



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:48 PM GMT

PDB ID : 2PJR
Title : HELICASE PRODUCT COMPLEX
Authors : Velankar, S.S.; Soultanas, P.; Dillingham, M.S.; Subramanya, H.S.; Wigley, D.B.
Deposited on : 1999-03-12
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

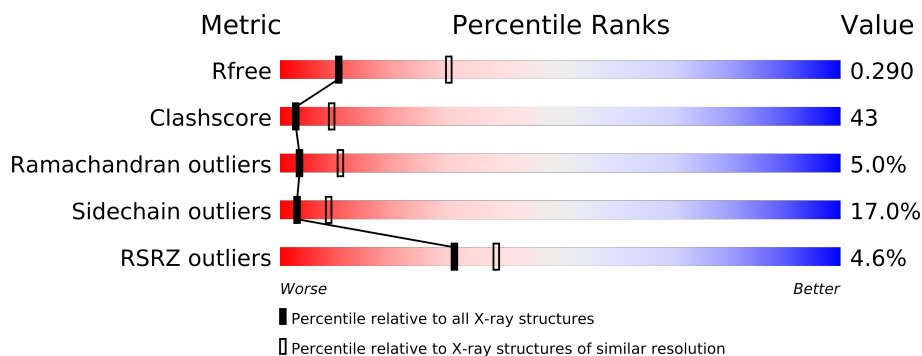
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	5	
1	D	5	
2	H	2	
3	I	5	
4	A	548	
4	F	548	
5	B	95	
5	G	95	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10671 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called DNA (5'-D(*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			
1	D	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	P	0	0	0
			98	48	18	28	4			

- Molecule 4 is a protein called PROTEIN (HELICASE PCRA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	542	Total	C	N	O	S	0	0	0
			4409	2792	775	829	13			
4	F	544	Total	C	N	O	S	0	0	0
			4424	2802	777	832	13			

- Molecule 5 is a protein called PROTEIN (HELICASE PCRA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	95	Total	C	N	O	S	0	0	0
			749	471	125	147	6			
5	G	95	Total	C	N	O	S	0	0	0
			749	471	125	147	6			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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 (5'-D(*TP*TP*TP*TP*T)-3')

Chain C: 

T13
T14
T15
T16
T17

- Molecule 1: DNA (5'-D(*TP*TP*TP*TP*T)-3')

Chain D: 

T13
T14
T15
T16
T17

- Molecule 2: DNA (5'-D(*GP*C)-3')

Chain H: 

G1
C2

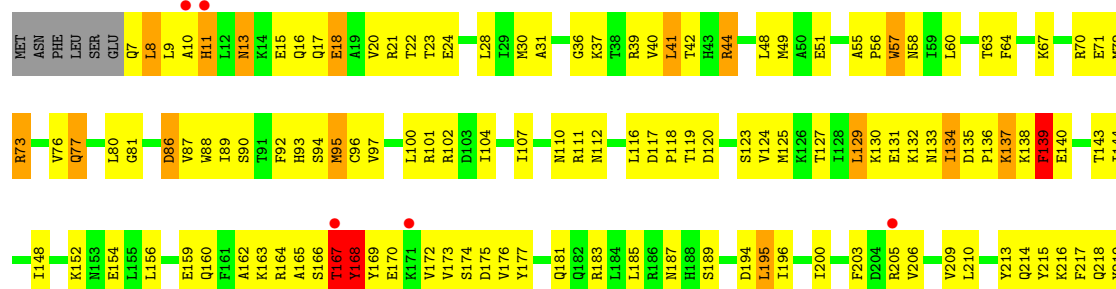
- Molecule 3: DNA (5'-D(*AP*CP*TP*GP*C)-3')

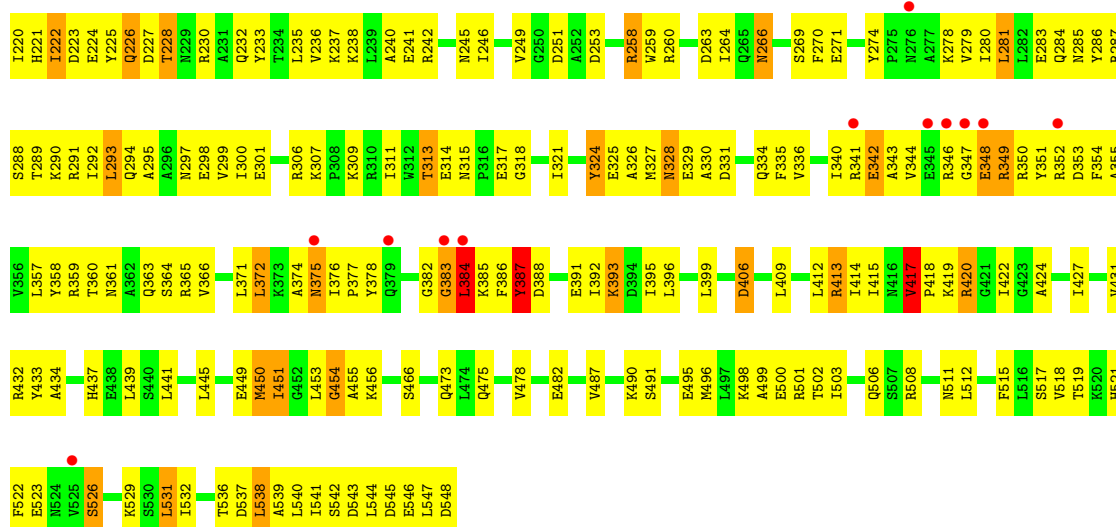
Chain I: 

A30
C31
T32
G33
C34

- Molecule 4: PROTEIN (HELICASE PCRA)

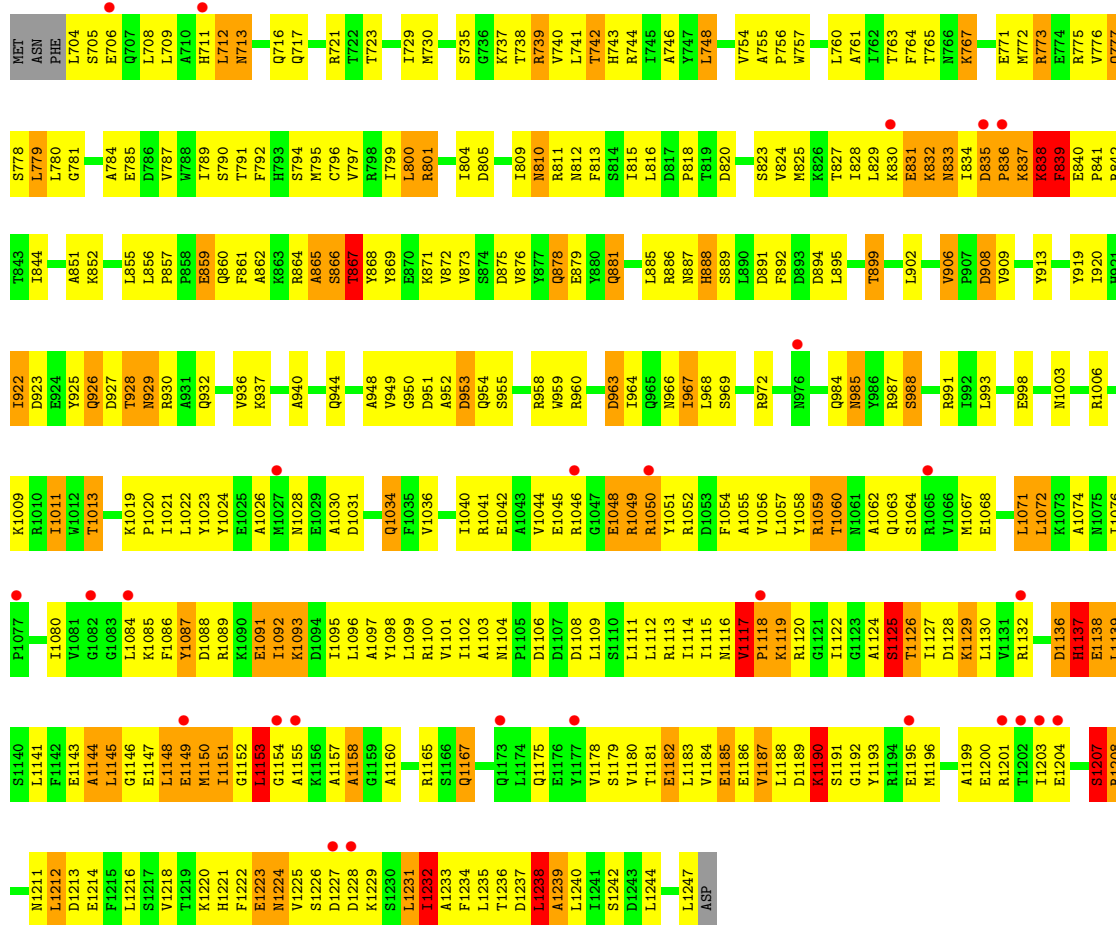
Chain A: 





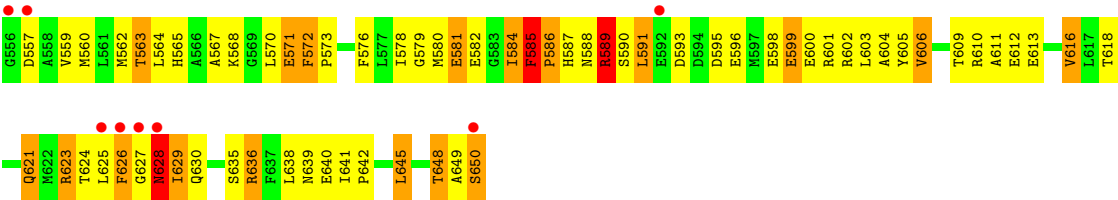
• Molecule 4: PROTEIN (HELICASE PCRA)

Chain F:



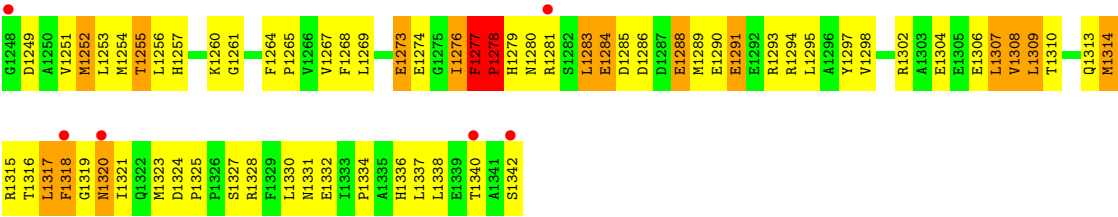
• Molecule 5: PROTEIN (HELICASE PCRA)

Chain B:



● Molecule 5: PROTEIN (HELICASE PCRA)

Chain G:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.05Å 62.60Å 141.83Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 14.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.90) 97.8 (14.98-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.296 0.242 , 0.290	Depositor DCC
R_{free} test set	1644 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32419 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10671	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	C	0.62	0/106	0.72	0/162
1	D	0.67	0/106	1.13	1/162 (0.6%)
2	H	1.79	2/42 (4.8%)	1.56	1/63 (1.6%)
3	I	2.09	4/109 (3.7%)	1.79	2/166 (1.2%)
4	A	0.52	0/4485	0.77	3/6059 (0.0%)
4	F	0.49	0/4500	0.78	8/6079 (0.1%)
5	B	0.63	1/762 (0.1%)	0.83	1/1028 (0.1%)
5	G	0.56	0/762	0.82	1/1028 (0.1%)
All	All	0.57	7/10872 (0.1%)	0.81	17/14747 (0.1%)

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
3	I	0	1
4	A	0	1
4	F	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	32	DT	O3'-P	-10.64	1.48	1.61
5	B	650	SER	CA-CB	7.21	1.63	1.52
3	I	33	DG	O3'-P	5.79	1.68	1.61
3	I	34	DC	C4'-C3'	5.35	1.58	1.53
3	I	34	DC	C3'-O3'	5.32	1.50	1.44
2	H	2	DC	P-O5'	-5.24	1.54	1.59
2	H	2	DC	O5'-C5'	-5.03	1.29	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	DT	O4'-C4'-C3'	-7.29	101.58	104.50
3	I	30	DA	O5'-C5'-C4'	7.16	128.89	111.00
3	I	33	DG	OP2-P-O3'	6.65	119.84	105.20
4	F	1117	VAL	C-N-CD	6.57	142.21	128.40
4	A	417	VAL	C-N-CD	6.39	141.82	128.40
4	F	1151	ILE	N-CA-C	-6.30	94.00	111.00
4	F	1190	LYS	N-CA-C	-6.13	94.46	111.00
4	A	548	ASP	CB-CG-OD1	6.02	123.72	118.30
5	G	1278	PRO	N-CA-C	-5.85	96.89	112.10
4	F	1207	SER	N-CA-C	-5.67	95.68	111.00
4	F	1238	LEU	N-CA-C	-5.59	95.91	111.00
4	F	1137	HIS	N-CA-C	-5.52	96.09	111.00
4	A	133	ASN	N-CA-C	5.40	125.57	111.00
5	B	585	PHE	C-N-CD	5.13	139.17	128.40
4	F	1118	PRO	N-CA-C	-5.12	98.80	112.10
4	F	866	SER	N-CA-C	-5.11	97.21	111.00
2	H	2	DC	C6-N1-C2	5.05	122.32	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	387	TYR	Sidechain
4	F	1193	TYR	Sidechain
3	I	34	DC	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	97	0	62	10	0
1	D	97	0	62	9	0
2	H	38	0	24	0	0
3	I	98	0	58	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4409	0	4432	355	0
4	F	4424	0	4450	447	0
5	B	749	0	731	104	0
5	G	749	0	731	89	0
6	A	5	0	0	1	0
6	F	5	0	0	0	0
All	All	10671	0	10550	919	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

All (919) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1096:LEU:HD21	4:F:1238:LEU:HD23	1.23	1.15
5:G:1316:THR:HG23	5:G:1320:ASN:HA	1.24	1.14
4:A:326:ALA:O	5:B:621:GLN:HG2	1.55	1.06
4:A:327:MET:HA	5:B:621:GLN:HG3	1.33	1.05
4:A:396:LEU:HD11	4:A:538:LEU:HD23	1.38	1.04
5:G:1256:LEU:HD21	5:G:1269:LEU:HD21	1.37	1.03
5:B:605:TYR:O	5:B:609:THR:HG22	1.61	1.00
4:F:1232:ILE:HD12	4:F:1232:ILE:H	1.25	0.99
4:F:1041:ARG:HB2	4:F:1076:ILE:HD11	1.45	0.98
4:F:780:LEU:HD12	4:F:784:ALA:HB2	1.43	0.98
5:B:585:PHE:O	5:B:587:HIS:N	1.97	0.97
4:F:832:LYS:HB3	4:F:833:ASN:ND2	1.80	0.96
4:F:713:ASN:HD21	4:F:716:GLN:HG3	1.31	0.96
4:F:1231:LEU:HD22	4:F:1235:LEU:HD11	1.48	0.96
4:A:13:ASN:ND2	4:A:13:ASN:H	1.64	0.95
1:D:16:DT:H2"	4:F:765:THR:HG22	1.48	0.95
4:A:298:GLU:HG2	5:B:642:PRO:HD3	1.46	0.94
4:F:929:ASN:HD22	4:F:929:ASN:N	1.66	0.94
4:F:1011:ILE:HD12	4:F:1011:ILE:H	1.31	0.93
5:B:642:PRO:HB2	5:B:645:LEU:HD12	1.51	0.93
4:F:929:ASN:ND2	4:F:929:ASN:H	1.57	0.93
4:A:73:ARG:HH11	4:A:73:ARG:HG3	1.33	0.93
4:A:293:LEU:HG	4:A:311:ILE:HG13	1.50	0.91
4:F:834:ILE:HG12	4:F:836:PRO:HD2	1.50	0.91
4:A:112:ASN:OD1	4:A:532:ILE:HG12	1.71	0.90
4:A:374:ALA:O	4:A:375:ASN:HB2	1.69	0.90
4:F:833:ASN:N	4:F:833:ASN:HD22	1.70	0.89
4:A:13:ASN:H	4:A:13:ASN:HD22	0.92	0.89
4:F:1190:LYS:C	4:F:1192:GLY:H	1.72	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:G:1298:VAL:O	5:G:1302:ARG:HG2	1.72	0.89
4:F:929:ASN:HD21	4:F:932:GLN:CD	1.76	0.89
4:A:100:LEU:HD22	4:A:104:ILE:HD13	1.54	0.89
5:B:564:LEU:HB3	5:B:603:LEU:HD22	1.55	0.89
4:A:139:PHE:H	4:A:139:PHE:HD1	1.17	0.88
4:A:215:TYR:HB3	4:A:242:ARG:HD3	1.55	0.87
4:F:742:THR:HG22	4:F:743:HIS:HD2	1.38	0.87
4:A:328:ASN:ND2	4:A:331:ASP:H	1.72	0.87
5:G:1277:PHE:HB3	5:G:1278:PRO:HD3	1.57	0.87
4:F:1087:TYR:HA	4:F:1092:ILE:HG21	1.58	0.86
4:F:1114:ILE:HA	4:F:1117:VAL:HG23	1.57	0.85
4:F:1050:ARG:NH1	5:G:1249:ASP:CG	2.29	0.85
5:G:1277:PHE:O	5:G:1279:HIS:N	2.08	0.85
4:A:13:ASN:N	4:A:13:ASN:HD22	1.76	0.84
4:A:13:ASN:HD21	4:A:16:GLN:CD	1.80	0.84
4:F:746:ALA:HB1	4:F:780:LEU:HD21	1.60	0.83
4:A:328:ASN:HD22	4:A:330:ALA:H	1.25	0.83
4:A:449:GLU:O	4:A:450:MET:HG2	1.79	0.83
4:A:287:ARG:HD3	5:B:571:GLU:HB3	1.62	0.82
5:B:636:ARG:HH11	5:B:636:ARG:HG2	1.45	0.82
4:F:1238:LEU:O	4:F:1240:LEU:N	2.13	0.82
4:F:833:ASN:N	4:F:833:ASN:ND2	2.27	0.81
4:A:336:VAL:HG12	4:A:340:ILE:HD11	1.61	0.81
4:F:1021:ILE:HG23	5:G:1307:LEU:HD23	1.62	0.81
4:A:73:ARG:NH1	4:A:73:ARG:HG3	1.92	0.81
4:A:336:VAL:O	4:A:340:ILE:HG13	1.81	0.81
4:F:988:SER:HB2	4:F:993:LEU:HD12	1.60	0.80
4:F:825:MET:HE1	4:F:844:ILE:HG21	1.61	0.80
4:F:1157:ALA:O	4:F:1160:ALA:N	2.14	0.80
4:A:298:GLU:HG2	5:B:642:PRO:CD	2.13	0.79
4:F:929:ASN:HD22	4:F:929:ASN:H	0.83	0.79
4:F:1178:VAL:CG1	4:F:1182:GLU:HB2	2.13	0.78
4:A:285:ASN:O	4:A:313:THR:HG23	1.82	0.78
4:F:1041:ARG:CB	4:F:1076:ILE:HD11	2.14	0.78
4:F:790:SER:OG	4:F:794:SER:HB3	1.84	0.78
5:B:606:VAL:O	5:B:610:ARG:HG2	1.84	0.77
4:A:163:LYS:HB2	4:F:1150:MET:CE	2.14	0.77
4:A:359:ARG:HH12	5:B:600:GLU:CD	1.87	0.77
1:D:15:DT:OP1	5:G:1255:THR:HG21	1.84	0.77
4:A:263:ASP:O	4:A:266:ASN:HB2	1.84	0.76
4:F:1049:ARG:N	4:F:1049:ARG:HD3	2.00	0.76
4:F:1099:LEU:HD23	4:F:1231:LEU:HD21	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:709:LEU:HA	4:F:712:LEU:HD12	1.68	0.75
4:F:1150:MET:C	4:F:1152:GLY:H	1.83	0.75
4:F:711:HIS:NE2	4:F:739:ARG:NH2	2.33	0.75
4:A:137:LYS:HD2	4:A:138:LYS:NZ	2.02	0.75
4:F:1048:GLU:CB	4:F:1049:ARG:HD3	2.17	0.75
4:A:154:GLU:HA	4:A:230:ARG:HB3	1.67	0.75
4:A:230:ARG:NH2	4:F:1139:LEU:HD21	2.01	0.75
4:F:1091:GLU:CD	4:F:1091:GLU:H	1.90	0.74
4:F:1114:ILE:HA	4:F:1117:VAL:CG2	2.16	0.74
4:F:1125:SER:O	4:F:1128:ASP:N	2.20	0.74
4:A:139:PHE:N	4:A:139:PHE:HD1	1.85	0.74
4:F:1050:ARG:HH11	4:F:1050:ARG:HG2	1.50	0.74
4:F:969:SER:HB2	4:F:972:ARG:HD2	1.70	0.74
5:B:628:ASN:N	5:B:628:ASN:HD22	1.83	0.74
4:A:23:THR:HB	4:A:48:LEU:HD21	1.69	0.74
5:B:585:PHE:HB3	5:B:586:PRO:HD3	1.67	0.74
4:A:165:ALA:HA	4:A:170:GLU:OE1	1.88	0.74
4:A:327:MET:HA	5:B:621:GLN:CG	2.14	0.74
4:F:1021:ILE:CG2	5:G:1307:LEU:HD23	2.18	0.74
4:A:352:ARG:HD2	4:A:352:ARG:O	1.87	0.74
4:F:1232:ILE:H	4:F:1232:ILE:CD1	1.97	0.73
5:B:606:VAL:O	5:B:610:ARG:CG	2.36	0.73
4:F:742:THR:HG22	4:F:743:HIS:CD2	2.23	0.73
4:F:985:ASN:ND2	4:F:987:ARG:H	1.87	0.73
5:B:564:LEU:CB	5:B:603:LEU:HD22	2.19	0.73
4:F:1086:PHE:CE1	4:F:1244:LEU:HD13	2.24	0.73
4:A:139:PHE:HA	4:A:144:ILE:HD11	1.71	0.73
4:F:1003:ASN:OD1	5:G:1290:GLU:HG2	1.87	0.73
4:F:1221:HIS:O	4:F:1224:ASN:HB2	1.89	0.73
4:A:20:VAL:HA	4:A:44:ARG:HG3	1.69	0.73
4:F:832:LYS:HB3	4:F:833:ASN:HD22	1.52	0.73
4:A:44:ARG:HE	4:A:221:HIS:HE1	1.36	0.73
4:F:746:ALA:CB	4:F:780:LEU:HD21	2.18	0.72
4:F:1048:GLU:HB3	4:F:1049:ARG:HD3	1.71	0.72
5:G:1307:LEU:HD21	5:G:1309:LEU:HD21	1.71	0.72
4:F:1178:VAL:HG13	4:F:1182:GLU:HB2	1.70	0.72
4:F:1056:VAL:HB	5:G:1253:LEU:HD12	1.71	0.72
4:F:713:ASN:HD22	4:F:713:ASN:N	1.87	0.72
4:F:1050:ARG:HH12	5:G:1249:ASP:CG	1.92	0.72
4:A:164:ARG:HB2	4:F:1150:MET:SD	2.30	0.72
5:G:1334:PRO:HB3	5:G:1336:HIS:NE2	2.05	0.72
4:A:230:ARG:HH22	4:F:1139:LEU:HD21	1.55	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1095:ILE:O	4:F:1099:LEU:HD12	1.89	0.71
4:A:139:PHE:N	4:A:139:PHE:CD1	2.54	0.71
3:I:32:DT:H2''	3:I:33:DG:O5'	1.90	0.71
4:F:991:ARG:HG2	5:G:1337:LEU:CD2	2.19	0.71
5:B:579:GLY:HA2	5:B:623:ARG:NH2	2.05	0.71
4:F:713:ASN:HD21	4:F:716:GLN:CG	2.03	0.71
4:A:13:ASN:ND2	4:A:16:GLN:OE1	2.23	0.71
4:F:1049:ARG:HH22	5:G:1306:GLU:CD	1.92	0.71
4:F:1096:LEU:HD21	4:F:1238:LEU:CD2	2.12	0.71
4:A:139:PHE:CZ	4:A:172:VAL:HG21	2.24	0.71
4:A:352:ARG:CD	5:B:560:MET:HE2	2.20	0.71
4:F:805:ASP:OD2	4:F:811:ARG:HD3	1.90	0.71
4:A:544:LEU:HG	4:A:544:LEU:O	1.91	0.71
5:G:1265:PRO:HA	5:G:1304:GLU:HB2	1.72	0.71
4:F:712:LEU:HB3	4:F:716:GLN:HB2	1.73	0.71
4:F:926:GLN:H	4:F:926:GLN:NE2	1.88	0.71
4:F:1149:GLU:O	4:F:1150:MET:HG3	1.91	0.71
4:A:125:MET:HE1	4:A:129:LEU:HD13	1.73	0.71
4:A:313:THR:HG21	4:A:315:ASN:ND2	2.05	0.70
4:F:773:ARG:NH1	4:F:789:ILE:HD12	2.05	0.70
4:A:13:ASN:ND2	4:A:16:GLN:CD	2.43	0.70
4:A:537:ASP:HB2	4:A:541:ILE:HD12	1.73	0.70
4:F:834:ILE:CG1	4:F:836:PRO:HD2	2.21	0.70
4:F:902:LEU:O	4:F:906:VAL:HG13	1.91	0.70
4:F:993:LEU:HD22	4:F:1013:THR:HG22	1.72	0.70
4:A:328:ASN:HD22	4:A:330:ALA:N	1.89	0.70
5:B:584:ILE:HG22	5:B:585:PHE:N	2.05	0.70
4:A:125:MET:CE	4:A:129:LEU:HD13	2.22	0.69
4:F:1044:VAL:HG21	4:F:1051:TYR:CE1	2.27	0.69
4:A:196:ILE:O	4:A:200:ILE:HD12	1.92	0.69
4:F:1068:GLU:O	4:F:1072:LEU:HB2	1.92	0.69
4:F:1057:LEU:HD22	5:G:1254:MET:HG2	1.73	0.69
4:A:44:ARG:HE	4:A:221:HIS:CE1	2.10	0.69
4:F:1044:VAL:HG21	4:F:1051:TYR:CD1	2.27	0.69
4:F:795:MET:O	4:F:799:ILE:HG13	1.92	0.69
4:F:1150:MET:CE	4:F:1152:GLY:HA2	2.23	0.69
4:F:1226:SER:O	4:F:1229:LYS:HE2	1.93	0.69
4:F:1054:PHE:HB2	5:G:1251:VAL:HG22	1.74	0.69
4:F:865:ALA:HB1	4:F:871:LYS:HG3	1.74	0.69
4:A:226:GLN:HG2	4:A:251:ASP:O	1.92	0.69
5:G:1257:HIS:HE1	5:G:1295:LEU:HD11	1.58	0.69
4:F:1235:LEU:HD12	4:F:1235:LEU:N	2.08	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1190:LYS:C	4:F:1192:GLY:N	2.45	0.69
4:F:865:ALA:O	4:F:871:LYS:HE2	1.92	0.69
5:B:636:ARG:NH1	5:B:636:ARG:HG2	2.06	0.69
4:F:1150:MET:C	4:F:1152:GLY:N	2.46	0.69
5:B:626:PHE:CD1	5:B:627:GLY:N	2.61	0.68
4:A:388:ASP:HA	4:A:393:LYS:HD2	1.75	0.68
4:F:928:THR:HG22	4:F:932:GLN:HB3	1.74	0.68
4:F:1150:MET:HE3	4:F:1152:GLY:HA2	1.76	0.68
4:F:1095:ILE:CD1	4:F:1187:VAL:HG11	2.24	0.68
5:G:1291:GLU:HG3	5:G:1294:ARG:NH2	2.08	0.68
4:F:834:ILE:HG12	4:F:836:PRO:CD	2.21	0.68
4:F:1058:TYR:CZ	4:F:1064:SER:HB3	2.29	0.68
4:A:298:GLU:CG	5:B:642:PRO:HD3	2.23	0.68
4:A:340:ILE:O	4:A:344:VAL:HG11	1.94	0.68
4:F:748:LEU:O	4:F:754:VAL:HG22	1.94	0.68
4:F:1099:LEU:CD2	4:F:1231:LEU:HD21	2.24	0.67
4:F:1139:LEU:HB2	4:F:1143:GLU:HB3	1.76	0.67
4:A:139:PHE:CE2	4:A:172:VAL:HG11	2.28	0.67
5:G:1252:MET:HG3	5:G:1264:PHE:CE2	2.30	0.67
4:A:417:VAL:O	4:A:419:LYS:N	2.27	0.67
4:A:258:ARG:NH2	5:B:595:ASP:HB2	2.10	0.67
4:A:386:PHE:CD1	4:A:544:LEU:HD22	2.30	0.67
4:F:859:GLU:O	4:F:862:ALA:HB3	1.94	0.67
4:F:729:ILE:HD13	4:F:740:VAL:HG11	1.77	0.67
4:A:478:VAL:HG13	4:A:482:GLU:HB2	1.76	0.67
4:F:825:MET:HE1	4:F:844:ILE:CG2	2.25	0.67
5:B:648:THR:HG23	5:B:650:SER:H	1.59	0.67
3:I:31:DC:C6	3:I:31:DC:H5'	2.30	0.67
4:A:116:LEU:HD13	4:A:189:SER:HB3	1.77	0.66
4:F:988:SER:HB2	4:F:993:LEU:CD1	2.25	0.66
4:A:127:THR:O	4:A:131:GLU:HG3	1.94	0.66
4:F:1050:ARG:NH1	4:F:1050:ARG:HG2	2.08	0.66
5:B:629:ILE:HD12	5:B:629:ILE:H	1.60	0.66
4:A:420:ARG:HG3	4:A:422:ILE:HD12	1.78	0.66
4:F:825:MET:HE3	4:F:829:LEU:HD13	1.77	0.66
4:F:844:ILE:HG23	4:F:873:VAL:HG13	1.77	0.66
4:A:96:CYS:SG	4:A:196:ILE:HD13	2.36	0.66
4:F:922:ILE:HG13	4:F:922:ILE:O	1.96	0.65
4:A:138:LYS:O	4:A:140:GLU:N	2.29	0.65
4:F:837:LYS:O	4:F:838:LYS:HB2	1.96	0.65
4:F:1114:ILE:HG22	4:F:1117:VAL:HG21	1.77	0.65
4:A:253:ASP:OD1	4:A:306:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1011:ILE:N	4:F:1011:ILE:HD12	2.09	0.65
4:F:985:ASN:HD21	4:F:988:SER:H	1.43	0.65
4:F:928:THR:HG22	4:F:932:GLN:CB	2.26	0.65
4:F:1060:THR:HG23	4:F:1062:ALA:H	1.61	0.65
4:F:742:THR:CG2	4:F:743:HIS:HD2	2.09	0.64
4:F:741:LEU:HD13	4:F:949:VAL:HG21	1.79	0.64
4:A:88:TRP:HE1	4:A:95:MET:HB2	1.62	0.64
4:F:1231:LEU:CD2	4:F:1235:LEU:HD11	2.26	0.64
4:A:73:ARG:HE	4:A:89:ILE:HD12	1.61	0.64
4:F:906:VAL:HG22	4:F:909:VAL:HG23	1.79	0.64
4:A:526:SER:O	4:A:529:LYS:NZ	2.31	0.64
4:A:291:ARG:HB2	4:A:317:GLU:O	1.97	0.64
5:B:590:SER:HB2	5:B:596:GLU:HB3	1.79	0.64
4:F:972:ARG:HH11	4:F:972:ARG:HG2	1.60	0.64
4:A:70:ARG:NH1	4:A:546:GLU:OE2	2.31	0.64
4:F:833:ASN:ND2	4:F:833:ASN:H	1.94	0.64
4:F:1030:ALA:O	4:F:1034:GLN:HB2	1.98	0.64
4:A:238:LYS:O	4:A:241:GLU:HB2	1.98	0.64
4:A:206:VAL:HG22	4:A:206:VAL:O	1.98	0.64
4:F:810:ASN:OD1	4:F:812:ASN:ND2	2.31	0.64
4:F:816:LEU:HD13	4:F:889:SER:HB3	1.78	0.64
4:F:861:PHE:O	4:F:864:ARG:O	2.15	0.63
4:A:328:ASN:ND2	4:A:331:ASP:N	2.44	0.63
4:A:386:PHE:CE1	4:A:544:LEU:HD22	2.33	0.63
4:A:101:ARG:O	4:A:111:ARG:HG2	1.98	0.63
4:F:1120:ARG:HH22	4:F:1191:SER:HA	1.63	0.63
4:F:1181:THR:O	4:F:1185:GLU:HB2	1.98	0.63
4:F:1087:TYR:HA	4:F:1092:ILE:CG2	2.28	0.63
4:F:1138:GLU:O	4:F:1138:GLU:HG3	1.98	0.63
4:A:134:ILE:HG13	4:A:136:PRO:HD2	1.80	0.63
4:A:285:ASN:HB3	4:A:293:LEU:HD21	1.81	0.63
4:F:1125:SER:O	4:F:1127:ILE:N	2.32	0.63
4:F:906:VAL:O	4:F:906:VAL:HG22	1.99	0.62
4:F:1048:GLU:C	4:F:1049:ARG:HD3	2.19	0.62
4:F:1231:LEU:HD22	4:F:1235:LEU:CD1	2.27	0.62
4:A:167:THR:O	4:A:168:TYR:O	2.18	0.62
5:G:1277:PHE:HB3	5:G:1278:PRO:CD	2.27	0.62
4:F:1151:ILE:HB	4:F:1153:LEU:HD22	1.81	0.62
4:A:7:GLN:O	4:A:9:LEU:N	2.33	0.62
4:F:1091:GLU:O	4:F:1095:ILE:HG22	2.00	0.61
5:G:1276:ILE:HG22	5:G:1277:PHE:N	2.14	0.61
5:G:1257:HIS:CE1	5:G:1295:LEU:HD11	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:857:PRO:HG2	4:F:860:GLN:HG3	1.81	0.61
4:F:1117:VAL:HG12	4:F:1118:PRO:CD	2.30	0.61
4:A:96:CYS:HB3	4:A:195:LEU:O	1.99	0.61
4:A:67:LYS:O	4:A:71:GLU:HG3	2.00	0.61
4:F:1021:ILE:HG12	5:G:1307:LEU:HD23	1.83	0.61
4:F:748:LEU:HD22	4:F:754:VAL:HG21	1.81	0.61
4:A:20:VAL:HG13	4:A:44:ARG:HA	1.81	0.61
5:B:625:LEU:HB3	5:B:630:GLN:NE2	2.15	0.61
4:F:773:ARG:O	4:F:777:GLN:HB2	2.01	0.61
4:F:713:ASN:HD22	4:F:713:ASN:H	1.47	0.61
1:C:14:DT:H2"	1:C:15:DT:H5'	1.82	0.61
4:F:1011:ILE:CD1	4:F:1011:ILE:H	2.06	0.61
4:F:835:ASP:N	4:F:836:PRO:HD2	2.15	0.61
4:A:290:LYS:HE3	4:A:315:ASN:O	1.99	0.61
5:B:623:ARG:O	5:B:630:GLN:HG2	2.01	0.61
4:F:797:VAL:HG23	4:F:895:LEU:HD22	1.82	0.61
4:F:1144:ALA:O	4:F:1146:GLY:N	2.34	0.60
4:A:313:THR:HG21	4:A:315:ASN:HD22	1.65	0.60
4:A:375:ASN:H	4:A:376:ILE:HD12	1.65	0.60
4:F:920:ILE:HD12	4:F:940:ALA:HB2	1.83	0.60
4:A:163:LYS:HB2	4:F:1150:MET:SD	2.41	0.60
4:F:991:ARG:HG2	5:G:1337:LEU:HD23	1.83	0.60
4:A:357:LEU:HD22	5:B:567:ALA:HB2	1.82	0.60
4:F:837:LYS:C	4:F:838:LYS:HD2	2.21	0.60
4:A:376:ILE:N	4:A:376:ILE:HD12	2.15	0.60
4:A:137:LYS:HD2	4:A:138:LYS:HZ2	1.66	0.60
4:A:358:TYR:CZ	4:A:364:SER:HB3	2.37	0.60
1:C:13:DT:H5"	5:B:589:ARG:NH2	2.16	0.60
4:A:340:ILE:HG21	5:B:559:VAL:HG21	1.82	0.60
4:A:451:ILE:HB	4:A:453:LEU:HG	1.84	0.60
4:A:125:MET:HE1	4:A:176:VAL:HG11	1.84	0.60
4:F:1235:LEU:H	4:F:1235:LEU:HD12	1.67	0.60
4:A:160:GLN:O	4:F:1150:MET:SD	2.60	0.60
4:F:1144:ALA:O	4:F:1147:GLU:N	2.16	0.60
4:F:1184:VAL:O	4:F:1188:LEU:HG	2.02	0.59
4:A:349:ARG:NH2	5:B:613:GLU:OE1	2.35	0.59
5:B:587:HIS:CE1	5:B:589:ARG:HD3	2.37	0.59
4:F:743:HIS:CD2	4:F:779:LEU:HD21	2.37	0.59
4:A:253:ASP:OD2	4:A:309:LYS:NZ	2.35	0.59
4:F:742:THR:HG22	4:F:743:HIS:N	2.17	0.59
4:A:206:VAL:O	4:A:206:VAL:CG2	2.49	0.59
4:A:227:ASP:OD2	5:B:568:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1024:TYR:O	5:G:1310:THR:HB	2.02	0.59
4:F:1234:PHE:O	4:F:1238:LEU:HB2	2.01	0.59
4:F:1064:SER:O	4:F:1068:GLU:HG3	2.02	0.59
4:A:281:LEU:HD22	4:A:283:GLU:CG	2.32	0.59
4:A:387:TYR:HA	4:A:392:ILE:HG21	1.85	0.59
4:A:374:ALA:HB3	4:A:376:ILE:CD1	2.33	0.59
4:F:1127:ILE:HG22	4:F:1128:ASP:N	2.17	0.59
4:A:387:TYR:CZ	4:A:542:SER:HB3	2.37	0.59
4:F:1148:LEU:O	4:F:1149:GLU:C	2.41	0.59
4:A:363:GLN:NE2	5:B:579:GLY:HA3	2.18	0.59
4:A:427:ILE:O	4:A:431:VAL:HG23	2.03	0.59
5:G:1294:ARG:O	5:G:1297:TYR:HB3	2.03	0.58
4:F:1049:ARG:CD	4:F:1049:ARG:N	2.66	0.58
5:B:585:PHE:O	5:B:586:PRO:C	2.41	0.58
4:A:163:LYS:HB2	4:F:1150:MET:HE1	1.83	0.58
4:A:359:ARG:NH1	5:B:600:GLU:OE2	2.30	0.58
5:B:626:PHE:CG	5:B:627:GLY:N	2.71	0.58
4:A:348:GLU:HG2	4:A:349:ARG:HG2	1.85	0.58
4:F:1203:ILE:CG2	4:F:1203:ILE:O	2.51	0.58
5:G:1319:GLY:C	5:G:1320:ASN:HD22	2.06	0.58
4:A:328:ASN:HD21	4:A:331:ASP:N	2.01	0.58
4:F:1148:LEU:O	4:F:1150:MET:N	2.37	0.58
4:A:119:THR:HB	4:A:393:LYS:HE2	1.86	0.58
4:A:417:VAL:O	4:A:418:PRO:C	2.37	0.58
4:F:964:ILE:HG12	4:F:968:LEU:HD12	1.85	0.58
5:G:1314:MET:HB2	5:G:1323:MET:HG2	1.84	0.58
4:A:293:LEU:HD22	4:A:313:THR:OG1	2.02	0.58
4:A:138:LYS:HB2	4:A:139:PHE:CD1	2.39	0.58
4:A:160:GLN:HA	4:F:1150:MET:HE1	1.86	0.58
4:F:810:ASN:HD22	4:F:888:HIS:CD2	2.22	0.58
5:G:1289:MET:HE2	5:G:1328:ARG:HD2	1.84	0.57
4:A:363:GLN:HE22	5:B:579:GLY:HA3	1.67	0.57
4:F:1122:ILE:HG23	4:F:1126:THR:HG22	1.87	0.57
3:I:31:DC:H5'	3:I:31:DC:H6	1.68	0.57
4:F:785:GLU:HG3	4:F:785:GLU:O	2.02	0.57
4:A:237:LYS:HZ1	4:F:1138:GLU:HB2	1.69	0.57
4:A:544:LEU:O	4:A:544:LEU:CG	2.52	0.57
4:A:164:ARG:HG2	4:A:164:ARG:O	2.05	0.57
4:F:1117:VAL:HG12	4:F:1118:PRO:N	2.19	0.57
5:G:1273:GLU:OE2	5:G:1315:ARG:NH1	2.38	0.57
4:A:259:TRP:CE3	4:A:260:ARG:HG2	2.40	0.57
4:A:300:ILE:HG13	4:A:300:ILE:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:334:GLN:O	4:A:334:GLN:HG2	2.03	0.57
4:F:1120:ARG:HB2	4:F:1122:ILE:HD12	1.86	0.57
4:A:328:ASN:ND2	4:A:330:ALA:HB3	2.19	0.57
4:F:985:ASN:HB2	4:F:1011:ILE:HG22	1.87	0.57
4:F:922:ILE:HG12	4:F:925:TYR:HD1	1.69	0.56
4:A:433:TYR:O	4:A:433:TYR:CD2	2.58	0.56
4:A:23:THR:OG1	4:A:24:GLU:OE1	2.23	0.56
4:F:708:LEU:HD11	4:F:746:ALA:O	2.06	0.56
4:F:717:GLN:HE21	4:F:721:ARG:HH21	1.52	0.56
4:F:1139:LEU:CB	4:F:1143:GLU:HB3	2.35	0.56
4:A:166:SER:O	4:A:167:THR:O	2.23	0.56
4:F:804:ILE:HG12	4:F:809:ILE:HB	1.85	0.56
4:F:1054:PHE:O	5:G:1252:MET:HG2	2.05	0.56
5:B:570:LEU:N	5:B:570:LEU:HD12	2.19	0.56
4:F:881:GLN:HA	4:F:881:GLN:NE2	2.20	0.56
4:F:713:ASN:ND2	4:F:716:GLN:H	2.03	0.56
4:A:437:HIS:O	4:A:439:LEU:HD13	2.06	0.56
4:F:993:LEU:HD23	4:F:1011:ILE:O	2.05	0.56
4:F:1120:ARG:NH2	4:F:1191:SER:HA	2.21	0.56
4:A:523:GLU:HG3	4:A:529:LYS:HE3	1.87	0.56
4:A:72:MET:O	4:A:76:VAL:HG23	2.06	0.56
4:F:909:VAL:O	4:F:913:TYR:HD2	1.88	0.56
4:F:1137:HIS:O	4:F:1138:GLU:CB	2.54	0.56
4:F:713:ASN:ND2	4:F:716:GLN:CG	2.69	0.56
5:B:585:PHE:HB3	5:B:586:PRO:CD	2.33	0.55
4:F:790:SER:OG	4:F:794:SER:CB	2.54	0.55
4:F:763:THR:HG23	4:F:791:THR:HG22	1.87	0.55
4:F:1091:GLU:CD	4:F:1208:ARG:HD3	2.27	0.55
4:F:1127:ILE:O	4:F:1130:LEU:HB3	2.05	0.55
4:F:881:GLN:CA	4:F:881:GLN:HE21	2.18	0.55
4:F:952:ALA:C	4:F:954:GLN:H	2.10	0.55
4:F:801:ARG:HD3	4:F:811:ARG:O	2.07	0.55
4:A:295:ALA:HB2	4:A:321:ILE:CD1	2.36	0.55
1:C:17:DT:O3'	4:A:540:LEU:HD22	2.06	0.55
5:B:636:ARG:O	5:B:640:GLU:HG3	2.06	0.55
4:A:298:GLU:HG3	5:B:640:GLU:O	2.07	0.55
4:A:351:TYR:CE1	4:A:376:ILE:HG23	2.41	0.55
5:B:625:LEU:HB3	5:B:630:GLN:HE22	1.71	0.55
4:F:1067:MET:O	4:F:1071:LEU:HB2	2.06	0.55
4:F:820:ASP:O	4:F:824:VAL:HG23	2.07	0.55
4:A:49:MET:CE	4:A:56:PRO:HG3	2.37	0.55
4:F:1085:LYS:HB2	4:F:1088:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1223:GLU:HG2	4:F:1229:LYS:HD3	1.89	0.55
4:F:1144:ALA:O	4:F:1145:LEU:C	2.45	0.55
4:F:1097:ALA:O	4:F:1101:VAL:HG23	2.06	0.55
4:A:431:VAL:HA	4:A:441:LEU:HD21	1.87	0.54
4:A:437:HIS:HB3	4:A:439:LEU:HD13	1.88	0.54
4:F:959:TRP:CZ3	4:F:960:ARG:HG3	2.41	0.54
4:A:325:GLU:HG2	5:B:621:GLN:OE1	2.07	0.54
4:A:13:ASN:N	4:A:13:ASN:ND2	2.38	0.54
4:A:288:SER:HB3	4:A:292:ILE:HB	1.89	0.54
4:F:830:LYS:HG2	4:F:830:LYS:O	2.07	0.54
4:A:73:ARG:HD2	4:A:89:ILE:HB	1.88	0.54
4:F:909:VAL:O	4:F:913:TYR:CD2	2.60	0.54
4:F:1203:ILE:HG23	4:F:1203:ILE:O	2.07	0.54
4:F:742:THR:HG23	4:F:779:LEU:HD22	1.89	0.54
4:F:1207:SER:O	4:F:1208:ARG:C	2.45	0.54
4:A:351:TYR:CZ	4:A:377:PRO:HD2	2.42	0.54
4:A:55:ALA:HB1	4:A:57:TRP:CE2	2.42	0.54
4:F:730:MET:CE	4:F:967:ILE:HD11	2.37	0.54
4:A:288:SER:OG	5:B:611:ALA:O	2.20	0.54
4:F:869:TYR:O	4:F:873:VAL:HG23	2.08	0.54
4:A:532:ILE:H	4:A:532:ILE:HD12	1.73	0.54
5:B:628:ASN:H	5:B:628:ASN:HD22	1.56	0.54
5:G:1273:GLU:OE2	5:G:1315:ARG:HD2	2.08	0.54
4:A:383:GLY:O	4:A:384:LEU:HD12	2.07	0.54
4:F:713:ASN:ND2	4:F:716:GLN:HG3	2.12	0.54
4:F:1050:ARG:HB3	4:F:1052:ARG:HG2	1.89	0.54
4:F:756:PRO:O	4:F:787:VAL:HA	2.07	0.54
5:B:642:PRO:CB	5:B:645:LEU:HD12	2.32	0.53
4:F:878:GLN:HE21	4:F:878:GLN:HA	1.73	0.53
4:F:927:ASP:OD2	5:G:1260:LYS:NZ	2.40	0.53
4:A:228:THR:HA	4:A:232:GLN:OE1	2.08	0.53
4:A:341:ARG:O	4:A:344:VAL:HG22	2.06	0.53
4:F:1023:TYR:HA	5:G:1309:LEU:O	2.09	0.53
4:F:1060:THR:CG2	4:F:1062:ALA:H	2.21	0.53
4:F:922:ILE:HD12	4:F:923:ASP:O	2.08	0.53
4:F:825:MET:CE	4:F:876:VAL:HG11	2.39	0.53
4:A:508:ARG:HG2	4:A:508:ARG:HH11	1.74	0.53
5:B:588:ASN:HA	5:B:591:LEU:HD22	1.91	0.53
4:F:1199:ALA:O	4:F:1201:ARG:HG3	2.08	0.53
1:D:14:DT:H72	1:D:15:DT:O4	2.09	0.53
4:F:1059:ARG:HG2	5:G:1277:PHE:HA	1.89	0.53
4:A:168:TYR:O	4:A:170:GLU:N	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:G:1274:GLU:HB2	5:G:1325:PRO:HD2	1.91	0.53
4:F:820:ASP:OD1	4:F:1093:LYS:HE2	2.08	0.53
4:A:536:THR:HG22	4:A:537:ASP:N	2.23	0.53
5:G:1293:ARG:NH1	5:G:1332:GLU:OE2	2.42	0.53
4:F:761:ALA:HB1	4:F:772:MET:CE	2.40	0.53
4:F:864:ARG:O	4:F:865:ALA:HB2	2.10	0.52
4:A:42:THR:HG22	4:A:76:VAL:HG23	1.91	0.52
4:F:972:ARG:NH1	4:F:972:ARG:HG2	2.24	0.52
4:A:194:ASP:O	4:A:196:ILE:N	2.43	0.52
5:G:1285:ASP:HB3	5:G:1288:GLU:HB2	1.91	0.52
5:G:1268:PHE:CD1	5:G:1308:VAL:HG13	2.44	0.52
4:F:1116:ASN:ND2	4:F:1122:ILE:H	2.08	0.52
5:B:596:GLU:O	5:B:600:GLU:HG2	2.09	0.52
5:B:628:ASN:ND2	5:B:628:ASN:N	2.54	0.52
4:A:487:VAL:O	4:A:491:SER:HB3	2.09	0.52
4:F:704:LEU:C	4:F:706:GLU:H	2.13	0.52
4:A:41:LEU:HD13	4:A:249:VAL:HG21	1.92	0.52
4:F:855:LEU:HD12	4:F:930:ARG:NH2	2.25	0.52
4:F:1049:ARG:NH2	5:G:1306:GLU:OE1	2.38	0.52
4:A:258:ARG:NH2	5:B:595:ASP:CB	2.72	0.52
4:F:987:ARG:HG2	4:F:988:SER:N	2.24	0.52
5:B:564:LEU:HB3	5:B:603:LEU:CD2	2.34	0.52
4:A:24:GLU:OE2	4:A:219:TYR:OH	2.25	0.52
4:F:1055:ALA:HB3	5:G:1267:VAL:HG22	1.91	0.52
4:A:495:GLU:OE2	4:A:498:LYS:HE3	2.09	0.52
4:A:210:LEU:O	4:A:214:GLN:HG3	2.09	0.52
4:A:417:VAL:HG12	4:A:418:PRO:HD3	1.92	0.52
1:D:15:DT:H2"	1:D:16:DT:OP2	2.09	0.52
5:B:584:ILE:CG2	5:B:585:PHE:N	2.73	0.52
4:F:1117:VAL:O	4:F:1119:LYS:N	2.43	0.52
4:F:1244:LEU:HA	4:F:1247:LEU:HD12	1.92	0.52
4:F:908:ASP:N	4:F:908:ASP:OD1	2.43	0.52
4:A:313:THR:HG22	4:A:315:ASN:H	1.74	0.52
4:F:835:ASP:O	4:F:840:GLU:HA	2.10	0.52
4:A:543:ASP:OD1	4:A:545:ASP:HB2	2.10	0.52
5:B:587:HIS:ND1	5:B:589:ARG:HB2	2.25	0.51
4:F:1055:ALA:HB2	5:G:1264:PHE:CG	2.45	0.51
4:A:518:VAL:HG13	4:A:547:LEU:HB3	1.91	0.51
4:F:1167:GLN:OE1	4:F:1190:LYS:HG3	2.10	0.51
4:A:233:TYR:O	4:A:237:LYS:HB2	2.10	0.51
4:F:868:TYR:O	4:F:872:VAL:HG23	2.11	0.51
4:F:1231:LEU:O	4:F:1235:LEU:CD1	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1221:HIS:O	4:F:1225:VAL:HG22	2.09	0.51
5:B:601:ARG:NH1	5:B:640:GLU:OE2	2.43	0.51
4:A:73:ARG:HH11	4:A:73:ARG:CG	2.10	0.51
4:F:1044:VAL:C	4:F:1046:ARG:H	2.14	0.51
4:F:748:LEU:HD21	4:F:919:TYR:CE2	2.45	0.51
4:F:756:PRO:O	4:F:787:VAL:HG22	2.10	0.51
5:B:602:ARG:O	5:B:605:TYR:HB3	2.10	0.51
4:F:1129:LYS:HD3	4:F:1151:ILE:CG2	2.40	0.51
5:G:1328:ARG:O	5:G:1332:GLU:HG3	2.10	0.51
4:F:1091:GLU:OE1	4:F:1208:ARG:HD3	2.10	0.51
5:G:1291:GLU:HG3	5:G:1294:ARG:HH21	1.76	0.51
4:F:764:PHE:HE2	4:F:932:GLN:NE2	2.08	0.51
5:B:629:ILE:HD12	5:B:629:ILE:N	2.25	0.51
4:F:797:VAL:HG21	4:F:815:ILE:HD11	1.93	0.51
4:A:117:ASP:HB2	4:A:118:PRO:HD2	1.93	0.51
4:A:224:GLU:OE1	4:A:224:GLU:HA	2.11	0.51
4:F:954:GLN:HG2	5:G:1298:VAL:HG12	1.93	0.51
4:A:298:GLU:HG2	5:B:642:PRO:CG	2.41	0.51
4:F:1179:SER:H	4:F:1182:GLU:HG3	1.76	0.51
4:A:363:GLN:HE21	5:B:578:ILE:HD12	1.76	0.51
4:F:1092:ILE:O	4:F:1096:LEU:HB2	2.10	0.51
4:F:824:VAL:HG22	4:F:1109:LEU:HD13	1.93	0.51
4:F:742:THR:CG2	4:F:743:HIS:N	2.74	0.51
4:A:340:ILE:CG2	5:B:559:VAL:HG21	2.41	0.51
4:A:340:ILE:O	4:A:344:VAL:CG1	2.59	0.51
4:F:713:ASN:ND2	4:F:713:ASN:N	2.58	0.50
4:F:1095:ILE:HD13	4:F:1187:VAL:CG1	2.42	0.50
4:A:285:ASN:CB	4:A:293:LEU:HD21	2.40	0.50
4:F:985:ASN:CB	4:F:993:LEU:HD21	2.41	0.50
4:F:1112:LEU:HD13	4:F:1141:LEU:CD1	2.41	0.50
4:F:1115:ILE:HG23	4:F:1116:ASN:N	2.26	0.50
4:F:1120:ARG:HH12	4:F:1167:GLN:HE22	1.58	0.50
4:A:342:GLU:O	4:A:346:ARG:HG3	2.12	0.50
4:A:194:ASP:C	4:A:196:ILE:H	2.14	0.50
4:A:200:ILE:HD11	4:A:235:LEU:HB2	1.92	0.50
4:F:1060:THR:HB	4:F:1063:GLN:HE21	1.76	0.50
4:A:134:ILE:CG1	4:A:136:PRO:HD2	2.41	0.50
4:F:1024:TYR:HB3	5:G:1310:THR:HG22	1.93	0.50
5:G:1342:SER:OG	5:G:1342:SER:OXT	2.17	0.50
5:G:1277:PHE:CD1	5:G:1277:PHE:C	2.85	0.50
4:F:881:GLN:HA	4:F:881:GLN:HE21	1.74	0.50
4:A:28:LEU:HB3	4:A:279:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:216:LYS:HD3	4:A:216:LYS:O	2.11	0.50
4:F:824:VAL:O	4:F:828:ILE:HG13	2.12	0.50
4:A:264:ILE:C	4:A:266:ASN:H	2.15	0.50
4:F:895:LEU:O	4:F:899:THR:CG2	2.60	0.50
4:A:13:ASN:ND2	4:A:16:GLN:CG	2.75	0.50
4:F:998:GLU:HG3	5:G:1334:PRO:CG	2.42	0.50
3:I:30:DA:H2''	3:I:31:DC:OP2	2.09	0.50
4:F:926:GLN:H	4:F:926:GLN:HE21	1.60	0.50
5:G:1314:MET:CB	5:G:1323:MET:HG2	2.41	0.50
4:A:187:ASN:HA	4:A:406:ASP:O	2.11	0.50
4:F:1095:ILE:O	4:F:1098:TYR:HB2	2.11	0.50
4:F:929:ASN:HD21	4:F:932:GLN:NE2	2.10	0.50
4:F:834:ILE:O	4:F:834:ILE:HG23	2.12	0.50
4:A:295:ALA:O	4:A:299:VAL:HG23	2.11	0.50
4:F:1089:ARG:NH1	4:F:1211:ASN:HD21	2.10	0.50
4:A:77:GLN:O	4:A:81:GLY:HA2	2.12	0.50
4:A:137:LYS:HD2	4:A:138:LYS:HZ1	1.72	0.50
4:F:1151:ILE:HB	4:F:1153:LEU:CD2	2.41	0.50
4:F:1125:SER:O	4:F:1126:THR:C	2.49	0.49
4:F:1189:ASP:O	4:F:1190:LYS:CB	2.60	0.49
4:A:125:MET:HE2	4:A:129:LEU:HD22	1.93	0.49
4:F:1238:LEU:O	4:F:1239:ALA:C	2.51	0.49
4:A:359:ARG:NH1	5:B:600:GLU:OE1	2.45	0.49
4:A:120:ASP:O	4:A:124:VAL:HG23	2.12	0.49
4:F:952:ALA:O	4:F:954:GLN:N	2.45	0.49
5:G:1256:LEU:HD21	5:G:1269:LEU:CD2	2.26	0.49
5:B:587:HIS:HE1	5:B:589:ARG:HD3	1.76	0.49
4:A:294:GLN:HG2	5:B:645:LEU:HD11	1.94	0.49
4:F:985:ASN:ND2	4:F:988:SER:H	2.10	0.49
5:B:593:ASP:HB3	5:B:596:GLU:HB2	1.95	0.49
4:F:756:PRO:CB	4:F:787:VAL:HG23	2.42	0.49
4:F:1122:ILE:HG23	4:F:1126:THR:CG2	2.42	0.49
4:A:144:ILE:HD12	4:A:173:VAL:HG22	1.94	0.49
4:A:119:THR:CB	4:A:393:LYS:HE2	2.42	0.49
4:A:291:ARG:HG2	5:B:645:LEU:HD23	1.95	0.49
5:G:1277:PHE:C	5:G:1277:PHE:HD1	2.14	0.49
4:F:796:CYS:HB3	4:F:895:LEU:O	2.13	0.49
4:A:393:LYS:HB3	4:A:393:LYS:HZ2	1.77	0.49
4:A:396:LEU:CD1	4:A:538:LEU:HD23	2.27	0.49
4:A:97:VAL:HG21	4:A:540:LEU:HD11	1.94	0.49
3:I:31:DC:H2''	3:I:32:DT:C5'	2.43	0.49
3:I:31:DC:H2''	3:I:32:DT:H5'	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1223:GLU:O	4:F:1229:LYS:NZ	2.43	0.49
4:F:1137:HIS:O	4:F:1138:GLU:HB2	2.13	0.49
4:A:237:LYS:HZ3	4:F:1138:GLU:CD	2.16	0.49
4:A:37:LYS:NZ	4:A:223:ASP:OD2	2.46	0.49
4:F:839:PHE:HD1	4:F:869:TYR:HD1	1.61	0.49
5:G:1289:MET:CE	5:G:1328:ARG:HD2	2.42	0.49
4:F:851:ALA:O	4:F:856:LEU:HB2	2.12	0.49
4:A:313:THR:HG22	4:A:314:GLU:N	2.28	0.49
4:F:929:ASN:ND2	4:F:929:ASN:N	2.34	0.49
4:A:295:ALA:HB2	4:A:321:ILE:HD11	1.95	0.49
4:F:1139:LEU:HB3	4:F:1143:GLU:HG2	1.94	0.49
4:F:825:MET:HE1	4:F:876:VAL:HG11	1.94	0.48
4:F:835:ASP:N	4:F:836:PRO:CD	2.75	0.48
4:A:329:GLU:CD	5:B:624:THR:H	2.15	0.48
4:A:64:PHE:CD1	4:A:224:GLU:HB2	2.48	0.48
4:F:712:LEU:HB3	4:F:716:GLN:CB	2.42	0.48
4:A:290:LYS:HB2	4:A:317:GLU:HA	1.95	0.48
4:A:375:ASN:N	4:A:376:ILE:HD12	2.27	0.48
4:A:437:HIS:CB	4:A:439:LEU:HD13	2.43	0.48
4:A:222:ILE:HD11	4:A:228:THR:HG21	1.95	0.48
4:F:713:ASN:ND2	4:F:713:ASN:H	2.10	0.48
4:F:985:ASN:ND2	4:F:987:ARG:N	2.59	0.48
4:A:343:ALA:O	4:A:348:GLU:O	2.32	0.48
4:F:1095:ILE:HD13	4:F:1187:VAL:HG11	1.95	0.48
4:F:838:LYS:N	4:F:838:LYS:HD2	2.28	0.48
5:G:1273:GLU:HB2	5:G:1324:ASP:HB2	1.94	0.48
4:F:1050:ARG:NH1	5:G:1249:ASP:OD2	2.38	0.48
4:F:1148:LEU:HD12	4:F:1151:ILE:HD12	1.95	0.48
4:F:1028:ASN:O	4:F:1031:ASP:HB3	2.14	0.48
4:A:399:LEU:HB3	4:A:531:LEU:HD21	1.95	0.48
4:F:951:ASP:OD2	4:F:954:GLN:OE1	2.31	0.48
4:F:711:HIS:ND1	4:F:743:HIS:HE1	2.12	0.48
5:B:565:HIS:CE1	5:B:603:LEU:HD11	2.49	0.48
4:F:737:LYS:HB2	4:F:949:VAL:HG11	1.95	0.48
1:C:15:DT:OP1	5:B:563:THR:HG21	2.13	0.48
4:A:271:GLU:OE2	4:A:279:VAL:HG21	2.12	0.48
4:F:771:GLU:O	4:F:775:ARG:HG3	2.14	0.48
4:F:818:PRO:HD3	4:F:892:PHE:HE2	1.77	0.48
4:A:353:ASP:HA	5:B:573:PRO:HD2	1.95	0.48
4:A:328:ASN:HD21	4:A:330:ALA:HB3	1.79	0.48
4:F:1051:TYR:O	5:G:1251:VAL:HA	2.13	0.48
4:A:194:ASP:C	4:A:196:ILE:N	2.66	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:895:LEU:O	4:F:899:THR:HG22	2.13	0.48
4:F:1213:ASP:HA	4:F:1216:LEU:HD12	1.95	0.48
4:F:1120:ARG:NH1	4:F:1167:GLN:HE22	2.12	0.48
4:A:163:LYS:C	4:F:1150:MET:SD	2.92	0.48
4:A:230:ARG:HH22	4:F:1139:LEU:CD2	2.25	0.48
4:F:1003:ASN:OD1	5:G:1293:ARG:HD2	2.14	0.48
4:A:9:LEU:HD21	4:A:21:ARG:HG2	1.95	0.48
4:A:284:GLN:NE2	4:A:286:TYR:CZ	2.82	0.48
4:F:1117:VAL:HG12	4:F:1118:PRO:HD3	1.95	0.48
4:A:538:LEU:O	4:A:540:LEU:N	2.35	0.48
4:F:746:ALA:CB	4:F:779:LEU:HD23	2.44	0.48
4:A:352:ARG:HD3	5:B:560:MET:HE2	1.96	0.48
3:I:30:DA:H1'	3:I:31:DC:H5''	1.95	0.48
4:A:521:HIS:O	4:A:522:PHE:C	2.52	0.48
4:A:396:LEU:HD21	4:A:538:LEU:HD22	1.96	0.47
4:F:838:LYS:O	4:F:840:GLU:N	2.47	0.47
4:A:134:ILE:O	4:A:136:PRO:O	2.32	0.47
4:A:437:HIS:O	4:A:439:LEU:CD1	2.62	0.47
4:A:499:ALA:O	4:A:501:ARG:HG3	2.14	0.47
5:B:571:GLU:HA	5:B:610:ARG:O	2.14	0.47
4:A:13:ASN:HD21	4:A:16:GLN:CG	2.27	0.47
4:F:925:TYR:CG	4:F:948:ALA:HB1	2.49	0.47
4:F:839:PHE:CD1	4:F:839:PHE:N	2.78	0.47
4:F:1021:ILE:O	5:G:1338:LEU:HA	2.14	0.47
4:F:1150:MET:HE2	4:F:1152:GLY:HA2	1.95	0.47
4:F:711:HIS:O	4:F:711:HIS:CD2	2.66	0.47
4:A:293:LEU:CD2	4:A:313:THR:OG1	2.62	0.47
4:A:41:LEU:CD1	4:A:249:VAL:HG21	2.44	0.47
4:A:454:GLY:O	4:A:456:LYS:N	2.47	0.47
4:A:391:GLU:HG2	4:A:392:ILE:HD12	1.96	0.47
4:A:417:VAL:HG12	4:A:418:PRO:CD	2.45	0.47
5:B:582:GLU:OE2	5:B:636:ARG:HG2	2.15	0.47
4:F:1040:ILE:HG22	4:F:1041:ARG:N	2.29	0.47
4:F:1190:LYS:O	4:F:1191:SER:CB	2.62	0.47
4:A:137:LYS:HD3	4:A:137:LYS:HA	1.59	0.47
4:A:518:VAL:CG1	4:A:547:LEU:HB3	2.43	0.47
4:A:351:TYR:CE1	4:A:377:PRO:HD2	2.50	0.47
4:F:1122:ILE:HG22	4:F:1127:ILE:HG13	1.97	0.47
3:I:31:DC:H1'	3:I:32:DT:H5''	1.95	0.47
4:F:958:ARG:HB3	5:G:1291:GLU:OE2	2.14	0.47
4:A:30:MET:HB2	4:A:281:LEU:HA	1.96	0.47
4:A:517:SER:O	4:A:518:VAL:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:580:MET:C	5:B:581:GLU:HG3	2.33	0.47
4:F:1048:GLU:HB3	4:F:1049:ARG:CD	2.41	0.47
4:A:352:ARG:NE	5:B:560:MET:HE2	2.30	0.47
4:F:764:PHE:CE2	4:F:932:GLN:NE2	2.82	0.47
4:F:838:LYS:HB3	4:F:839:PHE:CD1	2.49	0.47
4:A:348:GLU:O	4:A:349:ARG:HB2	2.15	0.47
4:A:281:LEU:HD22	4:A:283:GLU:HG3	1.96	0.47
4:F:852:LYS:NZ	4:F:894:ASP:OD1	2.48	0.47
4:A:414:ILE:C	4:A:414:ILE:HD12	2.35	0.47
4:F:835:ASP:HA	4:F:839:PHE:O	2.14	0.47
5:G:1286:ASP:N	5:G:1286:ASP:OD1	2.48	0.47
4:A:515:PHE:HE1	4:A:538:LEU:HD21	1.80	0.46
1:D:14:DT:H2"	5:G:1257:HIS:CG	2.50	0.46
4:F:1074:ALA:HB3	4:F:1076:ILE:HD12	1.97	0.46
4:F:1091:GLU:OE1	4:F:1091:GLU:N	2.42	0.46
4:F:1111:LEU:HD22	4:F:1141:LEU:HB3	1.98	0.46
4:A:451:ILE:HD13	4:A:451:ILE:N	2.30	0.46
4:F:891:ASP:O	4:F:894:ASP:HB2	2.14	0.46
4:A:117:ASP:OD1	4:A:119:THR:HB	2.16	0.46
5:G:1295:LEU:O	5:G:1298:VAL:HG22	2.15	0.46
4:A:313:THR:CG2	4:A:315:ASN:ND2	2.76	0.46
4:F:1116:ASN:ND2	4:F:1120:ARG:H	2.13	0.46
4:F:1118:PRO:O	4:F:1119:LYS:C	2.53	0.46
5:B:628:ASN:O	5:B:629:ILE:O	2.33	0.46
4:A:28:LEU:HB2	4:A:270:PHE:CD2	2.50	0.46
5:G:1320:ASN:ND2	5:G:1320:ASN:N	2.63	0.46
4:A:313:THR:HG22	4:A:314:GLU:H	1.81	0.46
4:F:835:ASP:HB2	4:F:841:PRO:HD3	1.97	0.46
4:A:449:GLU:C	4:A:450:MET:HG2	2.35	0.46
4:A:129:LEU:O	4:A:132:LYS:N	2.44	0.46
4:A:326:ALA:O	5:B:621:GLN:CG	2.46	0.46
4:A:93:HIS:O	4:A:97:VAL:HG23	2.15	0.46
5:G:1256:LEU:HB3	5:G:1295:LEU:HD22	1.97	0.46
4:F:1232:ILE:HD12	4:F:1232:ILE:N	2.09	0.46
4:F:1098:TYR:O	4:F:1102:ILE:HG13	2.16	0.46
4:F:1060:THR:CG2	4:F:1062:ALA:HB3	2.46	0.46
4:F:887:ASN:ND2	4:F:887:ASN:N	2.64	0.46
1:D:13:DT:H5"	5:G:1318:PHE:HZ	1.81	0.46
4:A:500:GLU:O	4:A:502:THR:HG23	2.16	0.46
4:F:1087:TYR:C	4:F:1089:ARG:H	2.19	0.46
4:F:1108:ASP:O	4:F:1109:LEU:C	2.55	0.46
4:A:300:ILE:HG23	4:A:306:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:G:1281:ARG:HA	5:G:1281:ARG:HD3	1.82	0.46
4:A:246:ILE:HG21	4:A:274:TYR:CE1	2.50	0.46
5:B:598:GLU:O	5:B:602:ARG:HG3	2.16	0.46
5:G:1317:LEU:HD23	5:G:1317:LEU:HA	1.72	0.46
4:F:1050:ARG:HH11	5:G:1249:ASP:CG	2.16	0.46
5:B:578:ILE:HG22	5:B:618:THR:OG1	2.16	0.46
4:F:1187:VAL:HG12	4:F:1188:LEU:N	2.30	0.46
4:A:37:LYS:NZ	4:A:223:ASP:OD1	2.42	0.46
4:F:1092:ILE:HG22	4:F:1093:LYS:N	2.30	0.46
4:F:776:VAL:CG1	4:F:784:ALA:HB1	2.46	0.46
5:G:1327:SER:O	5:G:1330:LEU:HB2	2.16	0.46
4:F:887:ASN:O	4:F:888:HIS:C	2.54	0.45
4:F:755:ALA:HB1	4:F:757:TRP:CE2	2.50	0.45
4:A:328:ASN:ND2	4:A:330:ALA:H	2.04	0.45
4:F:887:ASN:HD22	4:F:887:ASN:N	2.13	0.45
4:F:730:MET:HE1	4:F:967:ILE:HD11	1.97	0.45
4:F:1087:TYR:CZ	4:F:1242:SER:HB3	2.51	0.45
4:F:1103:ALA:HB2	4:F:1231:LEU:HD13	1.99	0.45
4:A:290:LYS:CE	4:A:315:ASN:O	2.65	0.45
4:A:349:ARG:HB3	4:A:354:PHE:CE1	2.51	0.45
5:B:599:GLU:HG3	5:B:602:ARG:HH21	1.82	0.45
4:A:215:TYR:HB3	4:A:242:ARG:CD	2.37	0.45
4:F:922:ILE:HG12	4:F:925:TYR:CD1	2.51	0.45
4:A:328:ASN:ND2	4:A:330:ALA:N	2.62	0.45
4:F:796:CYS:O	4:F:800:LEU:HD22	2.17	0.45
4:A:42:THR:HG22	4:A:76:VAL:CG2	2.46	0.45
4:A:160:GLN:HB3	4:F:1150:MET:HE2	1.99	0.45
4:F:1003:ASN:CG	5:G:1290:GLU:HG2	2.37	0.45
4:A:258:ARG:HG3	4:A:259:TRP:N	2.31	0.45
4:A:348:GLU:O	4:A:349:ARG:CB	2.64	0.45
4:A:60:LEU:HB2	4:A:217:PHE:CD1	2.52	0.45
4:F:1087:TYR:O	4:F:1093:LYS:HG3	2.17	0.45
4:A:324:TYR:CE1	4:A:326:ALA:HA	2.51	0.45
4:A:119:THR:HG21	4:A:393:LYS:CE	2.47	0.45
4:A:392:ILE:O	4:A:396:LEU:HB2	2.16	0.45
4:A:511:ASN:O	4:A:515:PHE:N	2.49	0.45
4:A:522:PHE:O	4:A:526:SER:HB2	2.17	0.45
4:A:329:GLU:OE1	5:B:624:THR:N	2.47	0.45
5:B:576:PHE:CE1	5:B:616:VAL:HG11	2.52	0.45
4:A:341:ARG:HD3	4:A:376:ILE:HD11	1.99	0.45
4:A:363:GLN:NE2	5:B:578:ILE:HD12	2.32	0.45
4:A:523:GLU:CG	4:A:523:GLU:O	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:852:LYS:NZ	4:F:881:GLN:OE1	2.47	0.45
4:F:1199:ALA:O	4:F:1200:GLU:C	2.54	0.45
4:F:820:ASP:O	4:F:823:SER:HB3	2.17	0.45
4:A:393:LYS:HB2	4:A:413:ARG:NH2	2.32	0.45
4:A:433:TYR:CG	4:A:433:TYR:O	2.70	0.45
5:B:593:ASP:HB3	5:B:596:GLU:CB	2.46	0.45
4:A:281:LEU:HD22	4:A:283:GLU:HG2	1.98	0.45
4:F:1022:LEU:HB2	5:G:1308:VAL:HB	1.99	0.45
4:F:1120:ARG:CB	4:F:1122:ILE:HD12	2.46	0.44
1:C:16:DT:O4	4:A:227:ASP:HB3	2.17	0.44
4:A:8:LEU:O	4:A:11:HIS:CE1	2.70	0.44
4:A:359:ARG:HA	4:A:359:ARG:HD2	1.71	0.44
4:A:266:ASN:HD22	4:A:266:ASN:HA	1.51	0.44
4:A:154:GLU:HA	4:A:230:ARG:CB	2.42	0.44
4:F:953:ASP:OD1	4:F:1006:ARG:HD2	2.16	0.44
5:G:1284:GLU:CG	5:G:1285:ASP:N	2.80	0.44
4:A:112:ASN:HD21	4:A:532:ILE:HD11	1.83	0.44
4:A:413:ARG:O	4:A:417:VAL:HG23	2.17	0.44
4:F:711:HIS:HD1	4:F:743:HIS:HE1	1.66	0.44
4:F:834:ILE:HG12	4:F:836:PRO:CG	2.47	0.44
4:A:328:ASN:C	4:A:328:ASN:ND2	2.71	0.44
5:G:1276:ILE:CD1	5:G:1315:ARG:HD3	2.47	0.44
4:A:351:TYR:HB2	5:B:557:ASP:O	2.17	0.44
4:F:1190:LYS:HD2	4:F:1190:LYS:HA	1.76	0.44
4:F:816:LEU:CD1	4:F:889:SER:HB3	2.44	0.44
4:A:138:LYS:O	4:A:139:PHE:C	2.56	0.44
4:A:347:GLY:O	4:A:348:GLU:CB	2.66	0.44
5:B:635:SER:O	5:B:638:LEU:HB2	2.18	0.44
4:F:866:SER:O	4:F:867:THR:C	2.53	0.44
4:A:220:ILE:HD12	4:A:240:ALA:HB2	2.00	0.44
4:F:1118:PRO:O	4:F:1120:ARG:HG3	2.18	0.44
4:F:886:ARG:C	4:F:888:HIS:H	2.21	0.44
4:A:412:LEU:HG	4:A:441:LEU:CD1	2.48	0.44
4:A:11:HIS:CD2	4:A:39:ARG:HH21	2.35	0.44
4:F:1085:LYS:HB2	4:F:1088:ASP:HB2	2.00	0.44
4:A:391:GLU:O	4:A:395:ILE:HG22	2.18	0.44
4:F:1021:ILE:HG12	5:G:1307:LEU:CD2	2.47	0.44
4:A:130:LYS:HG3	4:A:130:LYS:O	2.18	0.44
4:F:801:ARG:HG2	4:F:813:PHE:CE2	2.53	0.44
4:F:789:ILE:O	4:F:789:ILE:HG22	2.18	0.44
5:B:573:PRO:HA	5:B:612:GLU:HB2	1.99	0.44
4:A:432:ARG:C	4:A:434:ALA:H	2.22	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:621:GLN:HG2	5:B:621:GLN:H	1.37	0.43
4:A:226:GLN:HG2	4:A:251:ASP:C	2.39	0.43
4:A:49:MET:HE1	4:A:56:PRO:HG3	1.99	0.43
4:F:866:SER:OG	4:F:867:THR:N	2.49	0.43
4:A:385:LYS:HG3	4:A:542:SER:HB2	2.00	0.43
4:A:372:LEU:CD1	4:A:378:TYR:HE2	2.31	0.43
4:F:1136:ASP:O	4:F:1137:HIS:CG	2.71	0.43
4:F:1145:LEU:C	4:F:1147:GLU:N	2.72	0.43
4:A:218:GLN:O	4:A:245:ASN:HB2	2.19	0.43
4:F:1026:ALA:HB1	4:F:1031:ASP:HB3	1.99	0.43
4:A:18:GLU:HB3	4:A:280:ILE:HD13	2.00	0.43
4:A:162:ALA:HA	4:A:174:SER:OG	2.18	0.43
4:F:1178:VAL:HG12	4:F:1179:SER:N	2.33	0.43
4:F:1019:LYS:HD2	4:F:1019:LYS:HA	1.81	0.43
1:C:17:DT:H3'	4:A:540:LEU:O	2.19	0.43
5:G:1257:HIS:CE1	5:G:1295:LEU:HD21	2.52	0.43
4:F:1180:VAL:HG22	4:F:1231:LEU:HA	2.00	0.43
4:F:964:ILE:HG12	4:F:968:LEU:CD1	2.47	0.43
4:F:761:ALA:HB1	4:F:772:MET:HE1	2.00	0.43
5:B:587:HIS:HE1	5:B:589:ARG:CD	2.30	0.43
4:F:1208:ARG:O	4:F:1212:LEU:HD12	2.18	0.43
4:A:285:ASN:ND2	4:A:293:LEU:HD11	2.34	0.43
4:F:1113:ARG:O	4:F:1117:VAL:HG23	2.18	0.43
4:F:881:GLN:CA	4:F:881:GLN:NE2	2.80	0.43
4:A:56:PRO:O	4:A:87:VAL:HA	2.17	0.43
4:F:959:TRP:CD1	4:F:959:TRP:N	2.71	0.43
4:F:963:ASP:N	4:F:963:ASP:OD1	2.51	0.43
4:F:735:SER:HA	4:F:984:GLN:O	2.18	0.43
4:F:723:THR:HA	4:F:744:ARG:NH2	2.34	0.43
4:F:837:LYS:HB2	4:F:838:LYS:HD2	2.01	0.43
5:B:565:HIS:HE1	5:B:603:LEU:HD11	1.83	0.43
4:A:346:ARG:HB2	4:A:347:GLY:H	1.58	0.43
4:A:56:PRO:HB2	4:A:86:ASP:HB3	1.99	0.43
4:A:396:LEU:HD21	4:A:538:LEU:CD2	2.49	0.43
4:A:73:ARG:NE	4:A:89:ILE:HD12	2.30	0.43
4:F:878:GLN:HE21	4:F:878:GLN:CA	2.32	0.43
1:C:17:DT:H5'	4:A:64:PHE:O	2.19	0.43
4:F:1042:GLU:HA	4:F:1045:GLU:HG2	2.01	0.43
4:A:104:ILE:HD12	4:A:107:ILE:HD11	2.00	0.43
4:A:164:ARG:HB2	4:F:1150:MET:HG3	2.01	0.43
4:F:926:GLN:HE22	4:F:950:GLY:HA3	1.84	0.43
4:A:203:PHE:HE1	4:A:209:VAL:HG12	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:512:LEU:HD23	4:A:512:LEU:HA	1.83	0.43
4:F:824:VAL:HG12	4:F:828:ILE:HD11	2.01	0.43
5:B:636:ARG:HH11	5:B:636:ARG:CG	2.20	0.43
4:A:225:TYR:O	4:A:228:THR:OG1	2.37	0.43
4:A:387:TYR:C	4:A:387:TYR:CD1	2.92	0.42
4:A:433:TYR:CD2	4:A:451:ILE:HD12	2.54	0.42
4:A:102:ARG:HA	4:A:111:ARG:HD2	2.01	0.42
4:F:760:LEU:HD12	4:F:761:ALA:H	1.84	0.42
4:F:1036:VAL:HG22	5:G:1268:PHE:CD1	2.54	0.42
5:B:602:ARG:O	5:B:606:VAL:HG13	2.19	0.42
4:F:764:PHE:HE2	4:F:932:GLN:HE22	1.66	0.42
5:G:1276:ILE:HD11	5:G:1317:LEU:CD1	2.49	0.42
4:F:1153:LEU:N	4:F:1153:LEU:CD2	2.83	0.42
4:F:797:VAL:HG11	4:F:1236:THR:CG2	2.49	0.42
4:A:355:ALA:HB2	5:B:572:PHE:CG	2.54	0.42
4:F:1238:LEU:HD12	4:F:1238:LEU:HA	1.81	0.42
5:B:564:LEU:N	5:B:564:LEU:HD12	2.34	0.42
4:A:360:THR:O	4:A:363:GLN:HB2	2.19	0.42
4:F:1226:SER:O	4:F:1229:LYS:HG3	2.19	0.42
4:F:922:ILE:CG1	4:F:925:TYR:HD1	2.31	0.42
4:F:1228:ASP:OD2	4:F:1233:ALA:HB2	2.19	0.42
4:F:953:ASP:C	5:G:1294:ARG:HG2	2.39	0.42
1:D:13:DT:C7	5:G:1281:ARG:NH1	2.83	0.42
4:F:827:THR:O	4:F:831:GLU:HG2	2.19	0.42
4:F:776:VAL:HG12	4:F:784:ALA:CB	2.49	0.42
4:A:328:ASN:C	4:A:328:ASN:HD22	2.23	0.42
3:I:32:DT:H5'	3:I:32:DT:H6	1.83	0.42
4:A:56:PRO:HB3	4:A:87:VAL:HG23	2.02	0.42
4:A:148:ILE:HG23	4:A:177:TYR:CE1	2.54	0.42
4:F:838:LYS:HB3	4:F:839:PHE:CE1	2.54	0.42
4:F:1138:GLU:O	4:F:1138:GLU:CG	2.66	0.42
4:A:287:ARG:NH2	6:A:901:SO4:O2	2.52	0.42
4:F:832:LYS:HB3	4:F:833:ASN:HD21	1.78	0.42
4:F:1068:GLU:OE2	4:F:1080:ILE:HD11	2.20	0.42
4:F:1216:LEU:O	4:F:1220:LYS:HD2	2.20	0.42
5:B:641:ILE:O	5:B:642:PRO:C	2.58	0.42
4:A:519:THR:O	4:A:522:PHE:HB3	2.20	0.42
4:A:9:LEU:O	4:A:17:GLN:NE2	2.50	0.42
4:F:1084:LEU:HD23	4:F:1089:ARG:NH2	2.34	0.42
4:A:450:MET:C	4:A:451:ILE:HD13	2.40	0.42
4:F:1157:ALA:O	4:F:1158:ALA:C	2.58	0.42
4:F:1203:ILE:HA	4:F:1203:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1186:GLU:O	4:F:1186:GLU:HG3	2.20	0.42
5:G:1283:LEU:HD12	5:G:1283:LEU:HA	1.80	0.42
4:F:1085:LYS:HD2	4:F:1242:SER:HB2	2.01	0.41
4:F:780:LEU:HB2	4:F:781:GLY:H	1.63	0.41
4:F:1052:ARG:HB3	5:G:1249:ASP:HA	2.01	0.41
4:F:818:PRO:HD3	4:F:892:PHE:CE2	2.53	0.41
4:A:387:TYR:O	4:A:393:LYS:HG2	2.21	0.41
4:F:1041:ARG:O	4:F:1045:GLU:HG2	2.20	0.41
4:A:125:MET:HE1	4:A:129:LEU:CD1	2.47	0.41
4:F:729:ILE:HB	4:F:949:VAL:HG22	2.01	0.41
4:A:237:LYS:NZ	4:F:1138:GLU:HB2	2.34	0.41
5:B:562:MET:SD	5:B:567:ALA:HA	2.60	0.41
4:A:284:GLN:NE2	4:A:286:TYR:OH	2.53	0.41
4:A:36:GLY:O	4:A:40:VAL:HG23	2.20	0.41
4:A:409:LEU:HG	4:A:409:LEU:H	1.68	0.41
4:F:1218:VAL:HG12	4:F:1234:PHE:HE1	1.85	0.41
4:F:1231:LEU:O	4:F:1235:LEU:HD12	2.21	0.41
4:F:869:TYR:CZ	4:F:873:VAL:HG21	2.55	0.41
4:F:1060:THR:HB	4:F:1063:GLN:NE2	2.35	0.41
4:F:796:CYS:SG	4:F:899:THR:HG21	2.60	0.41
4:A:415:ILE:HG13	4:A:415:ILE:O	2.19	0.41
4:A:324:TYR:HB2	5:B:649:ALA:CB	2.50	0.41
4:F:1157:ALA:O	4:F:1160:ALA:HB3	2.20	0.41
4:F:1056:VAL:HB	5:G:1253:LEU:CD1	2.46	0.41
4:F:761:ALA:HB1	4:F:772:MET:HE3	2.01	0.41
4:A:152:LYS:NZ	4:A:181:GLN:NE2	2.68	0.41
5:B:584:ILE:HD12	5:B:584:ILE:HA	1.88	0.41
5:B:584:ILE:HG22	5:B:585:PHE:H	1.80	0.41
5:B:601:ARG:O	5:B:604:ALA:HB3	2.21	0.41
4:A:378:TYR:HA	5:B:559:VAL:O	2.20	0.41
4:A:361:ASN:C	4:A:363:GLN:H	2.24	0.41
4:A:213:TYR:HA	4:A:216:LYS:HB3	2.01	0.41
4:A:58:ASN:HA	4:A:216:LYS:O	2.20	0.41
4:A:58:ASN:HB3	4:A:218:GLN:HB2	2.02	0.41
4:F:1019:LYS:HA	4:F:1020:PRO:HD3	1.78	0.41
4:F:829:LEU:HD12	4:F:829:LEU:HA	1.88	0.41
4:F:1117:VAL:CG1	4:F:1118:PRO:HD3	2.50	0.41
4:F:998:GLU:HG3	5:G:1334:PRO:HG3	2.02	0.41
4:F:1055:ALA:HB1	5:G:1254:MET:HE3	2.03	0.41
4:F:866:SER:O	4:F:867:THR:O	2.38	0.41
1:D:14:DT:H72	1:D:15:DT:C4	2.56	0.41
4:A:351:TYR:HE1	4:A:376:ILE:HG23	1.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:1112:LEU:HD13	4:F:1141:LEU:HD11	2.01	0.41
4:F:1114:ILE:CG2	4:F:1117:VAL:HG21	2.48	0.41
4:F:1189:ASP:O	4:F:1190:LYS:HB2	2.21	0.41
1:C:15:DT:OP1	5:B:563:THR:CG2	2.68	0.41
4:F:1100:ARG:O	4:F:1104:ASN:N	2.48	0.41
4:F:1092:ILE:HG23	4:F:1096:LEU:HD12	2.02	0.41
4:F:1234:PHE:CE2	4:F:1238:LEU:HD22	2.56	0.41
4:F:1091:GLU:CD	4:F:1091:GLU:N	2.67	0.41
4:F:1225:VAL:O	4:F:1225:VAL:HG23	2.21	0.41
4:A:478:VAL:HG13	4:A:482:GLU:CB	2.48	0.41
1:C:14:DT:H2'	1:C:14:DT:H6	1.67	0.41
4:F:1087:TYR:HD1	4:F:1088:ASP:N	2.19	0.41
4:F:839:PHE:CD1	4:F:869:TYR:HD1	2.37	0.41
4:A:371:LEU:CD2	4:A:376:ILE:HB	2.51	0.41
4:F:1190:LYS:O	4:F:1192:GLY:N	2.53	0.41
4:F:1157:ALA:O	4:F:1160:ALA:CB	2.69	0.41
4:F:1152:GLY:O	4:F:1153:LEU:O	2.39	0.41
4:F:953:ASP:OD2	4:F:1009:LYS:HE3	2.21	0.41
4:A:37:LYS:HZ3	4:A:223:ASP:CG	2.22	0.41
1:D:13:DT:H73	5:G:1281:ARG:NH1	2.36	0.41
4:F:767:LYS:HG3	4:F:767:LYS:H	1.37	0.41
4:A:537:ASP:O	4:A:541:ILE:HB	2.21	0.41
4:F:1095:ILE:CD1	4:F:1187:VAL:CG1	2.97	0.41
4:A:164:ARG:HB2	4:F:1150:MET:CG	2.50	0.41
1:C:14:DT:H2''	1:C:15:DT:C5'	2.48	0.41
4:A:508:ARG:HG2	4:A:508:ARG:NH1	2.36	0.41
4:F:1200:GLU:O	4:F:1201:ARG:HB2	2.20	0.41
4:F:1104:ASN:HD21	4:F:1106:ASP:HB2	1.86	0.41
4:A:536:THR:O	4:A:540:LEU:HB2	2.21	0.40
5:G:1261:GLY:H	5:G:1302:ARG:NH1	2.18	0.40
4:A:532:ILE:N	4:A:532:ILE:HD12	2.35	0.40
4:A:22:THR:O	4:A:44:ARG:NH1	2.54	0.40
4:F:800:LEU:HG	4:F:804:ILE:HD12	2.02	0.40
4:A:289:THR:HG21	4:A:318:GLY:HA3	2.03	0.40
4:A:73:ARG:NH1	4:A:77:GLN:OE1	2.32	0.40
4:A:342:GLU:CG	4:A:346:ARG:HH21	2.34	0.40
4:F:964:ILE:HG12	4:F:964:ILE:O	2.21	0.40
4:A:326:ALA:O	5:B:621:GLN:N	2.41	0.40
4:F:925:TYR:O	4:F:928:THR:OG1	2.39	0.40
4:F:1111:LEU:O	4:F:1115:ILE:HB	2.21	0.40
4:A:44:ARG:HD2	4:A:44:ARG:HH11	1.69	0.40
3:I:31:DC:H2'	3:I:32:DT:H71	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:297:ASN:O	4:A:301:GLU:HB2	2.21	0.40
4:F:713:ASN:O	4:F:717:GLN:HG3	2.21	0.40
4:F:1111:LEU:HD22	4:F:1141:LEU:HD13	2.03	0.40
3:I:33:DG:H2''	3:I:34:DC:H5'	2.03	0.40
4:A:31:ALA:HB1	4:A:37:LYS:HB3	2.02	0.40
4:A:417:VAL:CG1	4:A:418:PRO:HD3	2.51	0.40
4:A:88:TRP:NE1	4:A:95:MET:HB2	2.32	0.40
4:A:342:GLU:HG3	4:A:346:ARG:NH2	2.37	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	
4	A	540/548 (98%)	456 (84%)	60 (11%)	24 (4%)	4	15
4	F	542/548 (99%)	448 (83%)	63 (12%)	31 (6%)	3	8
5	B	93/95 (98%)	80 (86%)	8 (9%)	5 (5%)	3	9
5	G	93/95 (98%)	81 (87%)	8 (9%)	4 (4%)	4	15
All	All	1268/1286 (99%)	1065 (84%)	139 (11%)	64 (5%)	3	11

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	134	ILE
4	A	139	PHE
4	A	167	THR
4	A	168	TYR
4	A	348	GLU
4	A	375	ASN
4	A	424	ALA
4	A	539	ALA
5	B	628	ASN
5	B	629	ILE

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Mol	Chain	Res	Type
4	F	831	GLU
4	F	836	PRO
4	F	839	PHE
4	F	865	ALA
4	F	953	ASP
4	F	1126	THR
4	F	1138	GLU
4	F	1144	ALA
4	F	1145	LEU
4	F	1149	GLU
4	F	1153	LEU
4	F	1154	GLY
4	F	1204	GLU
4	F	1208	ARG
4	F	1239	ALA
5	G	1321	ILE
4	A	342	GLU
4	A	350	ARG
4	A	382	GLY
4	A	384	LEU
4	A	454	GLY
4	A	538	LEU
4	F	838	LYS
4	F	867	THR
4	F	1048	GLU
4	F	1119	LYS
4	F	1124	ALA
4	F	1137	HIS
4	F	1158	ALA
4	F	1190	LYS
4	A	8	LEU
4	A	11	HIS
4	A	195	LEU
4	A	349	ARG
4	F	888	HIS
4	F	1155	ALA
4	A	10	ALA
4	A	169	TYR
4	A	383	GLY
5	B	589	ARG
4	F	832	LYS
4	F	1150	MET

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Mol	Chain	Res	Type
4	F	1238	LEU
5	G	1318	PHE
4	A	455	ALA
5	B	585	PHE
4	F	1117	VAL
4	F	1125	SER
4	A	365	ARG
5	B	586	PRO
4	F	1232	ILE
5	G	1277	PHE
5	G	1278	PRO
4	A	417	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	
4	A	472/478 (99%)	406 (86%)	66 (14%)	5	14
4	F	474/478 (99%)	390 (82%)	84 (18%)	3	8
5	B	81/81 (100%)	62 (76%)	19 (24%)	1	3
5	G	81/81 (100%)	62 (76%)	19 (24%)	1	3
All	All	1108/1118 (99%)	920 (83%)	188 (17%)	3	9

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	13	ASN
4	A	15	GLU
4	A	18	GLU
4	A	41	LEU
4	A	44	ARG
4	A	51	GLU
4	A	57	TRP
4	A	63	THR
4	A	73	ARG
4	A	77	GLN

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Mol	Chain	Res	Type
4	A	80	LEU
4	A	86	ASP
4	A	90	SER
4	A	92	PHE
4	A	94	SER
4	A	95	MET
4	A	110	ASN
4	A	123	SER
4	A	129	LEU
4	A	135	ASP
4	A	137	LYS
4	A	139	PHE
4	A	143	THR
4	A	156	LEU
4	A	159	GLU
4	A	167	THR
4	A	168	TYR
4	A	175	ASP
4	A	183	ARG
4	A	185	LEU
4	A	205	ARG
4	A	222	ILE
4	A	226	GLN
4	A	228	THR
4	A	236	VAL
4	A	258	ARG
4	A	266	ASN
4	A	269	SER
4	A	278	LYS
4	A	281	LEU
4	A	293	LEU
4	A	307	LYS
4	A	313	THR
4	A	324	TYR
4	A	328	ASN
4	A	335	PHE
4	A	366	VAL
4	A	372	LEU
4	A	384	LEU
4	A	387	TYR
4	A	393	LYS
4	A	406	ASP

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Mol	Chain	Res	Type
4	A	413	ARG
4	A	420	ARG
4	A	445	LEU
4	A	450	MET
4	A	451	ILE
4	A	466	SER
4	A	473	GLN
4	A	475	GLN
4	A	490	LYS
4	A	496	MET
4	A	503	ILE
4	A	506	GLN
4	A	526	SER
4	A	531	LEU
5	B	563	THR
5	B	571	GLU
5	B	572	PHE
5	B	581	GLU
5	B	584	ILE
5	B	585	PHE
5	B	589	ARG
5	B	591	LEU
5	B	599	GLU
5	B	606	VAL
5	B	616	VAL
5	B	621	GLN
5	B	623	ARG
5	B	626	PHE
5	B	628	ASN
5	B	636	ARG
5	B	639	ASN
5	B	645	LEU
5	B	648	THR
4	F	705	SER
4	F	712	LEU
4	F	713	ASN
4	F	738	THR
4	F	739	ARG
4	F	742	THR
4	F	748	LEU
4	F	767	LYS
4	F	773	ARG

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Mol	Chain	Res	Type
4	F	777	GLN
4	F	778	SER
4	F	779	LEU
4	F	792	PHE
4	F	800	LEU
4	F	801	ARG
4	F	810	ASN
4	F	833	ASN
4	F	835	ASP
4	F	837	LYS
4	F	838	LYS
4	F	839	PHE
4	F	842	ARG
4	F	859	GLU
4	F	867	THR
4	F	875	ASP
4	F	878	GLN
4	F	879	GLU
4	F	881	GLN
4	F	885	LEU
4	F	899	THR
4	F	906	VAL
4	F	908	ASP
4	F	922	ILE
4	F	926	GLN
4	F	928	THR
4	F	929	ASN
4	F	936	VAL
4	F	937	LYS
4	F	944	GLN
4	F	955	SER
4	F	963	ASP
4	F	966	ASN
4	F	967	ILE
4	F	985	ASN
4	F	988	SER
4	F	1011	ILE
4	F	1013	THR
4	F	1034	GLN
4	F	1049	ARG
4	F	1050	ARG
4	F	1059	ARG

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Mol	Chain	Res	Type
4	F	1060	THR
4	F	1071	LEU
4	F	1072	LEU
4	F	1087	TYR
4	F	1091	GLU
4	F	1092	ILE
4	F	1093	LYS
4	F	1125	SER
4	F	1129	LYS
4	F	1132	ARG
4	F	1136	ASP
4	F	1139	LEU
4	F	1148	LEU
4	F	1153	LEU
4	F	1165	ARG
4	F	1167	GLN
4	F	1175	GLN
4	F	1182	GLU
4	F	1183	LEU
4	F	1185	GLU
4	F	1187	VAL
4	F	1195	GLU
4	F	1196	MET
4	F	1207	SER
4	F	1212	LEU
4	F	1214	GLU
4	F	1222	PHE
4	F	1223	GLU
4	F	1224	ASN
4	F	1227	ASP
4	F	1231	LEU
4	F	1232	ILE
4	F	1237	ASP
5	G	1252	MET
5	G	1255	THR
5	G	1273	GLU
5	G	1276	ILE
5	G	1277	PHE
5	G	1280	ASN
5	G	1283	LEU
5	G	1284	GLU
5	G	1288	GLU

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Mol	Chain	Res	Type
5	G	1291	GLU
5	G	1307	LEU
5	G	1308	VAL
5	G	1309	LEU
5	G	1313	GLN
5	G	1314	MET
5	G	1317	LEU
5	G	1320	ASN
5	G	1331	ASN
5	G	1340	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	13	ASN
4	A	43	HIS
4	A	153	ASN
4	A	181	GLN
4	A	214	GLN
4	A	221	HIS
4	A	226	GLN
4	A	266	ASN
4	A	284	GLN
4	A	305	ASN
4	A	315	ASN
4	A	328	ASN
4	A	363	GLN
4	A	404	ASN
4	A	511	ASN
5	B	628	ASN
5	B	630	GLN
4	F	707	GLN
4	F	713	ASN
4	F	717	GLN
4	F	743	HIS
4	F	766	ASN
4	F	833	ASN
4	F	853	ASN
4	F	878	GLN
4	F	882	GLN
4	F	887	ASN
4	F	888	HIS

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Mol	Chain	Res	Type
4	F	914	GLN
4	F	918	GLN
4	F	926	GLN
4	F	929	ASN
4	F	932	GLN
4	F	944	GLN
4	F	965	GLN
4	F	976	ASN
4	F	984	GLN
4	F	985	ASN
4	F	994	GLN
4	F	1015	ASN
4	F	1034	GLN
4	F	1063	GLN
4	F	1104	ASN
4	F	1116	ASN
4	F	1170	GLN
4	F	1175	GLN
4	F	1206	GLN
4	F	1211	ASN
4	F	1224	ASN
5	G	1257	HIS
5	G	1280	ASN
5	G	1313	GLN
5	G	1320	ASN
5	G	1331	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	SO4	A	901	-	4,4,4	1.39	1 (25%)	6,6,6	0.48	0
6	SO4	F	1249	-	4,4,4	1.21	1 (25%)	6,6,6	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	901	-	-	0/0/0/0	0/0/0/0
6	SO4	F	1249	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	SO4	O4-S	-2.69	1.38	1.47
6	F	1249	SO4	O4-S	-2.32	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	C	5/5 (100%)	-0.49	0 100 100	22, 25, 37, 37	0
1	D	5/5 (100%)	-0.26	0 100 100	29, 32, 41, 55	0
2	H	2/2 (100%)	2.58	2 (100%) 0 0	53, 53, 53, 64	0
3	I	5/5 (100%)	0.54	0 100 100	39, 39, 43, 47	0
4	A	542/548 (98%)	-0.14	17 (3%) 47 55	7, 31, 68, 100	0
4	F	544/548 (99%)	0.08	27 (4%) 28 33	16, 42, 74, 101	0
5	B	95/95 (100%)	0.17	8 (8%) 11 14	11, 39, 79, 91	0
5	G	95/95 (100%)	0.23	6 (6%) 19 23	19, 41, 79, 91	0
All	All	1293/1303 (99%)	0.01	60 (4%) 31 38	7, 37, 74, 101	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	345	GLU	10.6
5	G	1318	PHE	6.3
5	B	650	SER	5.8
5	B	557	ASP	5.3
5	B	556	GLY	5.1
4	A	346	ARG	4.8
4	F	835	ASP	4.7
4	F	836	PRO	4.7
4	F	1155	ALA	4.2
4	F	830	LYS	4.2
4	F	1203	ILE	4.1
5	G	1248	GLY	4.0
4	F	1204	GLU	3.9
4	F	1227	ASP	3.8
4	F	1132	ARG	3.8
5	B	627	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
4	A	341	ARG	3.7
5	G	1342	SER	3.7
5	B	628	ASN	3.7
4	A	384	LEU	3.7
5	B	626	PHE	3.5
5	G	1320	ASN	3.4
4	F	1228	ASP	3.4
4	A	379	GLN	3.3
4	F	1201	ARG	3.1
4	F	1046	ARG	3.0
4	A	167	THR	2.9
4	F	711	HIS	2.8
2	H	1	DG	2.8
4	F	1027	MET	2.8
4	A	383	GLY	2.8
4	F	1077	PRO	2.7
4	A	348	GLU	2.7
4	A	205	ARG	2.6
4	A	11	HIS	2.5
4	A	347	GLY	2.5
5	B	625	LEU	2.5
4	A	276	ASN	2.5
4	F	1173	GLN	2.4
4	A	10	ALA	2.4
4	A	525	VAL	2.3
2	H	2	DC	2.3
4	A	375	ASN	2.3
4	F	1082	GLY	2.2
5	G	1281	ARG	2.2
4	F	1084	LEU	2.2
4	F	1202	THR	2.2
4	F	1154	GLY	2.2
4	A	352	ARG	2.2
5	G	1340	THR	2.2
4	F	1149	GLU	2.2
4	F	1065	ARG	2.1
4	F	1195	GLU	2.1
5	B	592	GLU	2.1
4	F	706	GLU	2.0
4	F	1177	TYR	2.0
4	A	171	LYS	2.0
4	F	1050	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	1118	PRO	2.0
4	F	976	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	901	5/5	0.12	-0.36	44,49,52,52	0
6	SO4	F	1249	5/5	0.10	-0.91	48,49,53,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.