89	0.54
3:D:282:LEU:HD21	5:F:410:ILE:CD1	2.33	0.54
5:F:383:ASN:N	5:F:383:ASN:OD1	2.40	0.54
5:F:395:THR:HG22	5:F:396:ASN:N	2.23	0.54
5:F:407:GLU:HG3	5:F:442:SER:OG	2.08	0.54
1:B:115:ILE:HG22	1:B:116:THR:H	1.73	0.54
6:N:15:DG:H8	6:N:15:DG:OP2	1.91	0.54
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.90	0.53
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.91	0.53
2:C:557:ARG:HG2	2:C:587:LEU:HB3	1.90	0.53
2:C:914:LYS:HG2	2:C:915:ASP:H	1.74	0.53
3:D:93:THR:HG22	3:D:94:GLN:H	1.73	0.53
3:D:502:PRO:HB3	3:D:506:VAL:CB	2.36	0.53
3:D:593:ASN:O	3:D:594:GLN:HG2	2.08	0.53
5:F:412:LEU:HB2	5:F:435:ILE:HD11	1.90	0.53
7:T:9:DC:C1'	7:T:10:DC:H5''	2.38	0.53
1:B:134:THR:HG22	1:B:135:ASP:H	1.73	0.53
2:C:42:ASP:OD2	2:C:44:GLU:HG2	2.08	0.53
2:C:102:LEU:CB	2:C:489:PRO:HG3	2.37	0.53
2:C:762:ASN:HD22	2:C:834:GLN:HA	1.74	0.53
2:C:1294:LYS:CB	3:D:347:VAL:HG13	2.39	0.53
2:C:118:LYS:HD3	2:C:485:ASP:OD1	2.09	0.53
2:C:1132:LEU:HD22	2:C:1177:ARG:NH2	2.23	0.53
2:C:1141:LEU:O	2:C:1145:ILE:HG13	2.08	0.53
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.38	0.53
3:D:355:ILE:HG21	3:D:466:MET:SD	2.48	0.53
3:D:417:ARG:NE	4:E:43:ASN:OD1	2.41	0.53
3:D:1243:LEU:HD13	3:D:1243:LEU:C	2.33	0.53
6:N:14:DT:C2'	6:N:15:DG:C8	2.91	0.53
1:A:218:ARG:CG	1:B:232:VAL:HA	2.38	0.53
1:B:71:LYS:HZ1	1:B:140:ILE:HB	1.74	0.53
3:D:154:LEU:HB3	3:D:158:GLN:OE1	2.08	0.53
3:D:212:THR:HA	3:D:215:LYS:HE2	1.90	0.53
3:D:506:VAL:HG13	3:D:625:MET:HA	1.90	0.53
5:F:126:GLY:O	5:F:130:VAL:HG13	2.09	0.53
5:F:313:ASP:OD1	5:F:341:LEU:HD12	2.09	0.53
1:A:22:THR:OG1	1:A:207:THR:O	2.19	0.53
2:C:1178:LYS:HG2	2:C:1178:LYS:O	2.09	0.53
3:D:514:THR:HG21	3:D:596:LEU:CG	2.39	0.53
3:D:851:PRO:HG3	3:D:876:SER:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:VAL:HG12	4:E:40:PRO:HD2	1.91	0.53
2:C:149:LEU:HD12	2:C:452:ARG:O	2.08	0.53
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.91	0.53
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.91	0.53
3:D:822:MET:HA	3:D:822:MET:CE	2.36	0.53
3:D:1021:ASP:OD2	3:D:1024:THR:N	2.42	0.53
3:D:1268:ASN:O	3:D:1269:ALA:HB3	2.09	0.53
5:F:99:ARG:HA	5:F:99:ARG:HE	1.74	0.53
1:B:59:VAL:HG22	1:B:144:ILE:HA	1.90	0.53
2:C:22:LEU:HD13	2:C:23:ASP:O	2.09	0.53
2:C:899:GLU:O	2:C:903:ARG:HG2	2.09	0.53
3:D:878:ASP:OD1	3:D:878:ASP:N	2.41	0.53
3:D:1220:ILE:HG23	3:D:1224:ARG:HD2	1.91	0.53
5:F:426:LYS:N	6:N:27:DA:OP2	2.33	0.53
6:N:14:DT:C2'	6:N:15:DG:N7	2.72	0.53
1:A:79:LEU:HD13	1:A:83:LEU:CD1	2.40	0.52
2:C:8:LYS:HG3	2:C:1171:ARG:NH2	2.24	0.52
2:C:263:VAL:HG22	2:C:273:HIS:CE1	2.43	0.52
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.42	0.52
3:D:289:ASP:O	3:D:292:VAL:HG22	2.09	0.52
3:D:555:TYR:HB2	3:D:585:LYS:O	2.08	0.52
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.91	0.52
5:F:119:ILE:O	5:F:123:ILE:HG13	2.08	0.52
5:F:271:ASN:O	5:F:275:VAL:HG23	2.09	0.52
2:C:15:PHE:CG	2:C:1190:ALA:HB2	2.44	0.52
2:C:61:SER:HB2	2:C:480:SER:OG	2.10	0.52
2:C:548:ARG:NE	2:C:569:ILE:HD12	2.24	0.52
3:D:26:SER:HB3	3:D:236:TRP:CZ2	2.44	0.52
5:F:114:GLU:HG3	5:F:115:GLY:N	2.23	0.52
5:F:115:GLY:HA2	5:F:118:ASP:OD1	2.09	0.52
2:C:1306:LYS:O	2:C:1309:VAL:HG22	2.09	0.52
1:B:205:MET:HE1	1:B:217:ILE:HG13	1.92	0.52
5:F:320:ILE:O	5:F:327:SER:OG	2.28	0.52
7:T:18:DG:H2''	7:T:19:DA:H5''	1.91	0.52
3:D:69:GLU:OE2	3:D:76:LYS:HE3	2.10	0.52
3:D:620:PHE:O	3:D:624:ILE:HG13	2.10	0.52
3:D:702:GLN:HG3	3:D:703:THR:HG23	1.91	0.52
3:D:746:LEU:N	3:D:746:LEU:HD23	2.24	0.52
5:F:363:ARG:O	5:F:367:ILE:HG13	2.10	0.52
2:C:285:ILE:HD12	2:C:285:ILE:O	2.09	0.52
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:677:ASN:H	2:C:677:ASN:ND2	2.08	0.52
3:D:973:LEU:HB3	3:D:1003:LEU:HB2	1.91	0.52
2:C:268:ARG:HH22	2:C:270:THR:HA	1.74	0.52
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.45	0.52
3:D:1208:ASP:OD1	3:D:1209:VAL:N	2.42	0.52
1:B:47:LEU:HD12	1:B:183:ILE:HD12	1.92	0.52
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.90	0.52
2:C:1163:THR:HB	2:C:1168:GLU:OE2	2.08	0.52
2:C:1212:LEU:HB2	2:C:1225:VAL:HG11	1.90	0.52
7:T:1:DA:H2"	7:T:2:DA:H8	1.74	0.52
1:B:83:LEU:HD23	1:B:83:LEU:C	2.34	0.52
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.91	0.52
3:D:20:ILE:CD1	3:D:1344:LEU:HD21	2.38	0.51
3:D:510:LEU:HA	3:D:513:MET:HE2	1.92	0.51
8:I:4:GLY:HA3	8:I:15:ARG:CA	2.39	0.51
2:C:1109:ILE:HD11	3:D:740:LEU:CD1	2.34	0.51
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.43	0.51
5:F:583:THR:HG22	5:F:584:ARG:N	2.21	0.51
1:A:66:HIS:HD2	2:C:874:GLY:HA2	1.76	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.91	0.51
2:C:898:GLU:HG2	5:F:541:ARG:HA	1.91	0.51
3:D:1348:LYS:O	3:D:1352:ILE:HG13	2.11	0.51
8:I:7:THR:HG23	8:I:17:GLY:HA2	1.91	0.51
2:C:748:ILE:HG13	2:C:966:ILE:HG22	1.93	0.51
2:C:1119:MET:HG2	2:C:1204:LEU:HD13	1.90	0.51
3:D:648:GLU:OE2	3:D:649:LYS:HG3	2.10	0.51
3:D:872:LEU:O	3:D:877:VAL:HG12	2.10	0.51
1:B:77:ASP:HB3	1:B:79:LEU:CD2	2.41	0.51
3:D:122:SER:O	3:D:126:LEU:HD23	2.10	0.51
3:D:531:LYS:H	3:D:531:LYS:HD2	1.75	0.51
3:D:678:ARG:O	3:D:682:VAL:HG23	2.10	0.51
3:D:801:VAL:O	3:D:805:GLN:HG3	2.10	0.51
3:D:1172:LYS:H	3:D:1172:LYS:HD2	1.76	0.51
5:F:94:THR:OG1	5:F:99:ARG:HG2	2.11	0.51
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.10	0.51
3:D:124:ILE:HG23	3:D:189:LEU:HD21	1.91	0.51
1:A:219:ARG:HA	1:A:222:THR:OG1	2.10	0.51
1:B:152:TYR:CE2	1:B:176:CYS:HB3	2.46	0.51
2:C:251:ALA:H	2:C:268:ARG:HA	1.75	0.51
2:C:524:ILE:HD13	2:C:712:SER:HB3	1.92	0.51
2:C:696:ASP:O	2:C:795:ALA:HB1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.44	0.51
3:D:133:ARG:O	3:D:137:ARG:HG2	2.11	0.51
3:D:520:ALA:HB1	3:D:543:SER:OG	2.11	0.51
3:D:597:GLY:N	12:D:1504:EPE:H51	2.24	0.51
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.41	0.51
3:D:1330:ARG:O	3:D:1334:GLU:HG3	2.11	0.51
2:C:254:ASP:HA	2:C:263:VAL:O	2.10	0.51
3:D:212:THR:HA	3:D:215:LYS:HG3	1.93	0.51
3:D:819:GLY:CA	3:D:883:ARG:HA	2.41	0.51
3:D:935:PHE:CB	8:I:13:ILE:HD11	2.40	0.51
3:D:1210:ILE:HD13	3:D:1210:ILE:N	2.24	0.51
5:F:402:LEU:O	5:F:405:ILE:HG13	2.10	0.51
3:D:514:THR:OG1	3:D:596:LEU:HB2	2.10	0.51
3:D:735:ALA:O	3:D:738:ARG:HG2	2.10	0.51
3:D:813:ASP:OD1	3:D:815:GLY:N	2.44	0.51
3:D:865:HIS:H	3:D:865:HIS:CD2	2.29	0.51
1:B:71:LYS:NZ	1:B:140:ILE:HB	2.26	0.51
2:C:255:ILE:HB	2:C:262:TYR:HB2	1.92	0.51
2:C:478:ARG:O	2:C:482:GLY:HA3	2.10	0.51
5:F:113:ARG:HH21	5:F:426:LYS:HD2	1.75	0.51
1:A:19:VAL:HG13	1:A:20:SER:H	1.77	0.50
2:C:246:LEU:HD12	2:C:246:LEU:N	2.18	0.50
2:C:1109:ILE:CD1	3:D:763:PHE:HB3	2.37	0.50
3:D:45:ASN:O	3:D:46:TYR:CD1	2.62	0.50
3:D:293:ARG:HH22	5:F:104:GLU:HG2	1.76	0.50
3:D:475:GLU:O	3:D:479:GLU:HG3	2.11	0.50
2:C:262:TYR:HD1	2:C:276:GLN:HE21	1.58	0.50
2:C:696:ASP:OD1	2:C:799:ASN:ND2	2.44	0.50
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.12	0.50
3:D:123:ARG:O	3:D:127:LEU:HB2	2.11	0.50
3:D:145:VAL:HA	3:D:158:GLN:O	2.11	0.50
3:D:1135:THR:CB	3:D:1136:GLY:HA2	2.42	0.50
5:F:479:THR:N	5:F:482:GLU:OE1	2.44	0.50
5:F:466:ILE:O	5:F:470:MET:HG3	2.10	0.50
1:B:136:GLU:HG2	1:B:137:ASN:N	2.24	0.50
2:C:118:LYS:NZ	2:C:485:ASP:O	2.44	0.50
2:C:675:ASP:HB2	2:C:1107:MET:CB	2.35	0.50
3:D:600:ALA:HB3	12:D:1504:EPE:H81	1.93	0.50
7:T:15:DG:H1'	7:T:16:DG:H5'	1.94	0.50
1:B:136:GLU:CG	1:B:137:ASN:N	2.74	0.50
2:C:1304:MET:HE2	2:C:1308:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:30:ILE:CG2	3:D:243:PRO:HG3	2.42	0.50
3:D:1244:GLN:O	3:D:1244:GLN:HG3	2.12	0.50
5:F:133:SER:HB2	5:F:365:MET:SD	2.51	0.50
6:N:14:DT:H2"	6:N:15:DG:C8	2.47	0.50
1:A:231:PHE:O	13:A:301:HOH:O	2.18	0.50
2:C:545:PHE:CE2	3:D:788:LEU:HD12	2.47	0.50
2:C:575:LEU:HD23	2:C:576:SER:O	2.11	0.50
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.94	0.50
2:C:1005:GLU:HG2	2:C:1006:GLU:H	1.77	0.50
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.17	0.50
3:D:1243:LEU:HD11	8:I:3:PRO:HD3	1.93	0.50
2:C:598:VAL:HG13	2:C:627:GLY:O	2.12	0.50
2:C:993:PRO:HG2	2:C:996:ARG:HD3	1.94	0.50
3:D:770:LEU:O	3:D:774:ILE:HG13	2.11	0.50
2:C:811:ASN:HA	2:C:815:SER:HB2	1.93	0.50
2:C:845:LEU:HB3	2:C:889:PRO:HB2	1.94	0.50
3:D:317:THR:HG22	3:D:322:ARG:O	2.12	0.50
3:D:552:ILE:HD12	3:D:552:ILE:O	2.12	0.50
3:D:1198:VAL:HB	3:D:1210:ILE:HG22	1.93	0.50
5:F:511:ILE:HG21	5:F:517:SER:HB3	1.93	0.50
6:N:2:DA:H2"	6:N:3:DC:H6	1.75	0.50
2:C:10:ARG:NH2	2:C:793:GLU:OE2	2.45	0.50
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.45	0.50
3:D:77:ARG:HB3	3:D:79:LYS:HG3	1.94	0.50
3:D:747:MET:HG3	3:D:775:SER:HA	1.92	0.50
3:D:747:MET:HE2	3:D:759:ILE:HG13	1.93	0.50
6:N:13:DA:N6	7:T:12:DT:H3	2.06	0.50
1:A:73:GLY:HA2	1:A:135:ASP:HB2	1.95	0.49
2:C:1294:LYS:HB2	3:D:347:VAL:HG13	1.93	0.49
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.94	0.49
5:F:333:VAL:HG22	5:F:337:VAL:HG23	1.94	0.49
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.93	0.49
2:C:540:ARG:HG2	2:C:568:ASN:HD21	1.78	0.49
3:D:140:TYR:HD2	5:F:100:MET:HE3	1.76	0.49
3:D:357:VAL:HG13	3:D:461:PHE:CZ	2.47	0.49
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.93	0.49
3:D:649:LYS:O	3:D:653:ILE:HG13	2.12	0.49
3:D:1149:ARG:HE	3:D:1153:PRO:HG2	1.77	0.49
2:C:968:GLU:HG2	2:C:1018:TYR:HE1	1.78	0.49
2:C:1326:LEU:HD22	3:D:342:LEU:HD11	1.93	0.49
3:D:268:LEU:CB	3:D:306:LEU:HD23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG13	1:B:125:LYS:HG3	1.94	0.49
1:B:211:ILE:HD11	1:B:215:GLU:HB3	1.93	0.49
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.46	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.27	0.49
3:D:963:VAL:HB	3:D:980:THR:HG23	1.94	0.49
6:N:10:DC:H2"	6:N:11:DT:H71	1.93	0.49
2:C:625:GLU:O	2:C:626:GLU:HG2	2.13	0.49
3:D:131:PRO:HG2	3:D:134:ASP:CG	2.37	0.49
2:C:297:VAL:HG12	2:C:315:MET:O	2.13	0.49
2:C:1287:LEU:O	2:C:1291:LEU:HG	2.11	0.49
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.95	0.49
3:D:885:VAL:HG13	3:D:894:VAL:HG11	1.94	0.49
3:D:1285:VAL:O	3:D:1289:ASN:HB3	2.13	0.49
2:C:815:SER:OG	3:D:357:VAL:HG22	2.13	0.49
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.93	0.49
2:C:1261:GLY:HA2	2:C:1263:ALA:HA	1.93	0.49
3:D:513:MET:HA	3:D:544:LEU:CD2	2.43	0.49
3:D:850:LYS:HG2	3:D:857:LEU:HG	1.94	0.49
7:T:3:DA:H2"	7:T:4:DC:C6	2.47	0.49
8:I:7:THR:CG2	8:I:17:GLY:HA2	2.42	0.49
2:C:231:GLU:OE2	2:C:233:ARG:NH1	2.45	0.49
2:C:300:ASP:OD1	2:C:313:ALA:N	2.46	0.49
2:C:400:VAL:CG1	2:C:584:TYR:HB3	2.37	0.49
3:D:205:LEU:O	3:D:205:LEU:HD13	2.12	0.49
3:D:901:ARG:O	3:D:902:ASP:HB2	2.13	0.49
8:I:2:THR:O	8:I:14:SER:HA	2.13	0.49
1:A:26:VAL:HG23	1:A:203:ILE:CG1	2.27	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.46	0.49
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.94	0.49
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.95	0.49
2:C:367:TYR:CD1	2:C:376:PRO:HB3	2.47	0.49
2:C:714:VAL:HB	2:C:787:PRO:HD2	1.95	0.49
2:C:1196:LYS:O	2:C:1200:LYS:HG3	2.13	0.49
2:C:1214:ASP:HB2	2:C:1221:PHE:CZ	2.47	0.49
3:D:195:GLU:O	3:D:199:GLU:HG3	2.12	0.49
3:D:347:VAL:HG12	3:D:348:ASP:O	2.12	0.49
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.95	0.49
1:A:182:ARG:HG2	1:A:183:ILE:N	2.28	0.49
2:C:68:LEU:HD21	2:C:100:LEU:HD13	1.94	0.49
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.95	0.49
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CD2	1:B:176:CYS:HB3	2.48	0.48
3:D:557:LYS:HA	3:D:563:LEU:HA	1.95	0.48
3:D:708:ASN:HA	3:D:712:GLN:O	2.13	0.48
3:D:903:LEU:HD11	3:D:913:GLU:OE2	2.13	0.48
5:F:316:PHE:CZ	5:F:333:VAL:HG13	2.48	0.48
5:F:426:LYS:HD3	6:N:28:DA:OP2	2.12	0.48
2:C:3:TYR:HB3	2:C:7:GLU:HB2	1.96	0.48
2:C:1332:SER:HB2	3:D:245:LEU:HD13	1.95	0.48
3:D:53:ARG:NH1	3:D:88:CYS:O	2.46	0.48
3:D:201:LEU:CD1	3:D:220:ARG:HD2	2.43	0.48
3:D:1004:ALA:HB3	3:D:1017:VAL:HG12	1.94	0.48
4:E:6:VAL:O	4:E:10:VAL:HG23	2.14	0.48
5:F:110:LEU:HD12	5:F:110:LEU:H	1.78	0.48
2:C:879:GLY:HA2	2:C:920:VAL:HB	1.96	0.48
3:D:337:ARG:NE	3:D:341:ASN:HD22	2.09	0.48
3:D:600:ALA:HB3	12:D:1504:EPE:C8	2.44	0.48
6:N:10:DC:C2'	6:N:11:DT:H71	2.44	0.48
1:B:104:LYS:HZ2	1:B:105:SER:N	2.12	0.48
2:C:232:ILE:HD13	2:C:237:LEU:HB3	1.95	0.48
2:C:1262:LYS:HA	2:C:1263:ALA:HA	1.55	0.48
3:D:97:VAL:HG21	3:D:101:ARG:NH1	2.29	0.48
3:D:868:TRP:O	3:D:872:LEU:HG	2.13	0.48
4:E:69:ARG:O	4:E:72:GLN:HB2	2.12	0.48
2:C:50:GLU:OE2	2:C:70:TYR:OH	2.24	0.48
2:C:103:VAL:HG12	2:C:117:ILE:HG22	1.95	0.48
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.12	0.48
3:D:515:ARG:HH21	3:D:717:VAL:HB	1.78	0.48
3:D:965:SER:HB3	3:D:973:LEU:HG	1.94	0.48
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.94	0.48
3:D:1167:LYS:HG3	3:D:1168:GLU:H	1.77	0.48
2:C:710:VAL:HA	2:C:715:THR:HG21	1.96	0.48
2:C:745:GLU:HG2	2:C:746:ALA:H	1.78	0.48
2:C:1247:SER:HB3	3:D:375:GLU:O	2.12	0.48
2:C:1262:LYS:HD2	2:C:1262:LYS:N	2.28	0.48
3:D:1226:VAL:HG21	3:D:1304:ARG:NE	2.29	0.48
5:F:262:VAL:HG12	5:F:264:LYS:H	1.79	0.48
5:F:554:ARG:HG3	5:F:580:PHE:CE2	2.45	0.48
1:A:38:THR:OG1	1:B:45:ARG:HD3	2.13	0.48
1:B:8:PHE:CE1	1:B:32:GLU:HG3	2.47	0.48
2:C:993:PRO:HG2	2:C:996:ARG:CD	2.44	0.48
3:D:1357:ILE:O	3:D:1362:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:OG1	1:B:232:VAL:CB	2.62	0.48
1:B:56:VAL:HG22	1:B:146:VAL:HG12	1.96	0.48
2:C:311:CYS:HB3	2:C:321:LEU:HD21	1.95	0.48
2:C:996:ARG:O	2:C:1000:LEU:HG	2.14	0.48
2:C:1148:ALA:HB1	2:C:1180:MET:HE1	1.96	0.48
3:D:84:ILE:H	3:D:84:ILE:HD12	1.79	0.48
5:F:572:THR:CG2	5:F:575:GLU:HB2	2.41	0.48
1:B:96:ASP:OD1	1:B:96:ASP:N	2.45	0.48
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.48	0.48
2:C:1137:GLU:O	2:C:1141:LEU:HD13	2.13	0.48
2:C:1143:GLU:OE2	2:C:1147:ARG:NH1	2.47	0.48
2:C:1244:HIS:ND1	2:C:1264:GLN:O	2.47	0.48
3:D:123:ARG:NH2	3:D:1334:GLU:HG2	2.29	0.48
3:D:694:SER:O	3:D:697:MET:HG3	2.13	0.48
3:D:1172:LYS:O	3:D:1173:ARG:HB2	2.14	0.48
1:B:218:ARG:O	1:B:222:THR:HG23	2.13	0.47
2:C:241:LEU:HD23	2:C:285:ILE:HG13	1.95	0.47
2:C:870:ILE:HD12	2:C:944:ARG:HG2	1.96	0.47
3:D:1327:GLU:CG	3:D:1330:ARG:HB3	2.42	0.47
4:E:39:VAL:HG23	4:E:53:GLU:HG2	1.96	0.47
2:C:540:ARG:HG2	2:C:568:ASN:ND2	2.29	0.47
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.49	0.47
3:D:198:CYS:SG	3:D:202:ARG:NH2	2.87	0.47
3:D:268:LEU:HB2	3:D:306:LEU:HD23	1.95	0.47
3:D:474:LEU:HB2	4:E:28:ARG:HH12	1.77	0.47
3:D:743:MET:O	3:D:743:MET:HG3	2.14	0.47
3:D:826:ILE:O	3:D:994:SER:HB3	2.14	0.47
3:D:1371:ARG:HH12	3:D:1372:ARG:HH21	1.61	0.47
2:C:46:GLN:O	2:C:51:ALA:HB2	2.13	0.47
2:C:849:GLU:O	2:C:886:LYS:HG3	2.14	0.47
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.97	0.47
3:D:289:ASP:O	3:D:290:ILE:C	2.57	0.47
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.96	0.47
3:D:1184:ASP:N	3:D:1185:PRO:CD	2.75	0.47
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.95	0.47
3:D:209:ASN:O	3:D:210:SER:HB2	2.13	0.47
4:E:71:GLU:HA	4:E:74:GLU:CG	2.44	0.47
5:F:423:ARG:HD3	6:N:25:DA:C6	2.49	0.47
8:I:4:GLY:HA3	8:I:14:SER:C	2.40	0.47
1:A:188:GLU:HG2	1:A:189:ALA:N	2.29	0.47
3:D:56:LEU:HD11	3:D:273:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.96	0.47
3:D:506:VAL:CG1	3:D:625:MET:HA	2.44	0.47
5:F:270:VAL:HA	5:F:273:MET:HE2	1.97	0.47
1:A:156:SER:OG	2:C:1059:ARG:NH2	2.47	0.47
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.96	0.47
2:C:445:ILE:H	2:C:445:ILE:HD12	1.78	0.47
2:C:518:ASN:O	2:C:691:PRO:HD3	2.14	0.47
2:C:592:ARG:NH1	2:C:653:MET:SD	2.87	0.47
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.80	0.47
2:C:672:GLU:CD	2:C:672:GLU:H	2.22	0.47
2:C:1126:ASP:OD1	2:C:1126:ASP:N	2.46	0.47
2:C:1333:LEU:C	2:C:1335:ILE:H	2.23	0.47
3:D:580:TRP:CD2	3:D:589:TYR:HD1	2.32	0.47
3:D:858:VAL:HG23	3:D:859:PRO:HD2	1.95	0.47
3:D:1005:LYS:C	3:D:1009:GLU:HG3	2.39	0.47
5:F:547:VAL:HG13	5:F:598:LEU:HD21	1.95	0.47
1:B:99:ILE:HG13	1:B:144:ILE:O	2.15	0.47
2:C:909:LYS:HG2	2:C:910:ALA:N	2.29	0.47
3:D:319:SER:O	3:D:319:SER:OG	2.33	0.47
3:D:473:THR:O	3:D:477:GLN:HG3	2.14	0.47
3:D:1344:LEU:O	3:D:1349:GLU:CG	2.62	0.47
4:E:32:VAL:O	4:E:34:GLY:N	2.47	0.47
5:F:540:LEU:HD23	5:F:540:LEU:O	2.14	0.47
1:A:37:HIS:HD2	1:B:45:ARG:HH12	1.61	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG3	1.96	0.47
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.49	0.47
2:C:322:LEU:HD23	2:C:325:LEU:HD11	1.96	0.47
2:C:572:ILE:HG22	2:C:572:ILE:O	2.15	0.47
2:C:1132:LEU:HD23	2:C:1132:LEU:O	2.14	0.47
3:D:377:PHE:O	3:D:381:ILE:HG13	2.14	0.47
3:D:593:ASN:C	3:D:594:GLN:HG2	2.39	0.47
3:D:599:LYS:O	3:D:602:SER:OG	2.32	0.47
3:D:819:GLY:HA3	3:D:883:ARG:HA	1.95	0.47
6:N:3:DC:H2"	6:N:4:DC:OP2	2.15	0.47
7:T:13:DC:H2"	7:T:14:DA:C8	2.50	0.47
1:A:28:LEU:HD21	1:B:231:PHE:HZ	1.79	0.47
1:A:83:LEU:HD23	2:C:694:ARG:CZ	2.45	0.47
2:C:231:GLU:OE1	2:C:331:LYS:HD3	2.15	0.47
3:D:201:LEU:HB3	3:D:217:LEU:CD1	2.45	0.47
3:D:709:ARG:O	3:D:709:ARG:HG3	2.14	0.47
3:D:768:ASN:H	3:D:768:ASN:ND2	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1221:LEU:C	3:D:1221:LEU:HD13	2.40	0.47
1:A:207:THR:HG22	1:A:208:ASN:H	1.80	0.47
1:B:81:ILE:O	1:B:85:LEU:HG	2.15	0.47
2:C:17:LYS:H	2:C:17:LYS:HG2	1.50	0.47
2:C:841:ARG:NH2	3:D:257:GLY:HA3	2.29	0.47
2:C:1029:LEU:O	2:C:1029:LEU:HD23	2.15	0.47
2:C:1151:LEU:HD21	2:C:1197:GLU:HB2	1.97	0.47
2:C:1244:HIS:CE1	3:D:352:ARG:HH21	2.33	0.47
3:D:488:ASN:ND2	4:E:16:ARG:HH12	2.13	0.47
3:D:745:GLY:C	3:D:746:LEU:HD23	2.39	0.47
3:D:875:ASN:N	3:D:875:ASN:OD1	2.45	0.47
5:F:112:THR:HA	5:F:113:ARG:HA	1.63	0.47
7:T:19:DA:H2''	7:T:20:DA:H5'	1.97	0.47
2:C:813:GLU:HB2	3:D:461:PHE:CD2	2.37	0.46
3:D:596:LEU:N	12:D:1504:EPE:H71	2.26	0.46
3:D:597:GLY:O	3:D:601:ILE:HG13	2.15	0.46
5:F:324:LYS:HD3	5:F:326:TRP:HE1	1.80	0.46
5:F:456:MET:O	5:F:460:ILE:HG13	2.15	0.46
7:T:17:DG:H2''	7:T:18:DG:C8	2.49	0.46
1:A:53:GLY:HA2	1:A:179:PRO:HG3	1.98	0.46
2:C:18:ARG:NH1	2:C:621:SER:H	2.11	0.46
2:C:553:THR:HG21	2:C:608:ALA:HB1	1.96	0.46
2:C:878:THR:OG1	2:C:879:GLY:N	2.48	0.46
2:C:970:GLY:O	2:C:973:SER:OG	2.30	0.46
3:D:47:ARG:O	3:D:47:ARG:HD3	2.15	0.46
4:E:26:ARG:HG3	4:E:30:MET:HE2	1.97	0.46
5:F:96:ASP:N	5:F:96:ASP:OD1	2.46	0.46
5:F:331:HIS:O	5:F:334:SER:OG	2.31	0.46
5:F:339:ARG:HH21	5:F:342:GLN:HE21	1.62	0.46
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.98	0.46
2:C:30:ILE:HD12	2:C:30:ILE:N	2.30	0.46
2:C:657:THR:HB	2:C:1187:PHE:HB2	1.97	0.46
2:C:748:ILE:N	2:C:748:ILE:HD13	2.30	0.46
2:C:1340:GLU:OE1	3:D:1341:ARG:NH2	2.41	0.46
3:D:384:LYS:O	3:D:388:ARG:HG3	2.15	0.46
3:D:615:LYS:HZ3	4:E:5:THR:HG23	1.80	0.46
3:D:841:GLY:HA2	3:D:901:ARG:HG2	1.96	0.46
3:D:1172:LYS:HD2	3:D:1172:LYS:N	2.31	0.46
2:C:228:VAL:HB	2:C:335:THR:OG1	2.16	0.46
2:C:961:SER:O	2:C:965:GLN:HG3	2.15	0.46
3:D:321:LYS:O	3:D:321:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.97	0.46
3:D:495:ASN:ND2	3:D:497:GLU:HB2	2.31	0.46
3:D:1023:HIS:O	3:D:1024:THR:O	2.33	0.46
1:B:77:ASP:OD1	1:B:78:ILE:N	2.49	0.46
1:B:82:LEU:CD2	1:B:173:VAL:HG22	2.45	0.46
2:C:17:LYS:HB3	2:C:1154:ASP:O	2.15	0.46
2:C:178:PRO:HA	2:C:397:LEU:HD12	1.97	0.46
2:C:1010:GLN:O	2:C:1014:LEU:HD13	2.16	0.46
2:C:1042:LEU:HB3	2:C:1046:VAL:CG1	2.44	0.46
3:D:749:LYS:HB3	3:D:750:PRO:HD2	1.98	0.46
3:D:850:LYS:HG2	3:D:857:LEU:CD2	2.46	0.46
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.16	0.46
5:F:572:THR:O	5:F:576:VAL:HG23	2.16	0.46
7:T:1:DA:H2"	7:T:2:DA:C8	2.50	0.46
1:A:162:GLU:O	1:A:163:GLU:C	2.59	0.46
1:B:51:MET:O	1:B:150:ARG:HA	2.16	0.46
1:B:180:VAL:HA	1:B:207:THR:HA	1.97	0.46
1:B:205:MET:CE	1:B:217:ILE:HG13	2.46	0.46
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.98	0.46
2:C:398:SER:O	2:C:401:GLY:N	2.48	0.46
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.97	0.46
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.46	0.46
2:C:1236:ASN:O	2:C:1236:ASN:ND2	2.31	0.46
3:D:120:LEU:HB3	3:D:121:PRO:CD	2.33	0.46
3:D:271:ARG:HH12	3:D:315:ALA:HB1	1.81	0.46
3:D:650:LYS:HZ1	3:D:762:ASN:HD22	1.64	0.46
3:D:918:ILE:HG13	3:D:919:ALA:N	2.30	0.46
3:D:1158:GLU:O	3:D:1206:ARG:NH1	2.49	0.46
5:F:136:GLU:O	5:F:353:LEU:HD11	2.16	0.46
2:C:204:LEU:HD13	2:C:208:ILE:HG21	1.98	0.46
2:C:389:PHE:HB2	2:C:390:PHE:CE1	2.51	0.46
2:C:626:GLU:O	2:C:626:GLU:HG3	2.15	0.46
2:C:824:GLN:NE2	2:C:1082:ILE:HD11	2.31	0.46
2:C:922:ASN:HD22	2:C:923:GLY:N	2.13	0.46
2:C:1033:ARG:HB3	2:C:1033:ARG:CZ	2.46	0.46
3:D:232:ASN:HD22	3:D:232:ASN:H	1.63	0.46
3:D:368:LEU:HD23	3:D:369:PRO:O	2.16	0.46
4:E:32:VAL:CG1	4:E:33:GLY:N	2.79	0.46
5:F:439:ILE:O	5:F:443:ILE:HG13	2.16	0.46
1:A:90:VAL:HG11	1:A:146:VAL:HG11	1.97	0.46
3:D:647:PRO:HG3	3:D:697:MET:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:937:ILE:N	8:I:11:ARG:O	2.49	0.46
3:D:1179:PRO:CG	3:D:1184:ASP:HA	2.39	0.46
3:D:1243:LEU:CD1	3:D:1243:LEU:C	2.89	0.46
3:D:1344:LEU:O	3:D:1345:ARG:C	2.58	0.46
7:T:10:DC:C4	7:T:11:DA:N6	2.85	0.46
1:B:26:VAL:HG21	1:B:217:ILE:HD13	1.97	0.45
2:C:1129:ASN:O	2:C:1133:LYS:N	2.37	0.45
3:D:35:PHE:CD2	3:D:101:ARG:HD2	2.51	0.45
3:D:768:ASN:HD21	3:D:771:GLN:CD	2.24	0.45
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.47	0.45
1:B:197:ASP:OD1	1:B:197:ASP:N	2.48	0.45
2:C:141:THR:HG23	9:C:1401:EDO:O2	2.17	0.45
2:C:170:VAL:HG23	2:C:170:VAL:O	2.16	0.45
2:C:521:LEU:HD13	2:C:521:LEU:C	2.41	0.45
2:C:1163:THR:O	2:C:1164:PHE:C	2.58	0.45
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.98	0.45
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.49	0.45
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.97	0.45
2:C:253:PHE:HA	2:C:265:LYS:HB2	1.97	0.45
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.99	0.45
2:C:1340:GLU:CD	3:D:1341:ARG:HE	2.25	0.45
3:D:432:LEU:HD13	3:D:499:ILE:HG21	1.99	0.45
3:D:1210:ILE:H	3:D:1210:ILE:CD1	2.24	0.45
3:D:1356:LEU:HD12	3:D:1365:TYR:CD2	2.51	0.45
5:F:106:GLY:HA2	5:F:385:ARG:NH2	2.31	0.45
5:F:492:ASP:OD1	5:F:493:LYS:HG3	2.16	0.45
2:C:1099:ASN:OD1	2:C:1101:LEU:HB2	2.16	0.45
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.99	0.45
3:D:919:ALA:HB1	3:D:1252:HIS:HB3	1.98	0.45
5:F:483:LEU:O	5:F:487:MET:HB2	2.16	0.45
5:F:510:PRO:HA	5:F:518:HIS:HD2	1.82	0.45
5:F:511:ILE:CG2	5:F:517:SER:HB3	2.47	0.45
7:T:10:DC:C5	7:T:11:DA:N6	2.84	0.45
3:D:360:TYR:OH	3:D:448:GLN:OE1	2.20	0.45
3:D:746:LEU:HD12	3:D:754:ILE:HD11	1.98	0.45
3:D:858:VAL:CG2	3:D:859:PRO:HD2	2.46	0.45
3:D:982:LEU:HB3	3:D:995:TYR:HB2	1.99	0.45
4:E:70:GLN:O	4:E:74:GLU:HG2	2.17	0.45
1:A:31:LEU:HB2	1:A:199:ASP:O	2.16	0.45
2:C:237:LEU:HD11	2:C:289:VAL:HA	1.97	0.45
3:D:197:GLU:OE1	3:D:220:ARG:NH2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:603:LYS:HG3	3:D:604:MET:N	2.31	0.45
3:D:705:THR:CG2	3:D:718:SER:HA	2.47	0.45
3:D:960:LEU:HD13	3:D:963:VAL:HG11	1.99	0.45
2:C:268:ARG:NH2	2:C:270:THR:HA	2.31	0.45
3:D:57:PHE:CZ	3:D:252:LEU:HB2	2.52	0.45
3:D:843:VAL:HG13	3:D:883:ARG:HB2	1.99	0.45
3:D:1280:VAL:HG22	3:D:1281:GLU:H	1.82	0.45
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.51	0.45
5:F:532:LEU:O	5:F:536:THR:HG23	2.16	0.45
1:A:11:PRO:HD2	1:B:227:GLN:O	2.17	0.45
2:C:237:LEU:HD23	2:C:237:LEU:N	2.29	0.45
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.98	0.45
2:C:1301:ARG:H	2:C:1301:ARG:HG3	1.61	0.45
6:N:17:DG:H2''	6:N:18:DA:C8	2.52	0.45
2:C:446:ASP:OD1	2:C:451:ARG:NH2	2.50	0.45
2:C:522:SER:HA	2:C:525:THR:HG22	1.99	0.45
2:C:943:LYS:HE2	2:C:943:LYS:HB3	1.82	0.45
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.44	0.45
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.17	0.45
3:D:798:ARG:O	3:D:801:VAL:HG22	2.17	0.45
3:D:1272:SER:O	3:D:1273:ASP:C	2.60	0.45
6:N:2:DA:H2''	6:N:3:DC:C6	2.51	0.45
2:C:745:GLU:CG	2:C:746:ALA:H	2.30	0.45
3:D:210:SER:O	3:D:212:THR:N	2.50	0.45
5:F:277:MET:CB	5:F:362:ASN:HD22	2.30	0.45
1:B:99:ILE:HD11	1:B:143:ARG:HG2	1.99	0.44
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.82	0.44
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.97	0.44
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.47	0.44
3:D:211:GLU:O	3:D:215:LYS:N	2.50	0.44
7:T:10:DC:H2''	7:T:11:DA:C4'	2.47	0.44
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.32	0.44
1:A:58:GLU:OE2	1:A:170:ARG:NH1	2.50	0.44
2:C:1164:PHE:O	2:C:1165:SER:C	2.60	0.44
3:D:260:PHE:O	5:F:504:PRO:HA	2.18	0.44
4:E:45:LYS:O	4:E:49:ILE:HG13	2.17	0.44
5:F:316:PHE:CZ	5:F:330:LEU:HD22	2.53	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD2	2.33	0.44
2:C:935:THR:N	2:C:1040:ASP:OD2	2.50	0.44
2:C:1205:PRO:HG3	2:C:1210:ILE:HG22	1.99	0.44
3:D:361:LEU:HA	3:D:365:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:782:GLY:O	3:D:786:THR:HG23	2.17	0.44
5:F:105:MET:HE1	5:F:385:ARG:HA	2.00	0.44
2:C:936:ARG:HG2	2:C:937:ASP:H	1.82	0.44
3:D:59:ALA:HB3	3:D:71:LEU:HD12	1.98	0.44
3:D:1021:ASP:CG	3:D:1024:THR:HG22	2.43	0.44
3:D:1348:LYS:O	3:D:1351:VAL:HG23	2.17	0.44
1:B:33:ARG:HG3	1:B:33:ARG:O	2.17	0.44
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.33	0.44
3:D:265:LEU:CD2	3:D:327:LEU:HG	2.47	0.44
3:D:564:VAL:HG23	3:D:564:VAL:O	2.16	0.44
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.17	0.44
5:F:360:ASP:HA	5:F:363:ARG:HH11	1.83	0.44
2:C:99:LYS:HA	2:C:121:GLU:HA	1.99	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:HB	1.99	0.44
2:C:1297:ASP:OD2	2:C:1300:GLY:HA3	2.17	0.44
3:D:56:LEU:H	3:D:56:LEU:HD22	1.82	0.44
3:D:76:LYS:O	3:D:77:ARG:CG	2.63	0.44
3:D:528:THR:HG23	3:D:529:GLY:N	2.33	0.44
3:D:774:ILE:HA	3:D:777:HIS:HD2	1.83	0.44
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.18	0.44
3:D:1367:GLN:HB3	13:D:1602:HOH:O	2.17	0.44
4:E:32:VAL:C	4:E:34:GLY:H	2.25	0.44
2:C:836:LEU:HD23	2:C:836:LEU:N	2.33	0.44
3:D:121:PRO:HB2	3:D:123:ARG:NH2	2.33	0.44
3:D:1343:GLU:C	3:D:1344:LEU:HG	2.43	0.44
6:N:13:DA:H2''	6:N:14:DT:H6	1.82	0.44
2:C:156:PHE:HZ	2:C:445:ILE:HG13	1.81	0.44
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.98	0.44
2:C:1193:ALA:O	2:C:1197:GLU:HG3	2.18	0.44
3:D:1241:TYR:CD1	3:D:1246:VAL:HG11	2.53	0.44
5:F:402:LEU:HD12	5:F:402:LEU:H	1.83	0.44
6:N:26:DT:H2''	6:N:27:DA:C8	2.53	0.44
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.91	0.43
2:C:727:VAL:HG21	2:C:772:SER:C	2.43	0.43
2:C:972:PHE:HD2	2:C:994:ARG:CZ	2.31	0.43
3:D:425:ARG:NE	3:D:427:PRO:HD2	2.30	0.43
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.18	0.43
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.32	0.43
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.33	0.43
2:C:370:MET:HE2	2:C:388:LEU:HD21	2.00	0.43
2:C:425:ILE:HG22	2:C:429:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:820:GLU:O	2:C:823:VAL:HG12	2.18	0.43
3:D:97:VAL:HG22	3:D:101:ARG:HG2	2.00	0.43
3:D:557:LYS:O	3:D:557:LYS:HG3	2.17	0.43
3:D:615:LYS:NZ	4:E:5:THR:HG23	2.32	0.43
2:C:553:THR:CG2	2:C:608:ALA:HB1	2.48	0.43
2:C:629:PHE:HE2	2:C:634:VAL:HG21	1.82	0.43
3:D:19:ALA:C	3:D:20:ILE:HD12	2.43	0.43
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.99	0.43
3:D:161:THR:CG2	3:D:164:GLN:HE21	2.13	0.43
3:D:490:ILE:O	3:D:499:ILE:HG22	2.18	0.43
5:F:326:TRP:HZ3	5:F:330:LEU:CD1	2.31	0.43
2:C:215:TYR:HE2	2:C:422:LYS:HD2	1.83	0.43
2:C:800:MET:HA	2:C:800:MET:HE2	2.01	0.43
2:C:1298:VAL:CA	2:C:1301:ARG:HD2	2.40	0.43
3:D:201:LEU:HD22	3:D:217:LEU:HD21	2.00	0.43
3:D:278:ARG:NH1	3:D:295:GLU:OE2	2.51	0.43
3:D:401:VAL:HG12	3:D:408:VAL:HG21	2.00	0.43
3:D:647:PRO:CG	3:D:697:MET:HB3	2.39	0.43
3:D:1005:LYS:HB3	3:D:1009:GLU:CB	2.49	0.43
3:D:1347:LEU:O	3:D:1351:VAL:HG22	2.19	0.43
5:F:479:THR:CG2	5:F:480:PRO:HD2	2.48	0.43
1:A:122:GLU:HG2	1:A:123:ILE:N	2.33	0.43
2:C:230:PHE:CD1	2:C:292:ILE:HD11	2.54	0.43
2:C:807:TRP:CE3	2:C:817:LEU:HD11	2.52	0.43
3:D:278:ARG:O	3:D:282:LEU:HG	2.18	0.43
3:D:853:THR:HG22	3:D:854:ALA:N	2.33	0.43
5:F:111:LEU:O	5:F:112:THR:HG23	2.19	0.43
2:C:360:LEU:HD22	2:C:378:ARG:NH2	2.34	0.43
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.19	0.43
3:D:245:LEU:O	3:D:250:ARG:NH2	2.51	0.43
3:D:1021:ASP:HB2	3:D:1022:PRO:HD2	1.99	0.43
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.18	0.43
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.99	0.43
1:B:229:GLU:HG2	1:B:229:GLU:O	2.18	0.43
2:C:1107:MET:O	2:C:1109:ILE:N	2.52	0.43
2:C:1172:LEU:HD22	2:C:1172:LEU:O	2.19	0.43
3:D:134:ASP:O	3:D:138:VAL:HG23	2.19	0.43
2:C:11:ILE:HB	2:C:1149:TYR:OH	2.18	0.43
2:C:130:MET:SD	2:C:134:GLY:HA2	2.59	0.43
2:C:1137:GLU:OE1	2:C:1140:LYS:HE2	2.19	0.43
2:C:1158:LYS:O	2:C:1158:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:294:ASN:O	3:D:298:MET:HG3	2.19	0.43
3:D:362:ARG:N	3:D:365:GLN:HE21	2.14	0.43
3:D:450:HIS:HB3	3:D:453:VAL:HG23	2.01	0.43
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.43	0.43
1:A:53:GLY:CA	1:A:179:PRO:HG3	2.48	0.43
2:C:95:PRO:HA	2:C:126:GLU:HG2	2.01	0.43
2:C:301:TYR:OH	2:C:334:GLU:HG2	2.19	0.43
2:C:569:ILE:H	2:C:569:ILE:HG13	1.47	0.43
2:C:848:GLU:OE1	2:C:886:LYS:NZ	2.43	0.43
4:E:42:GLU:O	4:E:43:ASN:HB3	2.19	0.43
4:E:63:ILE:HD12	4:E:63:ILE:N	2.34	0.43
5:F:451:ARG:HH22	6:N:20:DG:P	2.42	0.43
6:N:15:DG:OP2	6:N:15:DG:C8	2.70	0.43
1:A:77:ASP:O	1:A:81:ILE:HG13	2.19	0.43
2:C:191:LYS:HB3	2:C:191:LYS:HZ3	1.81	0.43
2:C:1080:ASN:ND2	2:C:1084:ASP:HB2	2.33	0.43
2:C:1148:ALA:CB	2:C:1180:MET:HE1	2.49	0.43
2:C:1225:VAL:HA	3:D:638:SER:CB	2.49	0.43
3:D:721:SER:O	3:D:725:MET:HG3	2.18	0.43
6:N:16:DG:C2	7:T:10:DC:O2	2.72	0.43
1:A:45:ARG:HD3	1:B:34:GLY:O	2.19	0.42
1:B:47:LEU:HD21	1:B:220:ALA:CB	2.35	0.42
1:B:78:ILE:HG22	1:B:82:LEU:HD12	2.00	0.42
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.81	0.42
2:C:325:LEU:O	2:C:330:HIS:HB2	2.19	0.42
2:C:701:GLY:O	2:C:1184:THR:N	2.43	0.42
2:C:1156:ARG:HG3	2:C:1156:ARG:O	2.19	0.42
3:D:105:ILE:HD13	3:D:273:ILE:HG12	2.01	0.42
3:D:515:ARG:HB3	3:D:545:HIS:HD2	1.83	0.42
3:D:580:TRP:CE3	3:D:589:TYR:HD1	2.36	0.42
3:D:872:LEU:HB3	3:D:877:VAL:HG11	2.01	0.42
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	2.01	0.42
5:F:418:LYS:O	5:F:418:LYS:HG2	2.19	0.42
2:C:271:ALA:HA	2:C:274:ILE:HD13	2.02	0.42
3:D:1179:PRO:CD	3:D:1184:ASP:HB3	2.43	0.42
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.19	0.42
5:F:277:MET:HG3	5:F:362:ASN:CB	2.49	0.42
5:F:339:ARG:HE	5:F:342:GLN:HG2	1.84	0.42
5:F:519:LEU:HD13	5:F:519:LEU:O	2.19	0.42
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.59	0.42
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:484:LEU:O	2:C:486:THR:N	2.52	0.42
2:C:675:ASP:OD1	2:C:676:ALA:N	2.53	0.42
2:C:1008:GLN:O	2:C:1012:GLU:HG3	2.19	0.42
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.54	0.42
3:D:255:LEU:O	3:D:259:ARG:O	2.37	0.42
3:D:858:VAL:HG23	3:D:868:TRP:CZ3	2.55	0.42
3:D:914:ALA:O	3:D:918:ILE:HG23	2.19	0.42
3:D:1266:ILE:HG22	3:D:1267:VAL:N	2.34	0.42
5:F:507:MET:O	5:F:520:GLY:N	2.46	0.42
6:N:15:DG:H1'	6:N:16:DG:H5'	2.01	0.42
1:A:32:GLU:HB2	1:A:35:PHE:CD1	2.54	0.42
2:C:176:ILE:HB	2:C:184:LEU:HB3	2.01	0.42
2:C:379:GLU:CD	2:C:379:GLU:H	2.27	0.42
2:C:1238:LEU:O	2:C:1242:LYS:HG2	2.19	0.42
3:D:646:ILE:H	3:D:646:ILE:HG13	1.69	0.42
3:D:950:ILE:HD13	3:D:995:TYR:HB3	2.02	0.42
1:A:14:VAL:HG13	1:A:15:ASP:H	1.84	0.42
1:B:81:ILE:HG23	1:B:130:ILE:O	2.20	0.42
2:C:275:ARG:HA	2:C:278:GLU:OE1	2.18	0.42
2:C:465:ARG:O	2:C:469:VAL:HG23	2.20	0.42
3:D:442:ILE:HG21	3:D:448:GLN:OE1	2.19	0.42
1:A:168:ILE:N	1:A:168:ILE:HD12	2.35	0.42
1:B:31:LEU:HD12	1:B:35:PHE:HB3	2.00	0.42
1:B:192:VAL:HG21	1:B:198:LEU:CD2	2.33	0.42
2:C:207:THR:HG21	2:C:351:LEU:HG	2.00	0.42
2:C:750:ILE:CD1	2:C:963:GLU:HG2	2.49	0.42
2:C:1306:LYS:HA	2:C:1309:VAL:HG22	2.02	0.42
3:D:514:THR:CB	3:D:596:LEU:HB2	2.50	0.42
3:D:850:LYS:HG2	3:D:857:LEU:HD21	2.01	0.42
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.35	0.42
1:A:79:LEU:HD13	1:A:83:LEU:HD13	2.01	0.42
2:C:562:GLU:HG2	2:C:574:SER:CB	2.50	0.42
2:C:562:GLU:HG2	2:C:574:SER:HB2	2.02	0.42
2:C:606:LEU:HD23	2:C:611:GLU:HA	2.02	0.42
2:C:1087:TYR:CE1	2:C:1213:TYR:HB2	2.54	0.42
3:D:57:PHE:HD2	3:D:98:ARG:HH22	1.66	0.42
3:D:114:ILE:HG13	3:D:118:LYS:HG3	2.02	0.42
4:E:40:PRO:O	4:E:52:ARG:NH2	2.52	0.42
5:F:586:ARG:O	5:F:590:ILE:HG13	2.20	0.42
7:T:11:DA:H8	7:T:11:DA:OP2	2.02	0.42
2:C:19:PRO:HA	2:C:1156:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ILE:HG21	2:C:325:LEU:HB3	2.01	0.42
2:C:603:ILE:HG13	2:C:603:ILE:O	2.20	0.42
2:C:1005:GLU:HG2	2:C:1006:GLU:N	2.33	0.42
3:D:1286:LYS:HA	3:D:1286:LYS:HD2	1.82	0.42
1:B:103:ASN:OD1	1:B:103:ASN:N	2.53	0.42
1:B:104:LYS:HZ2	1:B:105:SER:H	1.67	0.42
3:D:96:LYS:HD2	3:D:96:LYS:N	2.33	0.42
3:D:211:GLU:H	3:D:211:GLU:HG2	1.50	0.42
3:D:337:ARG:HD3	3:D:341:ASN:HB2	2.01	0.42
3:D:494:ALA:HB1	3:D:1248:ILE:HG22	2.02	0.42
5:F:530:LEU:H	5:F:530:LEU:CD2	2.30	0.42
7:T:17:DG:H2"	7:T:18:DG:H8	1.84	0.42
1:B:112:ALA:N	1:B:128:HIS:O	2.53	0.42
1:B:115:ILE:HG22	1:B:116:THR:N	2.34	0.42
1:B:219:ARG:O	1:B:223:ILE:HG13	2.20	0.42
2:C:242:VAL:HG12	2:C:244:GLU:H	1.85	0.42
2:C:478:ARG:NH1	2:C:487:LEU:HD13	2.35	0.42
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.47	0.42
2:C:1305:TYR:CE2	3:D:379:PRO:HG3	2.55	0.42
3:D:523:GLU:O	3:D:523:GLU:HG3	2.18	0.42
3:D:1212:ASP:OD2	3:D:1212:ASP:N	2.52	0.42
5:F:415:ALA:HB2	5:F:434:TRP:CD1	2.54	0.42
5:F:505:ILE:N	5:F:505:ILE:HD12	2.35	0.42
5:F:562:ARG:HH21	5:F:573:LEU:HA	1.85	0.42
2:C:22:LEU:HD22	2:C:23:ASP:H	1.84	0.41
2:C:165:HIS:O	2:C:166:SER:OG	2.32	0.41
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.55	0.41
2:C:621:SER:HB2	2:C:623:LEU:CD2	2.50	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.90	0.41
3:D:564:VAL:O	3:D:564:VAL:CG2	2.68	0.41
3:D:650:LYS:NZ	3:D:762:ASN:HD22	2.17	0.41
3:D:1188:GLU:HG2	3:D:1189:MET:H	1.84	0.41
3:D:1295:ASN:HB3	3:D:1297:LYS:HE3	2.02	0.41
5:F:342:GLN:HG3	5:F:343:LYS:N	2.35	0.41
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.88	0.41
1:A:45:ARG:HD3	1:B:38:THR:OG1	2.20	0.41
1:A:189:ALA:HA	1:A:198:LEU:O	2.19	0.41
1:A:228:LEU:HD12	1:A:231:PHE:HE1	1.85	0.41
2:C:1325:VAL:HG12	3:D:337:ARG:NH1	2.35	0.41
2:C:1326:LEU:O	2:C:1330:ILE:HG13	2.20	0.41
3:D:108:ALA:HB3	3:D:279:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:385:LEU:CD2	3:D:411:ILE:HG13	2.50	0.41
3:D:1361:THR:HG23	4:E:21:LEU:CD2	2.47	0.41
1:A:99:ILE:HG12	1:A:145:LYS:HG2	2.02	0.41
2:C:392:GLU:H	2:C:392:GLU:HG2	1.51	0.41
2:C:494:ASN:ND2	2:C:496:LYS:H	2.15	0.41
2:C:616:ILE:N	2:C:616:ILE:HD12	2.36	0.41
2:C:996:ARG:HD2	2:C:996:ARG:N	2.36	0.41
3:D:256:ASP:HA	3:D:257:GLY:C	2.44	0.41
3:D:331:ILE:HG22	3:D:1328:THR:HG21	2.03	0.41
3:D:705:THR:CG2	3:D:705:THR:O	2.67	0.41
3:D:803:VAL:O	3:D:803:VAL:HG22	2.20	0.41
3:D:1359:ALA:HA	3:D:1363:TYR:HB2	2.01	0.41
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.34	0.41
2:C:704:MET:HE3	2:C:704:MET:HB3	1.96	0.41
3:D:132:LEU:HD13	3:D:132:LEU:C	2.46	0.41
3:D:190:LYS:HG2	3:D:235:GLU:CG	2.50	0.41
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.01	0.41
5:F:277:MET:HG3	5:F:362:ASN:HB2	2.01	0.41
2:C:22:LEU:HD22	2:C:23:ASP:N	2.35	0.41
2:C:481:LEU:N	2:C:481:LEU:HD22	2.35	0.41
2:C:724:VAL:HG22	2:C:734:ILE:CD1	2.50	0.41
2:C:914:LYS:CG	2:C:915:ASP:H	2.32	0.41
3:D:365:GLN:HA	3:D:438:GLU:H	1.86	0.41
3:D:390:LEU:HD12	3:D:390:LEU:HA	1.82	0.41
3:D:709:ARG:O	3:D:712:GLN:HG2	2.20	0.41
3:D:785:ASP:O	3:D:789:LYS:HB3	2.20	0.41
6:N:3:DC:C2	6:N:4:DC:C5	3.09	0.41
1:B:11:PRO:HB3	1:B:30:PRO:O	2.20	0.41
2:C:287:VAL:HB	2:C:288:PRO:HD2	2.02	0.41
2:C:724:VAL:HG23	2:C:775:GLU:O	2.21	0.41
3:D:326:SER:O	3:D:330:MET:HG3	2.21	0.41
3:D:394:ILE:CG2	5:F:536:THR:HG22	2.49	0.41
3:D:397:ALA:O	3:D:401:VAL:HG13	2.20	0.41
3:D:1196:LEU:HD12	3:D:1198:VAL:HG12	2.02	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.20	0.41
2:C:268:ARG:O	2:C:268:ARG:HG3	2.21	0.41
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.02	0.41
2:C:339:ASN:HB3	2:C:343:HIS:H	1.86	0.41
2:C:575:LEU:CD2	2:C:579:ALA:HB3	2.51	0.41
2:C:1246:ARG:NH2	2:C:1258:PRO:HB3	2.35	0.41
3:D:216:LYS:HE3	3:D:216:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:385:LEU:HD21	3:D:411:ILE:HG13	2.02	0.41
3:D:1163:VAL:CG2	3:D:1175:LEU:HD11	2.49	0.41
3:D:1251:LYS:HB2	3:D:1251:LYS:HE3	1.77	0.41
4:E:39:VAL:HG12	4:E:40:PRO:CD	2.50	0.41
1:A:104:LYS:O	1:A:140:ILE:HG13	2.20	0.41
1:B:78:ILE:HA	1:B:81:ILE:CD1	2.50	0.41
2:C:517:GLN:O	2:C:518:ASN:OD1	2.39	0.41
2:C:1075:VAL:HG23	3:D:461:PHE:O	2.20	0.41
3:D:544:LEU:HD11	3:D:631:TYR:HE1	1.86	0.41
3:D:843:VAL:CG1	3:D:883:ARG:HD3	2.46	0.41
5:F:551:LEU:HD22	5:F:597:LYS:HD2	2.02	0.41
6:N:4:DC:C2'	6:N:5:DT:H71	2.51	0.41
1:B:31:LEU:O	1:B:198:LEU:HG	2.20	0.41
2:C:5:TYR:HA	2:C:8:LYS:HD3	2.02	0.41
2:C:78:PRO:HG3	2:C:129:LEU:HD12	2.03	0.41
2:C:99:LYS:HG3	2:C:121:GLU:HB3	2.02	0.41
2:C:156:PHE:CZ	2:C:445:ILE:HG13	2.56	0.41
2:C:734:ILE:HD12	2:C:777:VAL:HG21	2.03	0.41
2:C:1080:ASN:HD21	2:C:1084:ASP:CB	2.33	0.41
2:C:1223:ARG:O	2:C:1224:PRO:C	2.63	0.41
3:D:113:HIS:HD2	3:D:239:LEU:HD11	1.85	0.41
3:D:140:TYR:CD2	5:F:100:MET:HE3	2.56	0.41
3:D:211:GLU:HA	3:D:214:ARG:HB2	2.03	0.41
3:D:750:PRO:HA	3:D:781:LYS:HG3	2.02	0.41
3:D:865:HIS:CD2	3:D:868:TRP:HD1	2.39	0.41
3:D:877:VAL:O	3:D:877:VAL:CG1	2.69	0.41
3:D:919:ALA:O	3:D:923:ILE:HG13	2.20	0.41
3:D:1005:LYS:HB3	3:D:1009:GLU:CG	2.50	0.41
3:D:1268:ASN:N	3:D:1268:ASN:HD22	2.18	0.41
5:F:110:LEU:HD12	5:F:110:LEU:N	2.36	0.41
5:F:124:GLU:O	5:F:128:ASN:HB2	2.21	0.41
5:F:309:ASN:O	5:F:311:THR:HG23	2.21	0.41
5:F:330:LEU:HD23	5:F:330:LEU:HA	1.90	0.41
7:T:12:DT:C2'	7:T:13:DC:C5	3.02	0.41
2:C:4:SER:OG	2:C:7:GLU:HG2	2.20	0.41
2:C:79:VAL:HG21	5:F:476:ARG:NH1	2.34	0.41
2:C:204:LEU:O	2:C:205:PRO:C	2.64	0.41
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.56	0.41
2:C:646:SER:HB2	2:C:649:GLN:HG3	2.03	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.85	0.41
3:D:268:LEU:HD21	3:D:324:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:LEU:HG	3:D:904:ALA:HA	2.02	0.41
1:A:42:ALA:O	1:A:46:ILE:HG12	2.21	0.40
1:B:182:ARG:HG2	1:B:183:ILE:N	2.36	0.40
2:C:617:ALA:HA	2:C:636:CYS:SG	2.60	0.40
2:C:1060:ILE:HG23	2:C:1060:ILE:O	2.20	0.40
3:D:66:LYS:HB3	3:D:66:LYS:HE2	1.74	0.40
3:D:1371:ARG:NH1	3:D:1372:ARG:HH21	2.19	0.40
5:F:292:VAL:HG11	5:F:299:LYS:CE	2.51	0.40
2:C:106:GLU:HB2	2:C:114:VAL:CG2	2.48	0.40
2:C:148:GLN:HB2	2:C:511:LEU:HD11	2.03	0.40
2:C:985:GLU:O	2:C:986:ALA:C	2.64	0.40
2:C:998:LEU:HD23	2:C:998:LEU:HA	1.94	0.40
3:D:222:LYS:HE2	3:D:225:GLU:OE2	2.21	0.40
3:D:842:ARG:HH22	3:D:1254:GLU:CD	2.28	0.40
5:F:130:VAL:HB	5:F:365:MET:HG3	2.04	0.40
6:N:26:DT:C2'	6:N:27:DA:C8	3.04	0.40
2:C:145:ILE:HB	2:C:456:VAL:HB	2.03	0.40
2:C:195:PHE:CG	2:C:203:LYS:HG2	2.56	0.40
2:C:230:PHE:HD1	2:C:238:GLN:O	2.05	0.40
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.20	0.40
2:C:996:ARG:HD2	2:C:996:ARG:H	1.87	0.40
2:C:1005:GLU:C	2:C:1007:LYS:H	2.29	0.40
3:D:802:ASP:OD2	3:D:1313:SER:HB2	2.21	0.40
2:C:153:PRO:HB2	2:C:401:GLY:CA	2.51	0.40
2:C:1176:LEU:HD22	2:C:1180:MET:HA	2.03	0.40
2:C:1325:VAL:HG12	3:D:337:ARG:HH12	1.86	0.40
3:D:1173:ARG:HB3	3:D:1190:ILE:O	2.21	0.40
5:F:499:LYS:HE2	5:F:499:LYS:HB3	1.89	0.40
1:A:100:LEU:HD23	1:A:115:ILE:HG21	2.04	0.40
1:A:159:ILE:O	1:A:159:ILE:HG12	2.21	0.40
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.57	0.40
1:B:59:VAL:O	1:B:171:LEU:N	2.54	0.40
2:C:1101:LEU:HD22	3:D:731:ARG:HB2	2.04	0.40
3:D:128:LEU:HD13	3:D:188:LEU:HD22	2.04	0.40
3:D:646:ILE:HG22	3:D:647:PRO:CD	2.49	0.40
3:D:678:ARG:HG3	3:D:679:TYR:N	2.37	0.40
8:I:7:THR:HG21	8:I:17:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/239 (95%)	206 (91%)	19 (8%)	1 (0%)	30	59
1	B	213/239 (89%)	196 (92%)	14 (7%)	3 (1%)	9	33
2	C	1326/1342 (99%)	1245 (94%)	75 (6%)	6 (0%)	24	55
3	D	1231/1409 (87%)	1145 (93%)	83 (7%)	3 (0%)	43	70
4	E	77/90 (86%)	73 (95%)	3 (4%)	1 (1%)	9	34
5	F	391/613 (64%)	378 (97%)	13 (3%)	0	100	100
8	I	15/19 (79%)	12 (80%)	3 (20%)	0	100	100
All	All	3479/3951 (88%)	3255 (94%)	210 (6%)	14 (0%)	30	59

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	C	199	ASP
2	C	200	ARG
3	D	1345	ARG
2	C	235	ASN
3	D	211	GLU
2	C	485	ASP
3	D	1024	THR
1	B	135	ASP
2	C	398	SER
4	E	33	GLY
2	C	205	PRO
1	B	94	GLY
1	B	232	VAL

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	181/206 (88%)	162 (90%)	19 (10%)	6	24
1	B	181/206 (88%)	158 (87%)	23 (13%)	4	18
2	C	1144/1157 (99%)	1017 (89%)	127 (11%)	6	23
3	D	1035/1170 (88%)	908 (88%)	127 (12%)	4	19
4	E	67/74 (90%)	64 (96%)	3 (4%)	24	52
5	F	350/540 (65%)	309 (88%)	41 (12%)	5	21
8	I	13/15 (87%)	11 (85%)	2 (15%)	2	12
All	All	2971/3368 (88%)	2629 (88%)	342 (12%)	5	21

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	VAL
1	A	16	ILE
1	A	19	VAL
1	A	22	THR
1	A	26	VAL
1	A	67	GLU
1	A	76	GLU
1	A	79	LEU
1	A	92	VAL
1	A	124	VAL
1	A	129	VAL
1	A	140	ILE
1	A	173	VAL
1	A	183	ILE
1	A	203	ILE
1	A	207	THR
1	A	222	THR
1	A	231	PHE
1	B	8	PHE

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Mol	Chain	Res	Type
1	B	16	ILE
1	B	18	GLN
1	B	21	SER
1	B	57	THR
1	B	60	GLU
1	B	81	ILE
1	B	82	LEU
1	B	96	ASP
1	B	100	LEU
1	B	104	LYS
1	B	134	THR
1	B	136	GLU
1	B	144	ILE
1	B	146	VAL
1	B	173	VAL
1	B	176	CYS
1	B	186	ASN
1	B	192	VAL
1	B	194	GLN
1	B	214	GLU
1	B	215	GLU
1	B	226	GLU
2	C	2	VAL
2	C	6	THR
2	C	17	LYS
2	C	18	ARG
2	C	21	VAL
2	C	22	LEU
2	C	24	VAL
2	C	44	GLU
2	C	47	TYR
2	C	75	LEU
2	C	91	THR
2	C	99	LYS
2	C	107	ARG
2	C	113	THR
2	C	114	VAL
2	C	147	SER
2	C	160	ASP
2	C	192	ASP
2	C	204	LEU
2	C	217	THR

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Mol	Chain	Res	Type
2	C	227	LYS
2	C	230	PHE
2	C	233	ARG
2	C	237	LEU
2	C	241	LEU
2	C	246	LEU
2	C	252	SER
2	C	268	ARG
2	C	290	GLU
2	C	296	VAL
2	C	306	THR
2	C	308	GLU
2	C	309	LEU
2	C	316	GLU
2	C	321	LEU
2	C	322	LEU
2	C	331	LYS
2	C	353	VAL
2	C	354	ASP
2	C	377	THR
2	C	392	GLU
2	C	443	ASP
2	C	445	ILE
2	C	456	VAL
2	C	468	LEU
2	C	477	GLU
2	C	484	LEU
2	C	490	GLN
2	C	493	ILE
2	C	494	ASN
2	C	499	SER
2	C	504	GLU
2	C	510	GLN
2	C	524	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	562	GLU
2	C	569	ILE
2	C	573	ASN

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Mol	Chain	Res	Type
2	C	581	THR
2	C	582	ASN
2	C	609	ILE
2	C	611	GLU
2	C	615	VAL
2	C	622	ASN
2	C	635	THR
2	C	637	ARG
2	C	653	MET
2	C	672	GLU
2	C	677	ASN
2	C	680	LEU
2	C	681	MET
2	C	690	VAL
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	745	GLU
2	C	748	ILE
2	C	779	ARG
2	C	817	LEU
2	C	836	LEU
2	C	878	THR
2	C	894	GLN
2	C	908	GLU
2	C	916	SER
2	C	919	ARG
2	C	967	LEU
2	C	978	VAL
2	C	984	VAL
2	C	985	GLU
2	C	992	LEU
2	C	995	ASP
2	C	996	ARG
2	C	1009	ASN
2	C	1011	LEU
2	C	1027	LYS
2	C	1040	ASP
2	C	1041	ASP
2	C	1066	MET
2	C	1075	VAL
2	C	1082	ILE

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Mol	Chain	Res	Type
2	C	1092	THR
2	C	1105	SER
2	C	1106	ARG
2	C	1126	ASP
2	C	1151	LEU
2	C	1155	VAL
2	C	1157	GLN
2	C	1159	VAL
2	C	1162	SER
2	C	1168	GLU
2	C	1172	LEU
2	C	1198	LEU
2	C	1219	GLU
2	C	1220	GLN
2	C	1225	VAL
2	C	1227	VAL
2	C	1236	ASN
2	C	1253	LEU
2	C	1262	LYS
2	C	1298	VAL
2	C	1301	ARG
2	C	1339	LEU
2	C	1341	ASP
3	D	46	TYR
3	D	47	ARG
3	D	52	GLU
3	D	66	LYS
3	D	71	LEU
3	D	77	ARG
3	D	80	HIS
3	D	84	ILE
3	D	86	GLU
3	D	92	VAL
3	D	93	THR
3	D	94	GLN
3	D	101	ARG
3	D	124	ILE
3	D	135	ILE
3	D	152	THR
3	D	153	ASN
3	D	154	LEU
3	D	175	GLU

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Mol	Chain	Res	Type
3	D	188	LEU
3	D	194	LEU
3	D	195	GLU
3	D	196	GLN
3	D	205	LEU
3	D	211	GLU
3	D	216	LYS
3	D	217	LEU
3	D	232	ASN
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	270	ARG
3	D	279	LEU
3	D	324	LEU
3	D	332	LYS
3	D	340	GLN
3	D	357	VAL
3	D	386	GLU
3	D	390	LEU
3	D	394	ILE
3	D	425	ARG
3	D	429	LEU
3	D	441	LEU
3	D	453	VAL
3	D	460	ASP
3	D	472	LEU
3	D	474	LEU
3	D	490	ILE
3	D	491	LEU
3	D	506	VAL
3	D	507	VAL
3	D	544	LEU
3	D	547	ARG
3	D	552	ILE
3	D	560	ASN
3	D	571	ASP
3	D	572	THR
3	D	591	ILE
3	D	594	GLN
3	D	596	LEU
3	D	645	VAL

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Mol	Chain	Res	Type
3	D	648	GLU
3	D	663	GLU
3	D	664	ILE
3	D	667	GLN
3	D	674	THR
3	D	678	ARG
3	D	681	LYS
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	706	VAL
3	D	709	ARG
3	D	710	ASP
3	D	731	ARG
3	D	736	GLN
3	D	740	LEU
3	D	743	MET
3	D	746	LEU
3	D	768	ASN
3	D	770	LEU
3	D	783	LEU
3	D	789	LYS
3	D	801	VAL
3	D	818	GLU
3	D	826	ILE
3	D	830	ASP
3	D	840	LEU
3	D	849	LEU
3	D	862	THR
3	D	875	ASN
3	D	876	SER
3	D	878	ASP
3	D	886	VAL
3	D	890	THR
3	D	898	CYS
3	D	901	ARG
3	D	913	GLU
3	D	918	ILE
3	D	930	LEU
3	D	972	LYS
3	D	997	VAL
3	D	1011	VAL

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Mol	Chain	Res	Type
3	D	1024	THR
3	D	1025	MET
3	D	1143	ASP
3	D	1155	ILE
3	D	1168	GLU
3	D	1172	LYS
3	D	1184	ASP
3	D	1186	TYR
3	D	1189	MET
3	D	1192	LYS
3	D	1202	GLU
3	D	1209	VAL
3	D	1210	ILE
3	D	1221	LEU
3	D	1243	LEU
3	D	1268	ASN
3	D	1289	ASN
3	D	1301	THR
3	D	1320	ILE
3	D	1329	THR
3	D	1344	LEU
3	D	1351	VAL
3	D	1357	ILE
3	D	1372	ARG
4	E	4	VAL
4	E	25	ARG
4	E	36	ASP
5	F	105	MET
5	F	112	THR
5	F	113	ARG
5	F	118	ASP
5	F	130	VAL
5	F	131	GLN
5	F	132	CYS
5	F	293	GLU
5	F	331	HIS
5	F	338	HIS
5	F	342	GLN
5	F	364	ARG
5	F	383	ASN
5	F	395	THR
5	F	417	ASP

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Mol	Chain	Res	Type
5	F	421	TYR
5	F	437	GLN
5	F	450	ILE
5	F	472	GLN
5	F	485	GLU
5	F	486	ARG
5	F	487	MET
5	F	488	LEU
5	F	495	ARG
5	F	500	ILE
5	F	503	GLU
5	F	513	ASP
5	F	516	ASP
5	F	524	GLU
5	F	538	GLU
5	F	557	LYS
5	F	561	MET
5	F	568	ASN
5	F	573	LEU
5	F	574	GLU
5	F	578	LYS
5	F	579	GLN
5	F	581	ASP
5	F	599	ARG
5	F	603	ARG
5	F	606	VAL
8	I	5	PHE
8	I	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	66	HIS
1	A	186	ASN
1	B	18	GLN
1	B	23	HIS
1	B	84	ASN
1	B	127	GLN
1	B	147	GLN
1	B	194	GLN
2	C	31	GLN

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Mol	Chain	Res	Type
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	276	GLN
2	C	343	HIS
2	C	494	ASN
2	C	513	GLN
2	C	568	ASN
2	C	573	ASN
2	C	582	ASN
2	C	618	GLN
2	C	658	GLN
2	C	684	ASN
2	C	761	GLN
2	C	762	ASN
2	C	798	GLN
2	C	799	ASN
2	C	922	ASN
2	C	1080	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1157	GLN
2	C	1220	GLN
2	C	1264	GLN
2	C	1268	GLN
2	C	1314	GLN
3	D	153	ASN
3	D	164	GLN
3	D	200	GLN
3	D	232	ASN
3	D	341	ASN
3	D	365	GLN
3	D	495	ASN
3	D	545	HIS
3	D	594	GLN
3	D	669	GLN
3	D	690	ASN
3	D	700	ASN
3	D	702	GLN
3	D	762	ASN
3	D	768	ASN

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Mol	Chain	Res	Type
3	D	777	HIS
3	D	817	HIS
3	D	861	ASN
3	D	865	HIS
3	D	1010	GLN
3	D	1218	HIS
3	D	1227	HIS
3	D	1235	ASN
3	D	1268	ASN
3	D	1295	ASN
4	E	15	ASN
5	F	128	ASN
5	F	131	GLN
5	F	271	ASN
5	F	338	HIS
5	F	345	GLN
5	F	362	ASN
5	F	406	GLN
5	F	461	ASN
5	F	545	HIS
5	F	589	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	C	1401	-	3,3,3	0.41	0	2,2,2	0.61	0
12	EPE	D	1504	-	15,15,15	0.89	1 (6%)	19,20,20	1.94	6 (31%)

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
9	EDO	C	1401	-	-	0/1/1/1	-
12	EPE	D	1504	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1504	EPE	C10-S	3.07	1.81	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	1504	EPE	C7-N4-C5	4.18	122.38	111.24
12	D	1504	EPE	O2S-S-C10	3.30	111.71	106.73
12	D	1504	EPE	C5-N4-C3	3.27	115.88	108.84
12	D	1504	EPE	C7-N4-C3	2.73	118.52	111.24
12	D	1504	EPE	C6-N1-C2	2.49	114.21	108.84
12	D	1504	EPE	O3S-S-C10	2.06	110.04	106.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	1504	EPE	C9-C10-S-O3S
12	D	1504	EPE	C9-C10-S-O2S
12	D	1504	EPE	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1401	EDO	1	0
12	D	1504	EPE	7	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	228/239 (95%)	0.18	6 (2%) 57 38	73, 115, 173, 204	0
1	B	217/239 (90%)	0.37	9 (4%) 41 27	74, 133, 174, 188	0
2	C	1332/1342 (99%)	-0.13	10 (0%) 82 68	36, 92, 163, 211	0
3	D	1239/1409 (87%)	-0.02	11 (0%) 81 65	45, 104, 181, 218	0
4	E	79/90 (87%)	-0.19	1 (1%) 75 56	71, 95, 155, 183	0
5	F	395/613 (64%)	0.04	5 (1%) 75 56	68, 140, 182, 213	0
6	N	29/29 (100%)	0.13	2 (6%) 23 16	124, 171, 253, 256	0
7	T	24/24 (100%)	0.26	1 (4%) 40 26	114, 179, 256, 268	0
8	I	17/19 (89%)	0.25	1 (5%) 28 19	97, 108, 127, 131	0
All	All	3560/4004 (88%)	-0.02	46 (1%) 75 56	36, 107, 178, 268	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	134	ASP	4.6
1	B	142	MET	4.5
2	C	826	ASP	4.0
1	A	235	GLU	3.9
5	F	352	GLY	3.8
1	B	102	LEU	3.8
4	E	2	ALA	3.7
2	C	1244	HIS	3.6
5	F	125	ASP	3.4
3	D	665	GLN	3.4
3	D	973	LEU	3.2
1	A	175	ALA	3.1
3	D	1283	SER	3.1
1	B	61	ILE	3.1
1	A	90	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
6	N	12	DG	2.9
2	C	186	PHE	2.9
1	B	65	LEU	2.9
2	C	198	ILE	2.9
3	D	670	SER	2.8
5	F	132	CYS	2.8
5	F	469	GLN	2.8
1	B	234	LEU	2.7
3	D	1257	VAL	2.6
7	T	11	DA	2.6
1	B	23	HIS	2.5
5	F	266	PHE	2.5
3	D	892	PHE	2.4
3	D	121	PRO	2.4
2	C	116	ASP	2.4
2	C	230	PHE	2.4
6	N	1	DG	2.3
2	C	196	VAL	2.3
8	I	4	GLY	2.2
1	B	144	ILE	2.2
3	D	1198	VAL	2.1
2	C	1041	ASP	2.1
3	D	904	ALA	2.1
1	B	59	VAL	2.1
1	A	173	VAL	2.1
1	A	234	LEU	2.1
2	C	616	ILE	2.1
1	B	233	ASP	2.1
1	A	67	GLU	2.0
2	C	985	GLU	2.0
3	D	915	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	EPE	D	1504	15/15	0.61	0.10	114,143,172,178	0
9	EDO	C	1401	4/4	0.62	0.12	98,117,137,139	0
11	ZN	D	1502	1/1	0.97	0.05	126,126,126,126	0
11	ZN	D	1503	1/1	0.98	0.07	108,108,108,108	0
10	MG	D	1501	1/1	0.99	0.08	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.