



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:40 PM GMT

PDB ID : 2D5N
Title : Crystal structure of a bifunctional deaminase and reductase involved in riboflavin biosynthesis
Authors : Liaw, S.H.; Chen, S.J.; Chang, Y.C.
Deposited on : 2005-11-02
Resolution : 2.97 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>

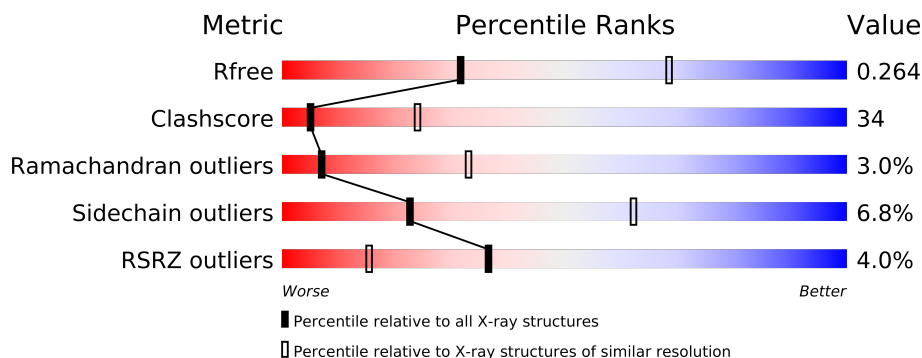
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.97 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	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (3.00-2.96)

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	A	373	
1	B	373	
1	C	373	
1	D	373	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11257 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 protein called Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	B	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	C	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	D	360	Total	C	N	O	S	0	0	0
			2747	1743	470	519	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	CLONING ARTIFACT	UNP P17618
A	-10	ARG	-	CLONING ARTIFACT	UNP P17618
A	-9	GLY	-	CLONING ARTIFACT	UNP P17618
A	-8	SER	-	CLONING ARTIFACT	UNP P17618
A	-7	HIS	-	CLONING ARTIFACT	UNP P17618
A	-6	HIS	-	CLONING ARTIFACT	UNP P17618
A	-5	HIS	-	CLONING ARTIFACT	UNP P17618
A	-4	HIS	-	CLONING ARTIFACT	UNP P17618
A	-3	HIS	-	CLONING ARTIFACT	UNP P17618
A	-2	HIS	-	CLONING ARTIFACT	UNP P17618
A	-1	GLY	-	CLONING ARTIFACT	UNP P17618
A	0	SER	-	CLONING ARTIFACT	UNP P17618
B	-11	MET	-	CLONING ARTIFACT	UNP P17618
B	-10	ARG	-	CLONING ARTIFACT	UNP P17618
B	-9	GLY	-	CLONING ARTIFACT	UNP P17618
B	-8	SER	-	CLONING ARTIFACT	UNP P17618
B	-7	HIS	-	CLONING ARTIFACT	UNP P17618
B	-6	HIS	-	CLONING ARTIFACT	UNP P17618
B	-5	HIS	-	CLONING ARTIFACT	UNP P17618
B	-4	HIS	-	CLONING ARTIFACT	UNP P17618
B	-3	HIS	-	CLONING ARTIFACT	UNP P17618

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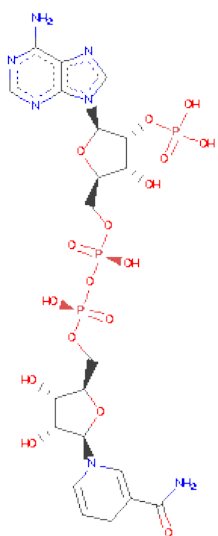
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	CLONING ARTIFACT	UNP P17618
B	-1	GLY	-	CLONING ARTIFACT	UNP P17618
B	0	SER	-	CLONING ARTIFACT	UNP P17618
C	-11	MET	-	CLONING ARTIFACT	UNP P17618
C	-10	ARG	-	CLONING ARTIFACT	UNP P17618
C	-9	GLY	-	CLONING ARTIFACT	UNP P17618
C	-8	SER	-	CLONING ARTIFACT	UNP P17618
C	-7	HIS	-	CLONING ARTIFACT	UNP P17618
C	-6	HIS	-	CLONING ARTIFACT	UNP P17618
C	-5	HIS	-	CLONING ARTIFACT	UNP P17618
C	-4	HIS	-	CLONING ARTIFACT	UNP P17618
C	-3	HIS	-	CLONING ARTIFACT	UNP P17618
C	-2	HIS	-	CLONING ARTIFACT	UNP P17618
C	-1	GLY	-	CLONING ARTIFACT	UNP P17618
C	0	SER	-	CLONING ARTIFACT	UNP P17618
D	-11	MET	-	CLONING ARTIFACT	UNP P17618
D	-10	ARG	-	CLONING ARTIFACT	UNP P17618
D	-9	GLY	-	CLONING ARTIFACT	UNP P17618
D	-8	SER	-	CLONING ARTIFACT	UNP P17618
D	-7	HIS	-	CLONING ARTIFACT	UNP P17618
D	-6	HIS	-	CLONING ARTIFACT	UNP P17618
D	-5	HIS	-	CLONING ARTIFACT	UNP P17618
D	-4	HIS	-	CLONING ARTIFACT	UNP P17618
D	-3	HIS	-	CLONING ARTIFACT	UNP P17618
D	-2	HIS	-	CLONING ARTIFACT	UNP P17618
D	-1	GLY	-	CLONING ARTIFACT	UNP P17618
D	0	SER	-	CLONING ARTIFACT	UNP P17618

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



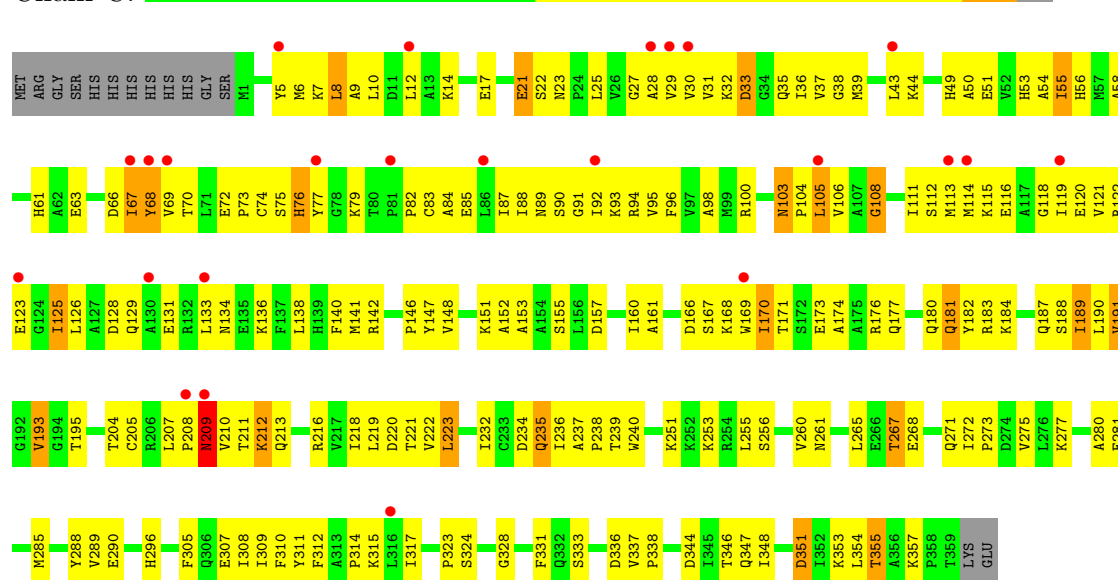
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	64	Total	O	0	0
			64	64		
4	C	54	Total	O	0	0
			54	54		
4	D	51	Total	O	0	0
			51	51		

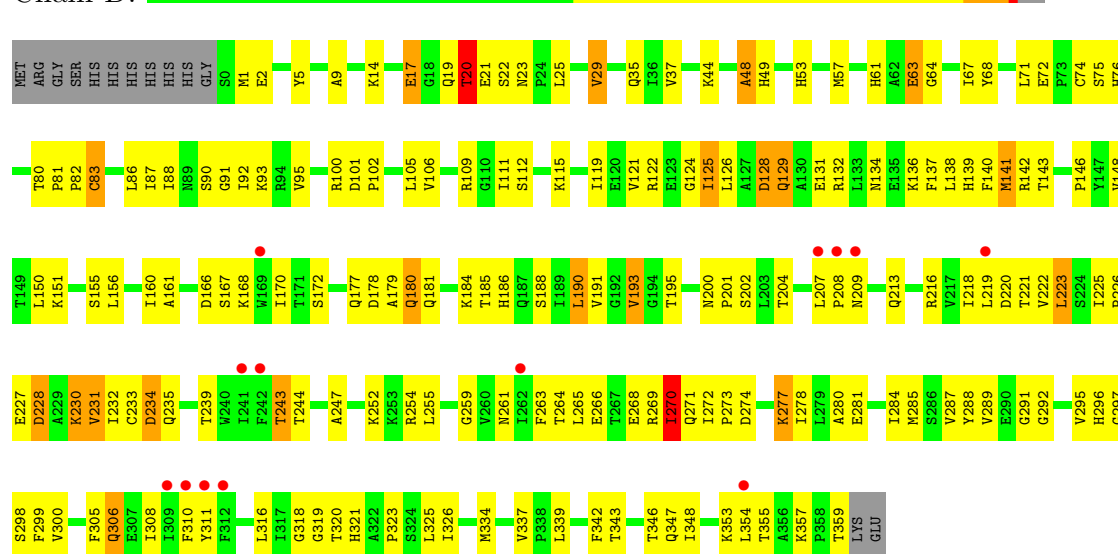
- Molecule 1: Riboflavin biosynthesis protein ribD

Chain C:



- Molecule 1: Riboflavin biosynthesis protein ribD

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.13Å 107.95Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.97 46.74 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.97) 97.2 (46.74-2.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.270 0.214 , 0.264	Depositor DCC
R_{free} test set	3566 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 35846 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11257	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: NDP, ZN

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	0.39	0/2792	0.67	1/3778 (0.0%)
1	B	0.38	0/2792	0.64	0/3778
1	C	0.37	0/2792	0.63	0/3778
1	D	0.37	0/2798	0.64	1/3786 (0.0%)
All	All	0.38	0/11174	0.65	2/15120 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	CYS	CA-CB-SG	6.18	125.13	114.00
1	D	83	CYS	CA-CB-SG	-5.45	104.19	114.00

There are no chirality outliers.

There are no planarity outliers.

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	A	2741	0	2782	156	0
1	B	2741	0	2782	232	0
1	C	2741	0	2782	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2747	0	2787	174	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	48	0	26	10	0
4	A	66	0	0	17	2
4	B	64	0	0	4	1
4	C	54	0	0	3	0
4	D	51	0	0	5	0
All	All	11257	0	11159	744	2

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 34.

All (744) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:309:ILE:HG12	1:B:355:THR:HG22	1.33	1.06
1:A:94:ARG:HA	4:A:1377:HOH:O	1.55	1.06
1:A:355:THR:HG22	4:A:1415:HOH:O	1.58	1.01
1:C:21:GLU:HG3	1:C:22:SER:H	1.26	1.00
1:D:270:ILE:H	1:D:270:ILE:HD13	1.24	0.98
1:B:308:ILE:HB	4:B:1362:HOH:O	1.64	0.97
1:B:181:GLN:HA	1:B:207:LEU:HD11	1.45	0.96
1:A:125:ILE:HD12	1:A:125:ILE:H	1.30	0.95
1:B:166:ASP:OD1	1:B:168:LYS:HG3	1.66	0.94
1:C:207:LEU:H	1:C:207:LEU:HD12	1.32	0.94
1:D:148:VAL:H	1:D:306:GLN:NE2	1.65	0.94
1:A:328:GLY:H	1:B:320:THR:HG22	1.36	0.91
1:A:95:VAL:HG11	1:A:114:MET:HE1	1.52	0.91
1:D:148:VAL:HB	1:D:305:PHE:HA	1.52	0.91
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.53	0.90
1:A:318:GLY:HA3	1:B:330:GLY:HA2	1.52	0.90
1:C:232:ILE:HD13	1:C:255:LEU:HD22	1.54	0.89
1:D:19:GLN:HG2	1:D:44:LYS:HD2	1.55	0.89
1:B:3:GLU:HB2	1:B:126:LEU:HD11	1.55	0.89
1:D:190:LEU:HB3	1:D:289:VAL:HG22	1.51	0.89
1:C:36:ILE:HD12	1:C:36:ILE:H	1.37	0.89
1:C:151:LYS:HD2	1:C:152:ALA:N	1.90	0.87
1:C:82:PRO:HD2	1:C:85:GLU:OE2	1.76	0.86
1:C:25:LEU:H	1:C:134:ASN:HD21	1.19	0.85
1:C:184:LYS:HZ1	1:C:207:LEU:HB2	1.42	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:VAL:H	1:B:306:GLN:HE21	1.18	0.84
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.57	0.83
1:D:25:LEU:H	1:D:134:ASN:HD21	1.25	0.83
1:C:32:LYS:HD2	1:C:61:HIS:O	1.78	0.83
1:C:309:ILE:CD1	1:C:355:THR:HB	2.09	0.83
1:A:64:GLY:HA2	1:A:93:LYS:HG2	1.58	0.83
1:A:184:LYS:NZ	1:A:207:LEU:HD12	1.93	0.82
1:C:94:ARG:HD3	1:C:96:PHE:CE2	2.14	0.82
1:B:206:ARG:HB2	1:B:206:ARG:NH1	1.94	0.82
1:A:134:ASN:O	1:A:138:LEU:HD13	1.77	0.82
1:C:204:THR:HB	1:C:213:GLN:NE2	1.95	0.82
1:C:180:GLN:HB3	1:C:207:LEU:HD11	1.62	0.81
1:B:301:LYS:HZ3	1:B:329:GLU:HG3	1.45	0.81
1:C:223:LEU:HD12	1:C:251:LYS:HD3	1.63	0.81
1:D:22:SER:HA	1:D:285:MET:HE1	1.63	0.81
1:C:111:ILE:O	1:C:115:LYS:HB2	1.82	0.80
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.11	0.80
1:D:190:LEU:CB	1:D:289:VAL:HG22	2.10	0.79
1:A:328:GLY:N	1:B:320:THR:HG22	1.96	0.79
1:B:88:ILE:HD11	1:B:114:MET:HA	1.65	0.78
1:B:161:ALA:HB3	1:B:323:PRO:CG	2.14	0.77
1:B:25:LEU:H	1:B:134:ASN:HD21	1.32	0.77
1:A:211:THR:HA	4:A:1369:HOH:O	1.85	0.76
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.68	0.75
1:B:72:GLU:OE1	1:B:111:ILE:HG12	1.86	0.75
1:C:105:LEU:H	1:C:105:LEU:HD23	1.51	0.75
1:B:137:PHE:HD1	1:B:138:LEU:HD12	1.51	0.75
1:A:62:ALA:O	1:A:92:ILE:HD13	1.87	0.75
1:C:309:ILE:HD13	1:C:355:THR:HB	1.68	0.75
1:C:181:GLN:HG3	1:C:182:TYR:N	2.02	0.74
1:A:72:GLU:OE2	1:A:111:ILE:HG12	1.87	0.74
1:C:94:ARG:HD3	1:C:96:PHE:CZ	2.22	0.74
1:B:234:ASP:O	1:B:236:ILE:N	2.20	0.73
1:A:120:GLU:N	4:A:1377:HOH:O	2.22	0.73
1:D:137:PHE:HD1	1:D:138:LEU:HD12	1.54	0.73
1:A:150:LEU:HB2	1:A:308:ILE:HD13	1.70	0.73
1:B:243:THR:HG22	1:B:244:THR:N	2.04	0.73
1:B:8:LEU:O	1:B:12:LEU:HD13	1.89	0.73
1:D:106:VAL:HG22	1:D:109:ARG:NH2	2.04	0.73
1:B:199:ASP:HB2	1:B:201:PRO:HD3	1.70	0.72
1:C:184:LYS:NZ	1:C:207:LEU:HB2	2.03	0.72
1:C:204:THR:HB	1:C:213:GLN:HE22	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:178:ASP:O	1:D:181:GLN:HG2	1.88	0.72
1:B:216:ARG:HD2	1:B:231:VAL:HG12	1.70	0.72
1:C:103:ASN:HD22	1:C:104:PRO:HD2	1.55	0.72
1:B:292:GLY:HA3	3:B:381:NDP:PA	2.29	0.72
1:A:44:LYS:HE3	1:C:35:GLN:NE2	2.05	0.72
1:D:193:VAL:HG13	1:D:220:ASP:HA	1.70	0.72
1:D:270:ILE:HD13	1:D:270:ILE:N	2.01	0.71
1:B:161:ALA:HB3	1:B:323:PRO:HG3	1.72	0.70
1:A:184:LYS:HZ2	1:A:207:LEU:HD12	1.55	0.70
1:A:125:ILE:N	1:A:125:ILE:HD12	2.06	0.70
1:C:181:GLN:O	1:C:184:LYS:HG2	1.92	0.70
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.74	0.70
1:B:187:GLN:HB3	1:B:284:ILE:HG23	1.74	0.70
1:B:184:LYS:HB2	1:B:205:CYS:SG	2.32	0.70
1:B:216:ARG:NH1	1:B:231:VAL:HA	2.07	0.69
1:C:220:ASP:OD2	1:C:223:LEU:HA	1.92	0.69
1:D:218:ILE:HD11	1:D:231:VAL:HG11	1.73	0.69
1:A:49:HIS:HD2	1:A:83:CYS:SG	2.15	0.69
1:C:85:GLU:HB3	1:C:89:ASN:HD21	1.58	0.69
1:C:87:ILE:HA	1:C:92:ILE:HD12	1.74	0.69
1:D:270:ILE:CD1	1:D:270:ILE:H	1.99	0.69
1:B:301:LYS:NZ	1:B:329:GLU:HG3	2.07	0.68
1:B:234:ASP:O	1:B:236:ILE:HG12	1.92	0.68
1:B:275:VAL:O	1:B:279:LEU:HG	1.94	0.68
1:D:93:LYS:HB2	4:D:1388:HOH:O	1.93	0.68
1:C:87:ILE:HG23	1:C:92:ILE:HD12	1.74	0.68
1:B:70:THR:O	1:B:98:ALA:HB3	1.94	0.68
1:B:265:LEU:CD1	1:B:270:ILE:HG23	2.24	0.68
1:A:329:GLU:HG2	4:A:1365:HOH:O	1.93	0.68
1:A:69:VAL:HG12	1:A:71:LEU:H	1.58	0.67
1:B:261:ASN:HB3	1:B:263:PHE:HE1	1.59	0.67
1:D:22:SER:HA	1:D:285:MET:CE	2.23	0.67
1:B:14:LYS:HD2	1:B:17:GLU:OE2	1.95	0.67
1:A:318:GLY:HA3	1:B:330:GLY:CA	2.24	0.67
1:B:98:ALA:O	1:B:127:ALA:HB2	1.95	0.67
4:A:1383:HOH:O	1:B:325:LEU:HB2	1.93	0.67
1:C:21:GLU:HG3	1:C:22:SER:N	2.07	0.67
1:B:166:ASP:OD2	1:B:168:LYS:HE2	1.95	0.67
1:C:93:LYS:O	1:C:119:ILE:HG23	1.94	0.67
1:C:25:LEU:N	1:C:134:ASN:HD21	1.91	0.67
1:B:134:ASN:O	1:B:138:LEU:HD13	1.95	0.67
1:B:63:GLU:HG3	1:B:91:GLY:HA3	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:LYS:HA	4:B:1367:HOH:O	1.95	0.66
1:B:71:LEU:HD13	1:B:72:GLU:N	2.10	0.66
1:D:346:THR:HG22	1:D:347:GLN:N	2.09	0.66
1:A:334:MET:HA	1:A:337:VAL:HG12	1.77	0.66
1:B:137:PHE:CD1	1:B:138:LEU:HD12	2.31	0.66
1:B:270:ILE:HB	3:B:381:NDP:C2A	2.26	0.65
1:A:64:GLY:HA2	1:A:93:LYS:CG	2.26	0.65
1:A:190:LEU:HA	1:A:217:VAL:O	1.95	0.65
1:B:41:ALA:O	1:B:43:LEU:HD22	1.97	0.65
1:B:206:ARG:HH11	1:B:206:ARG:HB2	1.60	0.65
1:B:211:THR:O	1:B:212:LYS:HB2	1.97	0.65
1:C:180:GLN:HA	1:C:183:ARG:HD2	1.78	0.65
4:A:1374:HOH:O	1:C:35:GLN:HB3	1.97	0.65
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.78	0.65
1:A:150:LEU:HD12	1:A:308:ILE:HD11	1.79	0.65
3:B:381:NDP:H8A	3:B:381:NDP:H52A	1.79	0.65
1:D:231:VAL:HB	1:D:239:THR:HG21	1.79	0.65
1:D:190:LEU:HD13	1:D:191:VAL:N	2.12	0.64
1:D:346:THR:HG22	1:D:347:GLN:H	1.62	0.64
1:D:230:LYS:O	1:D:234:ASP:HB3	1.96	0.64
1:A:311:TYR:OH	1:A:353:LYS:HE2	1.98	0.64
1:A:125:ILE:CD1	1:A:125:ILE:H	2.04	0.64
1:A:51:GLU:O	1:A:55:ILE:HG12	1.97	0.64
1:A:25:LEU:HB2	1:A:134:ASN:OD1	1.98	0.64
1:A:251:LYS:HG3	1:A:254:ARG:HH21	1.60	0.64
1:B:308:ILE:HG22	1:B:356:ALA:O	1.97	0.64
1:C:136:LYS:HG2	1:C:147:TYR:CG	2.32	0.64
1:D:141:MET:HA	1:D:141:MET:CE	2.26	0.64
1:C:75:SER:HA	1:C:82:PRO:HB3	1.79	0.64
1:C:6:MET:HB3	1:C:126:LEU:HD12	1.80	0.64
1:C:207:LEU:H	1:C:207:LEU:CD1	2.07	0.64
1:A:207:LEU:O	1:A:208:PRO:O	2.16	0.64
1:B:221:THR:HB	3:B:381:NDP:O3X	1.98	0.64
1:B:254:ARG:HG2	1:B:258:PHE:CE1	2.33	0.63
1:B:42:HIS:HD2	1:B:49:HIS:HA	1.62	0.63
1:B:84:ALA:O	1:B:88:ILE:HG12	1.99	0.63
1:D:243:THR:HG22	1:D:244:THR:H	1.63	0.63
1:C:151:LYS:HG3	1:C:288:TYR:OH	1.99	0.63
1:C:277:LYS:HE3	1:C:281:GLU:OE2	1.99	0.63
1:C:181:GLN:HG3	1:C:182:TYR:H	1.63	0.63
1:B:292:GLY:HA3	3:B:381:NDP:O2A	1.99	0.63
1:A:270:ILE:N	1:A:270:ILE:HD12	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:235:GLN:NE2	4:C:1395:HOH:O	2.32	0.63
1:D:277:LYS:NZ	1:D:277:LYS:HB3	2.13	0.63
1:D:111:ILE:HG22	1:D:115:LYS:HE3	1.81	0.62
1:B:243:THR:HG22	1:B:244:THR:H	1.62	0.62
1:D:125:ILE:H	1:D:125:ILE:HD12	1.63	0.62
1:B:216:ARG:CZ	1:B:231:VAL:HA	2.30	0.62
1:A:255:LEU:O	1:A:260:VAL:HG13	1.98	0.62
1:C:347:GLN:HG3	1:C:351:ASP:O	2.00	0.62
1:A:184:LYS:HZ3	1:A:207:LEU:HB2	1.63	0.62
1:A:312:PHE:CE2	1:A:354:LEU:HD12	2.33	0.62
1:B:161:ALA:HB3	1:B:323:PRO:HG2	1.80	0.62
1:D:310:PHE:CE2	1:D:325:LEU:HD13	2.35	0.62
1:D:49:HIS:ND1	1:D:74:CYS:SG	2.71	0.62
1:B:308:ILE:HD11	1:B:310:PHE:CE1	2.34	0.62
1:D:134:ASN:O	1:D:138:LEU:HD13	2.00	0.62
1:B:240:TRP:CD1	1:B:261:ASN:HB2	2.34	0.62
1:B:103:ASN:HD22	1:B:104:PRO:HD2	1.64	0.62
1:D:148:VAL:H	1:D:306:GLN:HE21	1.44	0.61
1:D:146:PRO:HD3	1:D:280:ALA:HB2	1.81	0.61
1:B:308:ILE:CG2	1:B:356:ALA:HB3	2.29	0.61
1:C:77:TYR:HA	1:C:82:PRO:HG3	1.81	0.61
1:C:88:ILE:HG13	1:C:89:ASN:N	2.15	0.61
1:B:79:LYS:O	1:B:80:THR:HG23	2.00	0.61
1:B:204:THR:HB	1:B:213:GLN:HE22	1.66	0.61
1:B:243:THR:HG21	1:B:247:ALA:HB2	1.83	0.61
1:B:291:GLY:O	1:B:295:VAL:HB	2.00	0.61
1:D:148:VAL:H	1:D:306:GLN:HE22	1.46	0.61
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.83	0.61
1:C:161:ALA:HB3	1:C:323:PRO:CG	2.30	0.61
1:B:148:VAL:H	1:B:306:GLN:NE2	1.95	0.61
1:C:173:GLU:HA	1:C:176:ARG:HD3	1.83	0.61
1:B:125:ILE:HD12	1:B:125:ILE:H	1.66	0.61
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.82	0.61
1:B:218:ILE:N	1:B:218:ILE:HD12	2.16	0.60
1:A:223:LEU:HD12	1:A:247:ALA:HB1	1.82	0.60
1:B:103:ASN:HD22	1:B:104:PRO:CD	2.14	0.60
1:B:67:ILE:HG22	1:B:92:ILE:HG21	1.83	0.60
1:D:343:THR:HG21	1:D:357:LYS:HG3	1.83	0.60
1:B:193:VAL:O	1:B:197:LYS:HG2	2.02	0.60
1:D:63:GLU:HB2	4:D:1394:HOH:O	2.01	0.60
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.83	0.60
1:D:150:LEU:CD2	1:D:289:VAL:HB	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:HIS:CD2	1:A:83:CYS:SG	2.94	0.60
1:C:311:TYR:HE1	1:C:353:LYS:HD2	1.66	0.60
1:C:95:VAL:HG11	1:C:114:MET:HE3	1.84	0.59
1:B:103:ASN:ND2	1:B:105:LEU:H	2.00	0.59
1:B:254:ARG:HG3	1:B:254:ARG:HH11	1.67	0.59
1:C:5:TYR:OH	1:C:31:VAL:HG21	2.01	0.59
1:C:152:ALA:HB3	1:C:310:PHE:CE1	2.38	0.59
1:C:67:ILE:CG2	1:C:95:VAL:HG23	2.32	0.59
1:B:199:ASP:CB	1:B:201:PRO:HD3	2.33	0.59
1:C:67:ILE:HG23	1:C:95:VAL:HG23	1.85	0.59
1:C:83:CYS:O	1:C:87:ILE:HG13	2.02	0.59
1:D:37:VAL:HG11	1:D:61:HIS:HB3	1.83	0.59
1:A:19:GLN:HE22	1:C:36:ILE:CD1	2.16	0.59
1:D:193:VAL:CG1	1:D:220:ASP:HA	2.33	0.59
1:B:292:GLY:HA2	3:B:381:NDP:H51N	1.84	0.58
4:A:1383:HOH:O	1:B:325:LEU:CB	2.49	0.58
1:D:72:GLU:OE1	1:D:111:ILE:HG12	2.03	0.58
1:C:161:ALA:HB3	1:C:323:PRO:HG3	1.84	0.58
1:B:74:CYS:SG	1:B:83:CYS:N	2.67	0.58
1:D:190:LEU:HD11	1:D:219:LEU:HD22	1.85	0.58
1:D:80:THR:HB	1:D:81:PRO:HD2	1.83	0.58
1:C:125:ILE:HD13	1:C:125:ILE:N	2.17	0.58
1:C:191:VAL:HG21	1:C:195:THR:HG21	1.85	0.58
1:B:284:ILE:N	1:B:284:ILE:HD12	2.19	0.58
1:B:44:LYS:NZ	1:D:35:GLN:HE22	2.02	0.58
1:D:150:LEU:HD23	1:D:289:VAL:HB	1.84	0.58
1:C:188:SER:C	1:C:189:ILE:HD13	2.23	0.58
1:B:302:GLU:OE2	1:B:302:GLU:HA	2.03	0.58
1:C:103:ASN:HD22	1:C:104:PRO:CD	2.17	0.58
1:B:129:GLN:C	1:B:131:GLU:H	2.06	0.58
1:A:118:GLY:HA3	4:A:1403:HOH:O	2.04	0.58
1:A:83:CYS:O	1:A:87:ILE:HG12	2.04	0.57
1:B:177:GLN:O	1:B:180:GLN:HB2	2.04	0.57
1:D:269:ARG:HB2	4:D:1368:HOH:O	2.02	0.57
1:C:10:LEU:HD23	1:C:70:THR:HG21	1.87	0.57
1:B:134:ASN:HB2	1:B:138:LEU:HD13	1.86	0.57
1:B:167:SER:O	1:B:169:TRP:N	2.37	0.57
1:C:157:ASP:HA	1:D:325:LEU:CD1	2.34	0.57
1:A:19:GLN:HE22	1:C:36:ILE:HD12	1.70	0.57
1:B:176:ARG:HH11	1:B:176:ARG:HG2	1.70	0.57
1:B:200:ASN:N	1:B:201:PRO:CD	2.67	0.57
1:B:270:ILE:HB	3:B:381:NDP:H2A	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:348:ILE:N	1:B:348:ILE:HD12	2.20	0.57
1:B:204:THR:O	1:B:206:ARG:HG3	2.05	0.57
1:C:193:VAL:HG13	1:C:220:ASP:HB2	1.86	0.57
1:B:191:VAL:CG1	1:B:195:THR:HB	2.34	0.57
1:D:178:ASP:OD1	1:D:348:ILE:HG13	2.04	0.57
1:C:180:GLN:CB	1:C:207:LEU:HD11	2.35	0.56
1:A:150:LEU:HD12	1:A:308:ILE:CD1	2.35	0.56
1:B:243:THR:CG2	1:B:244:THR:N	2.67	0.56
1:D:83:CYS:O	1:D:87:ILE:HG13	2.05	0.56
1:C:207:LEU:N	1:C:207:LEU:HD12	2.13	0.56
1:A:20:THR:HB	1:A:23:ASN:HB2	1.87	0.56
1:C:25:LEU:H	1:C:134:ASN:ND2	1.96	0.56
1:D:334:MET:O	1:D:337:VAL:HG12	2.05	0.56
1:B:243:THR:CG2	1:B:244:THR:H	2.18	0.56
1:A:290:GLU:O	1:A:296:HIS:CE1	2.58	0.56
1:C:205:CYS:SG	1:C:210:VAL:HG11	2.46	0.56
1:B:31:VAL:O	1:B:65:ALA:HB1	2.06	0.56
1:D:101:ASP:OD1	1:D:102:PRO:HD2	2.06	0.56
1:B:125:ILE:HD12	1:B:125:ILE:N	2.21	0.56
1:B:234:ASP:C	1:B:234:ASP:OD2	2.44	0.56
1:C:55:ILE:HD11	1:C:92:ILE:HD11	1.87	0.55
1:C:28:ALA:HB3	1:C:50:ALA:O	2.05	0.55
1:A:66:ASP:OD2	1:A:94:ARG:HB2	2.06	0.55
1:C:94:ARG:HD3	1:C:96:PHE:HE2	1.64	0.55
1:C:131:GLU:OE1	1:C:142:ARG:NH2	2.32	0.55
1:D:17:GLU:HA	1:D:25:LEU:HD21	1.88	0.55
1:B:258:PHE:HD1	1:B:258:PHE:N	2.05	0.55
1:B:176:ARG:HG2	1:B:176:ARG:NH1	2.21	0.55
1:C:166:ASP:OD1	1:C:168:LYS:HG3	2.07	0.55
1:B:103:ASN:HD21	1:B:105:LEU:HD13	1.70	0.55
1:C:148:VAL:HB	1:C:305:PHE:HA	1.89	0.55
1:B:240:TRP:CH2	1:B:284:ILE:HD11	2.42	0.55
1:B:308:ILE:HG21	1:B:356:ALA:HB3	1.87	0.55
1:D:296:HIS:O	1:D:300:VAL:HG23	2.05	0.55
1:C:265:LEU:HD11	1:C:275:VAL:HG22	1.89	0.55
1:D:23:ASN:HD22	1:D:23:ASN:N	2.03	0.55
1:C:120:GLU:HB3	4:C:1383:HOH:O	2.07	0.55
1:C:190:LEU:HD21	1:C:219:LEU:HD21	1.88	0.55
1:C:111:ILE:HG23	1:C:121:VAL:HG11	1.89	0.55
1:B:301:LYS:HZ3	1:B:329:GLU:CG	2.18	0.54
1:C:221:THR:HG22	1:C:222:VAL:HG13	1.88	0.54
1:B:233:CYS:O	1:B:235:GLN:N	2.39	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:324:SER:HB3	4:C:1387:HOH:O	2.07	0.54
1:B:151:LYS:HD3	1:B:151:LYS:C	2.28	0.54
1:A:222:VAL:HG22	1:A:222:VAL:O	2.06	0.54
1:D:320:THR:HG22	1:D:321:HIS:H	1.72	0.54
1:A:1:MET:N	4:A:1368:HOH:O	2.40	0.54
1:D:243:THR:HG21	1:D:247:ALA:HB2	1.88	0.54
1:B:278:ILE:O	1:B:281:GLU:HB2	2.07	0.54
1:C:93:LYS:HB3	1:C:93:LYS:HZ2	1.72	0.54
1:B:293:SER:OG	1:B:327:SER:HB2	2.08	0.54
1:C:10:LEU:HD23	1:C:70:THR:CG2	2.38	0.54
1:B:200:ASN:OD1	1:B:229:ALA:HA	2.07	0.54
1:D:161:ALA:HB3	1:D:323:PRO:HG3	1.89	0.54
1:A:105:LEU:HG	1:A:105:LEU:O	2.07	0.54
1:C:211:THR:O	1:C:212:LYS:HB2	2.07	0.54
1:B:17:GLU:HA	1:B:25:LEU:HD21	1.89	0.53
1:B:258:PHE:N	1:B:258:PHE:CD1	2.76	0.53
1:D:111:ILE:O	1:D:115:LYS:HG3	2.07	0.53
1:A:344:ASP:HB3	1:A:355:THR:CG2	2.39	0.53
1:B:35:GLN:OE1	1:D:19:GLN:HB2	2.09	0.53
1:A:137:PHE:HD1	1:A:138:LEU:HD12	1.73	0.53
1:C:93:LYS:HB3	1:C:93:LYS:NZ	2.23	0.53
1:A:1:MET:HA	1:A:1:MET:CE	2.38	0.53
1:C:103:ASN:HD21	1:C:105:LEU:HD21	1.74	0.53
1:A:190:LEU:HD23	1:A:191:VAL:N	2.23	0.53
1:A:9:ALA:O	1:A:27:GLY:HA3	2.08	0.53
1:B:25:LEU:H	1:B:134:ASN:ND2	2.04	0.53
1:A:32:LYS:HE3	1:A:63:GLU:O	2.09	0.53
1:D:202:SER:O	1:D:204:THR:HG23	2.07	0.53
1:C:223:LEU:HD12	1:C:251:LYS:CD	2.37	0.53
1:B:137:PHE:HD1	1:B:138:LEU:CD1	2.21	0.53
1:C:235:GLN:HA	1:C:235:GLN:OE1	2.08	0.53
1:C:125:ILE:HD13	1:C:125:ILE:H	1.73	0.53
1:C:312:PHE:CE2	1:C:354:LEU:HD12	2.42	0.53
1:D:19:GLN:O	1:D:20:THR:HG23	2.09	0.53
1:A:207:LEU:HB3	1:A:208:PRO:HD2	1.90	0.53
1:C:168:LYS:HE3	1:C:169:TRP:CZ3	2.44	0.53
1:A:184:LYS:HB2	1:A:184:LYS:NZ	2.23	0.52
1:C:157:ASP:HA	1:D:325:LEU:HD12	1.91	0.52
1:C:9:ALA:HB2	1:C:29:VAL:HG12	1.90	0.52
1:D:232:ILE:HD12	1:D:255:LEU:HD22	1.92	0.52
1:A:26:VAL:O	1:A:41:ALA:HA	2.09	0.52
1:C:153:ALA:HB1	1:C:171:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:LYS:HZ3	1:A:207:LEU:HD12	1.71	0.52
1:B:206:ARG:CB	1:B:206:ARG:HH11	2.21	0.52
1:B:254:ARG:CG	1:B:254:ARG:HH11	2.21	0.52
1:B:251:LYS:HA	1:B:254:ARG:NH2	2.24	0.52
1:D:337:VAL:HG13	1:D:337:VAL:O	2.08	0.52
1:D:101:ASP:OD2	1:D:106:VAL:HB	2.09	0.52
1:D:218:ILE:CD1	1:D:231:VAL:HG21	2.39	0.52
1:D:191:VAL:HG13	1:D:195:THR:HB	1.90	0.52
1:C:37:VAL:O	1:C:37:VAL:HG22	2.10	0.52
1:C:87:ILE:CG2	1:C:92:ILE:HD12	2.39	0.52
1:B:20:THR:HB	1:B:23:ASN:HB2	1.90	0.52
1:D:291:GLY:O	1:D:295:VAL:HB	2.09	0.52
1:C:87:ILE:HG23	1:C:92:ILE:CD1	2.38	0.52
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.89	0.52
1:A:35:GLN:OE1	1:C:44:LYS:HE3	2.10	0.52
1:D:265:LEU:N	1:D:265:LEU:HD12	2.25	0.52
1:A:277:LYS:HB3	1:A:277:LYS:NZ	2.24	0.52
1:D:19:GLN:HE21	1:D:44:LYS:HD2	1.75	0.52
1:D:216:ARG:O	1:D:239:THR:HA	2.09	0.52
1:A:190:LEU:HG	1:A:217:VAL:HG12	1.92	0.52
1:A:193:VAL:HG13	1:A:220:ASP:HB2	1.90	0.52
1:B:99:MET:HE2	1:B:100:ARG:O	2.09	0.52
1:A:251:LYS:HG3	1:A:254:ARG:NH2	2.25	0.52
1:B:217:VAL:C	1:B:218:ILE:HD12	2.30	0.52
1:B:55:ILE:HD11	1:B:92:ILE:HD11	1.92	0.52
1:A:325:LEU:HD12	1:B:157:ASP:HA	1.91	0.52
1:B:308:ILE:HD11	1:B:310:PHE:CZ	2.45	0.52
1:C:12:LEU:HD21	1:C:39:MET:HB3	1.91	0.52
1:A:16:GLY:O	1:A:19:GLN:HB2	2.09	0.52
1:C:136:LYS:HG2	1:C:147:TYR:CD2	2.45	0.52
1:C:169:TRP:O	1:C:315:LYS:HE3	2.10	0.51
1:C:160:ILE:HG12	1:C:323:PRO:O	2.09	0.51
1:B:335:LYS:C	1:B:335:LYS:HD2	2.30	0.51
1:D:177:GLN:HG3	4:D:1365:HOH:O	2.10	0.51
1:A:344:ASP:HB3	1:A:355:THR:HG23	1.92	0.51
1:D:271:GLN:HG2	1:D:273:PRO:HD2	1.91	0.51
1:C:234:ASP:O	1:C:235:GLN:C	2.48	0.51
1:B:7:LYS:HA	1:B:10:LEU:HD12	1.91	0.51
1:C:90:SER:OG	1:C:92:ILE:HG13	2.09	0.51
1:C:187:GLN:HE22	1:C:285:MET:HG3	1.74	0.51
1:D:177:GLN:O	1:D:180:GLN:HB2	2.11	0.51
1:A:146:PRO:HA	1:A:285:MET:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:164:THR:O	1:B:164:THR:HG22	2.11	0.51
1:D:48:ALA:HB3	1:D:53:HIS:CE1	2.45	0.51
1:B:102:PRO:HG2	1:B:137:PHE:HE1	1.76	0.51
1:C:8:LEU:HD22	1:C:12:LEU:HD13	1.92	0.51
1:B:28:ALA:HA	1:B:68:TYR:O	2.11	0.51
1:D:222:VAL:O	1:D:222:VAL:HG22	2.10	0.51
1:A:109:ARG:HG3	4:A:1391:HOH:O	2.09	0.51
1:C:36:ILE:CD1	1:C:36:ILE:H	2.15	0.51
1:B:184:LYS:NZ	1:B:210:VAL:HA	2.26	0.51
1:D:9:ALA:HB2	1:D:29:VAL:HG12	1.93	0.50
1:B:169:TRP:HA	1:B:169:TRP:HE3	1.76	0.50
1:A:334:MET:CE	1:B:170:ILE:HA	2.41	0.50
1:D:190:LEU:HD21	1:D:219:LEU:HD13	1.94	0.50
1:D:146:PRO:HG3	1:D:284:ILE:O	2.10	0.50
1:D:128:ASP:O	1:D:132:ARG:HG3	2.11	0.50
1:A:20:THR:O	1:A:21:GLU:HB2	2.10	0.50
1:A:57:MET:HG3	1:C:53:HIS:CE1	2.47	0.50
1:B:1:MET:N	4:B:1384:HOH:O	2.43	0.50
1:C:25:LEU:HD23	1:C:133:LEU:HD11	1.93	0.50
1:D:148:VAL:HG23	1:D:306:GLN:HE22	1.76	0.50
1:B:131:GLU:OE2	1:B:138:LEU:HD23	2.11	0.50
1:A:112:SER:O	1:A:116:GLU:HB2	2.11	0.50
1:A:74:CYS:O	1:A:82:PRO:HB2	2.11	0.50
1:A:175:ALA:O	1:A:178:ASP:N	2.44	0.50
1:C:72:GLU:CD	1:C:111:ILE:HG12	2.32	0.50
1:C:37:VAL:HG22	1:C:58:ALA:HA	1.94	0.50
1:A:325:LEU:CD1	1:B:157:ASP:HA	2.42	0.50
1:B:335:LYS:HD2	1:B:336:ASP:N	2.26	0.50
1:B:169:TRP:HA	1:B:169:TRP:CE3	2.46	0.49
1:D:72:GLU:CD	1:D:111:ILE:HG12	2.33	0.49
1:A:318:GLY:CA	1:B:330:GLY:HA2	2.35	0.49
1:C:49:HIS:ND1	1:C:83:CYS:SG	2.77	0.49
1:D:220:ASP:CG	1:D:223:LEU:HA	2.31	0.49
1:D:63:GLU:HA	1:D:91:GLY:HA3	1.93	0.49
1:B:308:ILE:HG23	1:B:308:ILE:O	2.12	0.49
1:A:150:LEU:HB2	1:A:308:ILE:CD1	2.40	0.49
1:D:188:SER:OG	1:D:287:VAL:HG22	2.11	0.49
1:C:68:TYR:N	1:C:68:TYR:CD2	2.79	0.49
1:A:320:THR:HG23	1:A:321:HIS:CD2	2.47	0.49
1:A:136:LYS:HE3	1:A:185:THR:O	2.13	0.49
1:B:55:ILE:HG13	1:B:86:LEU:CD1	2.43	0.49
1:B:193:VAL:HG11	1:B:220:ASP:CG	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:160:ILE:HG22	1:D:160:ILE:O	2.12	0.49
1:A:157:ASP:OD2	1:A:159:LYS:HD3	2.13	0.49
1:D:289:VAL:HG21	1:D:299:PHE:CZ	2.47	0.49
1:A:44:LYS:HE3	1:C:35:GLN:HE21	1.74	0.49
1:C:14:LYS:HE3	1:C:17:GLU:OE2	2.13	0.49
1:A:334:MET:HE2	1:B:170:ILE:HA	1.93	0.49
1:B:312:PHE:CE2	1:B:354:LEU:HD12	2.48	0.49
1:C:208:PRO:O	1:C:209:ASN:HB2	2.12	0.49
1:C:180:GLN:O	1:C:183:ARG:HB2	2.11	0.49
1:B:25:LEU:N	1:B:134:ASN:HD21	2.06	0.49
1:D:200:ASN:O	1:D:230:LYS:HG3	2.13	0.49
1:B:66:ASP:HA	1:B:94:ARG:O	2.13	0.49
1:A:29:VAL:O	1:A:67:ILE:HA	2.13	0.49
1:D:272:ILE:CG1	1:D:298:SER:HB3	2.43	0.49
1:A:170:ILE:HG12	1:B:334:MET:HE1	1.95	0.49
1:C:267:THR:HG22	1:C:268:GLU:H	1.78	0.49
1:B:3:GLU:CB	1:B:126:LEU:HD11	2.37	0.49
1:C:67:ILE:O	1:C:67:ILE:HG23	2.13	0.49
1:B:14:LYS:HE3	4:B:1374:HOH:O	2.11	0.49
1:A:312:PHE:HE2	1:A:354:LEU:HD12	1.75	0.49
1:B:255:LEU:O	1:B:260:VAL:HB	2.13	0.49
1:A:184:LYS:HB2	1:A:184:LYS:HZ2	1.78	0.48
1:B:65:ALA:O	1:B:92:ILE:HG23	2.13	0.48
1:C:95:VAL:HG12	1:C:121:VAL:HG22	1.95	0.48
1:D:223:LEU:HD23	1:D:225:ILE:HG22	1.95	0.48
1:C:87:ILE:CA	1:C:92:ILE:HD12	2.42	0.48
1:D:75:SER:HB2	1:D:109:ARG:HD2	1.95	0.48
1:A:74:CYS:SG	1:A:83:CYS:N	2.76	0.48
1:A:272:ILE:N	1:A:273:PRO:CD	2.76	0.48
1:C:333:SER:HB3	1:C:336:ASP:OD2	2.14	0.48
1:D:156:LEU:HB3	1:D:316:LEU:HD23	1.95	0.48
1:A:67:ILE:CG2	1:A:95:VAL:HG22	2.44	0.48
1:D:19:GLN:CG	1:D:44:LYS:HD2	2.37	0.48
1:A:180:GLN:HB3	1:A:207:LEU:HD21	1.95	0.48
1:B:254:ARG:HG2	1:B:258:PHE:CZ	2.49	0.48
1:D:14:LYS:O	1:D:17:GLU:HB2	2.13	0.48
1:C:68:TYR:N	1:C:68:TYR:HD2	2.12	0.48
1:C:6:MET:HE1	1:C:69:VAL:O	2.14	0.48
1:D:200:ASN:N	1:D:201:PRO:CD	2.76	0.48
1:D:343:THR:HG21	1:D:357:LYS:HE2	1.95	0.48
1:A:20:THR:O	1:A:45:TYR:HD1	1.97	0.48
1:D:339:LEU:O	1:D:359:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:287:VAL:HG12	1:D:289:VAL:HG23	1.96	0.47
1:A:184:LYS:HZ3	1:A:207:LEU:CB	2.27	0.47
1:B:272:ILE:HB	1:B:273:PRO:HD3	1.96	0.47
1:B:202:SER:CB	1:B:230:LYS:HD2	2.44	0.47
1:A:90:SER:OG	1:A:92:ILE:HG12	2.14	0.47
1:B:191:VAL:HG13	1:B:291:GLY:HA3	1.97	0.47
1:B:345:ILE:HG23	1:B:354:LEU:HD23	1.97	0.47
1:B:234:ASP:O	1:B:235:GLN:C	2.52	0.47
1:B:210:VAL:O	1:B:212:LYS:N	2.47	0.47
1:A:202:SER:O	1:A:216:ARG:HD2	2.14	0.47
1:C:84:ALA:O	1:C:88:ILE:HG23	2.14	0.47
1:D:140:PHE:CG	1:D:285:MET:HG2	2.49	0.47
1:C:112:SER:O	1:C:115:LYS:N	2.47	0.47
1:B:102:PRO:HG2	1:B:137:PHE:CE1	2.49	0.47
1:D:263:PHE:CD2	1:D:278:ILE:HG21	2.48	0.47
1:A:42:HIS:HE1	1:A:47:GLU:O	1.97	0.47
1:D:19:GLN:CG	1:D:44:LYS:HA	2.45	0.47
1:C:103:ASN:HD21	1:C:105:LEU:CD2	2.27	0.47
1:B:12:LEU:CD2	1:B:39:MET:HB3	2.44	0.47
1:B:67:ILE:HG23	1:B:67:ILE:O	2.15	0.47
1:C:314:PRO:HG3	1:D:342:PHE:CE2	2.49	0.47
1:C:33:ASP:OD2	1:C:33:ASP:N	2.48	0.47
1:D:140:PHE:CD2	1:D:285:MET:HG2	2.49	0.47
1:C:95:VAL:HG11	1:C:114:MET:CE	2.44	0.47
1:C:240:TRP:CD1	1:C:261:ASN:HB2	2.50	0.47
1:A:123:GLU:O	1:A:125:ILE:HD12	2.14	0.47
1:D:64:GLY:HA2	1:D:93:LYS:HG2	1.96	0.47
1:D:311:TYR:CE1	1:D:353:LYS:HD2	2.50	0.47
1:D:1:MET:HG3	1:D:5:TYR:CE2	2.50	0.47
1:C:103:ASN:HB3	1:C:106:VAL:HG22	1.97	0.46
1:C:9:ALA:HB2	1:C:29:VAL:CG1	2.45	0.46
1:B:301:LYS:CE	1:B:329:GLU:HB2	2.45	0.46
1:B:301:LYS:HD3	1:B:329:GLU:HB2	1.96	0.46
1:A:222:VAL:HG12	4:A:1395:HOH:O	2.15	0.46
1:B:35:GLN:CD	1:D:19:GLN:HB2	2.36	0.46
1:C:85:GLU:O	1:C:88:ILE:N	2.47	0.46
1:A:207:LEU:HB3	1:A:208:PRO:CD	2.46	0.46
1:B:254:ARG:HB2	1:B:254:ARG:NH1	2.31	0.46
1:B:168:LYS:O	1:B:169:TRP:HB2	2.16	0.46
1:C:7:LYS:O	1:C:10:LEU:HB2	2.15	0.46
1:C:100:ARG:HH21	1:C:108:GLY:HA2	1.79	0.46
1:B:202:SER:HB2	1:B:230:LYS:HD2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:56:HIS:NE2	1:C:56:HIS:NE2	2.64	0.46
1:C:129:GLN:CD	1:C:129:GLN:H	2.18	0.46
1:B:213:GLN:HB3	1:B:237:ALA:HB2	1.98	0.46
1:B:301:LYS:NZ	1:B:329:GLU:CB	2.79	0.46
1:B:301:LYS:NZ	1:B:329:GLU:CG	2.77	0.46
1:B:193:VAL:HG13	1:B:219:LEU:O	2.16	0.46
1:B:85:GLU:HG2	1:B:89:ASN:HD21	1.80	0.46
1:B:198:ALA:O	1:B:199:ASP:OD1	2.33	0.46
1:D:88:ILE:HA	1:D:119:ILE:HD11	1.97	0.46
1:C:85:GLU:HB3	1:C:89:ASN:ND2	2.27	0.46
1:D:226:PRO:C	1:D:228:ASP:N	2.68	0.46
1:B:53:HIS:HB3	1:D:57:MET:HE3	1.98	0.46
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.45	0.45
1:A:134:ASN:HB2	1:A:138:LEU:CD1	2.46	0.45
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.15	0.45
1:B:95:VAL:HG23	1:B:119:ILE:HG21	1.98	0.45
1:C:23:ASN:N	1:C:23:ASN:HD22	2.14	0.45
1:C:66:ASP:CG	1:C:94:ARG:HD2	2.37	0.45
1:A:30:VAL:HG12	1:A:37:VAL:CG2	2.47	0.45
1:D:180:GLN:HB3	1:D:180:GLN:HE21	1.53	0.45
1:C:85:GLU:O	1:C:88:ILE:HG12	2.17	0.45
1:C:37:VAL:HG21	1:C:61:HIS:CD2	2.52	0.45
1:A:64:GLY:CA	1:A:93:LYS:HG2	2.40	0.45
1:A:71:LEU:O	1:A:72:GLU:C	2.55	0.45
1:C:315:LYS:HE2	1:D:339:LEU:HD13	1.98	0.45
1:C:151:LYS:HD2	1:C:151:LYS:C	2.37	0.45
1:D:277:LYS:HB3	1:D:277:LYS:HZ3	1.82	0.45
1:A:170:ILE:HG12	1:B:334:MET:CE	2.46	0.45
1:B:263:PHE:CD2	1:B:278:ILE:HG21	2.52	0.45
1:C:153:ALA:HB1	1:C:171:THR:HG23	1.97	0.45
1:C:331:PHE:CE1	1:C:338:PRO:HD2	2.51	0.45
1:D:155:SER:N	1:D:170:ILE:HD11	2.32	0.45
1:B:134:ASN:HB3	1:B:137:PHE:HB3	1.99	0.45
1:B:277:LYS:O	1:B:281:GLU:HG3	2.17	0.45
1:C:216:ARG:HD2	1:C:237:ALA:HB3	1.98	0.45
1:B:310:PHE:CE1	1:B:325:LEU:HD22	2.51	0.45
1:C:82:PRO:O	1:C:85:GLU:N	2.47	0.45
1:C:157:ASP:HA	1:D:325:LEU:HD13	1.99	0.45
1:B:92:ILE:O	1:B:119:ILE:HD12	2.17	0.45
1:C:167:SER:HA	1:D:334:MET:HE2	1.97	0.45
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.46	0.45
1:C:311:TYR:CE1	1:C:353:LYS:HD2	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:237:ALA:HB1	1:C:238:PRO:CD	2.47	0.45
1:C:85:GLU:HA	1:C:88:ILE:HG12	1.99	0.45
1:C:55:ILE:O	1:C:58:ALA:N	2.36	0.45
1:D:346:THR:CG2	1:D:347:GLN:N	2.78	0.45
1:D:252:LYS:HE3	1:D:264:THR:HG21	1.98	0.45
1:C:55:ILE:CD1	1:C:92:ILE:HD11	2.46	0.45
1:D:181:GLN:O	1:D:184:LYS:HB3	2.16	0.45
1:A:348:ILE:HD11	1:A:353:LYS:HE3	1.99	0.45
1:A:32:LYS:HB2	1:A:37:VAL:HG11	1.99	0.45
1:C:346:THR:O	1:C:353:LYS:HB3	2.17	0.44
1:C:116:GLU:C	1:C:118:GLY:H	2.19	0.44
1:A:334:MET:HA	1:A:337:VAL:CG1	2.47	0.44
1:D:72:GLU:HG3	1:D:111:ILE:CD1	2.47	0.44
1:D:19:GLN:HG2	1:D:44:LYS:CD	2.37	0.44
1:C:88:ILE:CG1	1:C:89:ASN:N	2.79	0.44
1:B:204:THR:HB	1:B:213:GLN:NE2	2.32	0.44
1:A:193:VAL:HG11	1:A:220:ASP:CG	2.38	0.44
1:C:189:ILE:N	1:C:189:ILE:HD13	2.32	0.44
1:C:285:MET:HE3	1:C:285:MET:HB2	1.77	0.44
1:C:56:HIS:C	1:C:56:HIS:ND1	2.71	0.44
1:B:293:SER:H	3:B:381:NDP:H52N	1.82	0.44
1:D:326:ILE:O	1:D:326:ILE:HG22	2.17	0.44
1:A:85:GLU:HB2	1:A:113:MET:HE3	1.99	0.44
1:D:190:LEU:HD21	1:D:219:LEU:CD1	2.47	0.44
1:C:32:LYS:HG2	1:C:33:ASP:OD2	2.17	0.44
1:C:6:MET:O	1:C:10:LEU:HG	2.18	0.44
1:B:223:LEU:HB2	1:B:243:THR:HG21	1.99	0.44
1:C:5:TYR:CZ	1:C:31:VAL:HG21	2.52	0.44
1:D:23:ASN:ND2	1:D:23:ASN:N	2.66	0.44
1:A:49:HIS:HD2	1:A:74:CYS:SG	2.40	0.44
1:D:230:LYS:O	1:D:232:ILE:N	2.50	0.44
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.83	0.44
1:A:148:VAL:HB	1:A:305:PHE:HA	2.00	0.44
1:B:261:ASN:HB3	1:B:263:PHE:CE1	2.45	0.44
1:B:195:THR:O	1:B:196:VAL:C	2.56	0.44
1:C:129:GLN:CD	1:C:129:GLN:N	2.71	0.44
1:D:300:VAL:HG21	1:D:326:ILE:CD1	2.45	0.44
1:A:311:TYR:CZ	1:A:353:LYS:HE2	2.52	0.44
1:D:204:THR:HB	1:D:213:GLN:NE2	2.33	0.44
1:A:199:ASP:O	1:A:200:ASN:C	2.56	0.44
1:C:174:ALA:HB1	1:C:348:ILE:HG22	2.00	0.44
1:A:308:ILE:O	1:A:355:THR:HA	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:272:ILE:HB	1:D:273:PRO:CD	2.39	0.44
1:D:134:ASN:HB3	1:D:137:PHE:HB3	2.00	0.44
1:C:28:ALA:H	1:C:50:ALA:HB1	1.82	0.44
1:D:160:ILE:CG2	1:D:160:ILE:O	2.66	0.44
1:C:337:VAL:HG23	1:C:337:VAL:O	2.16	0.44
1:D:76:HIS:O	1:D:82:PRO:HB3	2.18	0.44
1:A:342:PHE:HA	1:A:356:ALA:HB2	2.00	0.44
1:D:151:LYS:HE2	1:D:179:ALA:HB1	2.00	0.44
1:A:12:LEU:CD1	1:A:39:MET:HB3	2.48	0.44
1:A:159:LYS:NZ	4:A:1383:HOH:O	2.35	0.44
1:D:137:PHE:CD1	1:D:138:LEU:HD12	2.43	0.44
1:C:6:MET:CB	1:C:126:LEU:HD12	2.45	0.44
1:A:329:GLU:O	1:B:319:GLY:HA2	2.17	0.44
1:B:80:THR:HB	1:B:81:PRO:HD2	2.00	0.44
1:B:348:ILE:HD13	1:B:353:LYS:HB2	2.00	0.44
1:D:274:ASP:O	1:D:278:ILE:HG12	2.18	0.44
1:A:157:ASP:HB2	4:A:1383:HOH:O	2.18	0.43
1:D:272:ILE:CB	1:D:273:PRO:HD3	2.35	0.43
1:B:61:HIS:NE2	1:D:44:LYS:HE2	2.33	0.43
1:C:344:ASP:HB3	1:C:355:THR:HG23	2.00	0.43
1:C:96:PHE:N	1:C:96:PHE:CD2	2.86	0.43
1:A:134:ASN:HB2	1:A:138:LEU:HD11	1.99	0.43
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.39	0.43
1:B:311:TYR:OH	1:B:353:LYS:HE3	2.17	0.43
1:A:175:ALA:O	1:A:176:ARG:C	2.56	0.43
1:C:184:LYS:HB3	1:C:184:LYS:HE2	1.82	0.43
1:A:181:GLN:HA	1:A:207:LEU:HD11	1.99	0.43
1:A:17:GLU:HA	1:A:25:LEU:HD11	1.99	0.43
1:C:167:SER:HA	1:D:334:MET:CE	2.48	0.43
1:A:114:MET:O	1:A:115:LYS:C	2.57	0.43
1:A:32:LYS:HB2	1:A:37:VAL:CG1	2.47	0.43
1:C:312:PHE:HE2	1:C:354:LEU:HD12	1.82	0.43
1:C:331:PHE:CD1	1:C:337:VAL:HG12	2.54	0.43
1:C:63:GLU:HA	1:C:91:GLY:O	2.19	0.43
1:B:221:THR:O	1:B:243:THR:HG23	2.18	0.43
1:B:42:HIS:CD2	1:B:49:HIS:HD2	2.37	0.43
1:B:82:PRO:O	1:B:85:GLU:N	2.52	0.43
1:A:359:THR:HG22	4:A:1416:HOH:O	2.19	0.43
1:D:124:GLY:O	1:D:125:ILE:C	2.55	0.43
1:C:29:VAL:HG13	1:C:68:TYR:HB2	1.99	0.43
1:C:328:GLY:O	1:D:319:GLY:HA2	2.18	0.43
1:A:319:GLY:HA3	1:A:322:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:ALA:O	1:A:323:PRO:HD2	2.18	0.43
1:A:55:ILE:HD11	1:A:67:ILE:HD12	2.00	0.43
1:D:190:LEU:HD13	1:D:191:VAL:H	1.82	0.43
1:C:95:VAL:CG1	1:C:121:VAL:HG22	2.48	0.43
1:B:254:ARG:NH1	1:B:254:ARG:CG	2.81	0.43
1:D:277:LYS:O	1:D:281:GLU:HG3	2.18	0.43
1:A:19:GLN:CD	1:C:35:GLN:HB2	2.39	0.43
1:C:12:LEU:CD2	1:C:39:MET:HB3	2.49	0.43
1:B:252:LYS:O	1:B:256:SER:HB3	2.19	0.43
1:B:138:LEU:O	1:B:142:ARG:HG3	2.19	0.43
1:D:337:VAL:CG1	1:D:337:VAL:O	2.67	0.43
1:A:290:GLU:O	1:A:296:HIS:NE2	2.51	0.43
1:C:28:ALA:HA	1:C:68:TYR:O	2.19	0.43
1:A:32:LYS:HD3	1:A:32:LYS:C	2.39	0.42
1:D:208:PRO:O	1:D:209:ASN:HB2	2.19	0.42
1:C:181:GLN:NE2	1:C:182:TYR:CE2	2.88	0.42
1:C:152:ALA:HB3	1:C:310:PHE:CD1	2.54	0.42
1:D:272:ILE:HG12	1:D:298:SER:HB3	2.00	0.42
1:B:103:ASN:HD22	1:B:103:ASN:C	2.21	0.42
1:C:146:PRO:HA	1:C:285:MET:O	2.19	0.42
1:D:131:GLU:OE1	1:D:142:ARG:NH2	2.45	0.42
1:D:139:HIS:O	1:D:143:THR:HG23	2.19	0.42
1:B:198:ALA:C	1:B:199:ASP:OD1	2.57	0.42
1:B:83:CYS:O	1:B:87:ILE:HG13	2.19	0.42
1:D:150:LEU:HB2	1:D:308:ILE:HD13	2.02	0.42
1:D:184:LYS:HD2	1:D:207:LEU:HD23	2.01	0.42
1:B:202:SER:O	1:B:203:LEU:HB2	2.18	0.42
1:C:140:PHE:HE1	1:C:280:ALA:HB1	1.85	0.42
1:A:36:ILE:O	1:C:43:LEU:HD13	2.18	0.42
1:A:14:LYS:O	1:A:14:LYS:HG3	2.19	0.42
1:A:248:ASP:O	1:A:252:LYS:HG3	2.19	0.42
1:B:258:PHE:HD1	1:B:258:PHE:H	1.66	0.42
1:C:173:GLU:O	1:C:177:GLN:HB2	2.20	0.42
1:B:51:GLU:OE1	1:B:83:CYS:CB	2.67	0.42
1:C:28:ALA:CB	1:C:51:GLU:HA	2.49	0.42
1:C:8:LEU:HD22	1:C:12:LEU:CD1	2.49	0.42
1:D:227:GLU:OE2	1:D:254:ARG:HD2	2.20	0.42
1:C:239:THR:O	1:C:260:VAL:HG13	2.19	0.42
1:A:13:ALA:HB2	1:A:27:GLY:N	2.34	0.42
1:B:9:ALA:O	1:B:27:GLY:HA3	2.20	0.42
1:B:176:ARG:N	1:B:176:ARG:HD3	2.35	0.42
1:C:100:ARG:NH1	1:C:123:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:345:ILE:N	1:A:345:ILE:HD12	2.34	0.42
1:B:284:ILE:N	1:B:284:ILE:CD1	2.83	0.42
1:C:9:ALA:HB1	1:C:27:GLY:O	2.20	0.42
1:B:296:HIS:HB3	1:B:326:ILE:HD12	2.02	0.42
1:D:67:ILE:HG22	1:D:95:VAL:HG22	2.01	0.42
1:A:157:ASP:HB3	1:A:316:LEU:HD22	2.02	0.42
1:B:210:VAL:HG23	1:B:211:THR:N	2.35	0.42
1:C:234:ASP:O	1:C:236:ILE:HG13	2.19	0.42
1:C:234:ASP:O	1:C:236:ILE:N	2.52	0.42
1:C:191:VAL:O	1:C:218:ILE:HA	2.20	0.42
1:A:84:ALA:HB3	1:A:113:MET:CE	2.50	0.42
1:B:126:LEU:C	1:B:128:ASP:N	2.74	0.41
1:B:213:GLN:HB3	1:B:237:ALA:CB	2.49	0.41
1:C:6:MET:CE	1:C:98:ALA:HB2	2.50	0.41
1:D:216:ARG:CZ	1:D:231:VAL:HA	2.49	0.41
1:B:227:GLU:CD	1:B:227:GLU:H	2.23	0.41
1:A:15:GLN:O	1:C:36:ILE:HD13	2.20	0.41
1:B:206:ARG:CB	1:B:206:ARG:NH1	2.76	0.41
1:D:230:LYS:HB2	4:D:1404:HOH:O	2.19	0.41
1:B:218:ILE:CD1	1:B:218:ILE:N	2.82	0.41
1:C:272:ILE:HB	1:C:273:PRO:HD3	2.02	0.41
1:C:290:GLU:O	1:C:296:HIS:NE2	2.54	0.41
1:D:72:GLU:HB2	1:D:100:ARG:HA	2.02	0.41
1:C:72:GLU:HA	1:C:73:PRO:HD3	1.92	0.41
1:B:102:PRO:HB2	1:B:141:MET:CB	2.49	0.41
1:D:218:ILE:HD11	1:D:231:VAL:HG21	2.01	0.41
1:B:115:LYS:HB2	1:B:115:LYS:HE3	1.85	0.41
1:B:308:ILE:O	1:B:355:THR:HA	2.20	0.41
1:B:102:PRO:HB2	1:B:141:MET:HB2	2.02	0.41
1:C:28:ALA:O	1:C:54:ALA:HB2	2.21	0.41
1:A:115:LYS:HE2	1:A:121:VAL:HB	2.02	0.41
1:B:129:GLN:C	1:B:131:GLU:N	2.72	0.41
1:D:125:ILE:HG22	1:D:126:LEU:HG	2.02	0.41
1:B:103:ASN:HD22	1:B:104:PRO:N	2.18	0.41
1:B:125:ILE:H	1:B:125:ILE:CD1	2.32	0.41
1:D:343:THR:CG2	1:D:357:LYS:HG3	2.50	0.41
1:A:1:MET:HA	1:A:1:MET:HE2	2.01	0.41
1:D:161:ALA:HB3	1:D:323:PRO:CG	2.50	0.41
1:A:147:TYR:N	1:A:285:MET:O	2.44	0.41
1:C:272:ILE:N	1:C:273:PRO:CD	2.83	0.41
1:A:132:ARG:O	1:A:135:GLU:HB2	2.20	0.41
1:C:69:VAL:HG21	1:C:73:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:29:VAL:HG13	1:D:68:TYR:HB2	2.02	0.41
1:D:289:VAL:HG21	1:D:299:PHE:CE2	2.56	0.41
1:A:24:PRO:HD3	1:A:137:PHE:CE2	2.56	0.41
1:B:292:GLY:HA2	3:B:381:NDP:C5D	2.51	0.41
1:A:191:VAL:O	1:A:218:ILE:HA	2.20	0.41
1:B:103:ASN:ND2	1:B:103:ASN:C	2.74	0.41
1:C:30:VAL:HB	1:C:38:GLY:HA3	2.01	0.41
1:D:136:LYS:HE3	1:D:185:THR:O	2.19	0.41
1:B:12:LEU:N	1:B:12:LEU:HD12	2.36	0.41
1:D:23:ASN:H	1:D:23:ASN:ND2	2.18	0.41
1:A:176:ARG:HD2	4:A:1385:HOH:O	2.21	0.41
1:B:292:GLY:HA3	3:B:381:NDP:O1A	2.20	0.41
1:D:75:SER:CB	1:D:109:ARG:HD2	2.51	0.41
1:C:190:LEU:HD12	1:C:289:VAL:HG13	2.01	0.41
1:A:30:VAL:O	1:A:37:VAL:HG22	2.21	0.41
1:C:170:ILE:HG22	1:C:171:THR:N	2.35	0.41
1:D:226:PRO:C	1:D:228:ASP:H	2.25	0.41
1:D:233:CYS:O	1:D:235:GLN:N	2.54	0.41
1:B:32:LYS:HE2	1:B:33:ASP:OD2	2.21	0.41
1:D:166:ASP:OD1	1:D:168:LYS:HG3	2.20	0.41
1:C:307:GLU:CD	1:C:357:LYS:HZ3	2.25	0.41
1:A:103:ASN:HA	1:A:104:PRO:HD3	1.94	0.41
1:A:334:MET:HB2	1:B:168:LYS:HB2	2.03	0.41
1:C:181:GLN:NE2	1:C:182:TYR:CD2	2.87	0.41
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.56	0.41
1:C:253:LYS:HA	1:C:256:SER:OG	2.21	0.41
1:A:276:LEU:HA	1:A:276:LEU:HD23	1.87	0.41
1:D:186:HIS:CD2	1:D:288:TYR:HB2	2.56	0.41
1:C:96:PHE:HA	1:C:122:ARG:O	2.21	0.40
1:B:6:MET:HG2	1:B:125:ILE:O	2.21	0.40
1:D:37:VAL:HG11	1:D:61:HIS:CB	2.50	0.40
1:B:155:SER:HB3	1:B:317:ILE:HG13	2.03	0.40
1:C:155:SER:HB3	1:C:317:ILE:HG12	2.02	0.40
1:D:129:GLN:HB3	1:D:129:GLN:HE21	1.68	0.40
1:A:337:VAL:HA	1:A:338:PRO:HD3	1.87	0.40
1:A:25:LEU:HA	4:A:1375:HOH:O	2.21	0.40
1:B:51:GLU:O	1:B:55:ILE:HG12	2.21	0.40
1:B:86:LEU:O	1:B:86:LEU:HD13	2.21	0.40
1:D:9:ALA:HB2	1:D:29:VAL:CG1	2.51	0.40
1:D:20:THR:O	1:D:21:GLU:HB2	2.21	0.40
1:C:82:PRO:C	1:C:84:ALA:N	2.75	0.40
1:B:79:LYS:O	1:B:80:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:VAL:HG12	1:B:27:GLY:N	2.36	0.40
1:D:19:GLN:HE21	1:D:44:LYS:NZ	2.19	0.40
1:D:101:ASP:HA	1:D:102:PRO:HD3	1.79	0.40
1:C:116:GLU:C	1:C:118:GLY:N	2.74	0.40
1:C:174:ALA:CB	1:C:348:ILE:HG22	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1398:HOH:O	4:B:1422:HOH:O[3_645]	1.93	0.27
4:A:1410:HOH:O	4:A:1419:HOH:O[3_645]	2.19	0.01

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	357/373 (96%)	310 (87%)	41 (12%)	6 (2%)	14	53
1	B	357/373 (96%)	303 (85%)	44 (12%)	10 (3%)	8	36
1	C	357/373 (96%)	303 (85%)	43 (12%)	11 (3%)	7	32
1	D	358/373 (96%)	309 (86%)	33 (9%)	16 (4%)	4	21
All	All	1429/1492 (96%)	1225 (86%)	161 (11%)	43 (3%)	7	33

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
1	A	329	GLU
1	B	168	LYS
1	B	208	PRO
1	B	211	THR
1	B	212	LYS
1	B	234	ASP
1	B	235	GLN

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Mol	Chain	Res	Type
1	C	67	ILE
1	C	209	ASN
1	C	212	LYS
1	C	235	GLN
1	D	20	THR
1	D	167	SER
1	A	211	THR
1	B	78	GLY
1	B	196	VAL
1	B	292	GLY
1	C	79	LYS
1	D	17	GLU
1	D	92	ILE
1	D	125	ILE
1	D	234	ASP
1	A	48	ALA
1	C	21	GLU
1	C	108	GLY
1	A	21	GLU
1	B	21	GLU
1	C	76	HIS
1	D	172	SER
1	D	221	THR
1	D	230	LYS
1	D	259	GLY
1	A	290	GLU
1	C	170	ILE
1	D	48	ALA
1	D	270	ILE
1	C	113	MET
1	D	228	ASP
1	D	231	VAL
1	D	318	GLY
1	C	55	ILE
1	D	292	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/305 (96%)	276 (94%)	17 (6%)	28	70
1	B	293/305 (96%)	277 (94%)	16 (6%)	30	72
1	C	293/305 (96%)	272 (93%)	21 (7%)	21	59
1	D	294/305 (96%)	268 (91%)	26 (9%)	14	47
All	All	1173/1220 (96%)	1093 (93%)	80 (7%)	22	62

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	25	LEU
1	A	80	THR
1	A	86	LEU
1	A	171	THR
1	A	177	GLN
1	A	181	GLN
1	A	193	VAL
1	A	231	VAL
1	A	256	SER
1	A	260	VAL
1	A	277	LYS
1	A	282	GLU
1	A	298	SER
1	A	350	ARG
1	A	355	THR
1	B	43	LEU
1	B	70	THR
1	B	101	ASP
1	B	103	ASN
1	B	109	ARG
1	B	128	ASP
1	B	176	ARG
1	B	187	GLN
1	B	212	LYS
1	B	228	ASP
1	B	234	ASP
1	B	235	GLN
1	B	249	GLU
1	B	258	PHE
1	B	320	THR
1	B	335	LYS

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Mol	Chain	Res	Type
1	C	8	LEU
1	C	33	ASP
1	C	68	TYR
1	C	74	CYS
1	C	76	HIS
1	C	103	ASN
1	C	105	LEU
1	C	125	ILE
1	C	128	ASP
1	C	138	LEU
1	C	141	MET
1	C	181	GLN
1	C	189	ILE
1	C	191	VAL
1	C	193	VAL
1	C	209	ASN
1	C	223	LEU
1	C	267	THR
1	C	271	GLN
1	C	351	ASP
1	C	355	THR
1	D	2	GLU
1	D	20	THR
1	D	29	VAL
1	D	63	GLU
1	D	71	LEU
1	D	86	LEU
1	D	90	SER
1	D	105	LEU
1	D	112	SER
1	D	122	ARG
1	D	128	ASP
1	D	129	GLN
1	D	141	MET
1	D	180	GLN
1	D	190	LEU
1	D	193	VAL
1	D	223	LEU
1	D	243	THR
1	D	261	ASN
1	D	266	GLU
1	D	268	GLU

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Mol	Chain	Res	Type
1	D	270	ILE
1	D	277	LYS
1	D	306	GLN
1	D	354	LEU
1	D	355	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	19	GLN
1	A	49	HIS
1	A	139	HIS
1	A	177	GLN
1	A	187	GLN
1	A	209	ASN
1	A	235	GLN
1	A	321	HIS
1	A	341	GLN
1	A	347	GLN
1	B	23	ASN
1	B	35	GLN
1	B	42	HIS
1	B	89	ASN
1	B	103	ASN
1	B	134	ASN
1	B	186	HIS
1	B	187	GLN
1	B	296	HIS
1	B	306	GLN
1	B	341	GLN
1	B	347	GLN
1	C	15	GLN
1	C	23	ASN
1	C	35	GLN
1	C	89	ASN
1	C	103	ASN
1	C	134	ASN
1	C	186	HIS
1	C	187	GLN
1	C	209	ASN
1	C	261	ASN

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Mol	Chain	Res	Type
1	C	341	GLN
1	D	19	GLN
1	D	23	ASN
1	D	35	GLN
1	D	53	HIS
1	D	56	HIS
1	D	89	ASN
1	D	129	GLN
1	D	134	ASN
1	D	180	GLN
1	D	181	GLN
1	D	186	HIS
1	D	271	GLN
1	D	306	GLN
1	D	347	GLN

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 ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	B	381	-	52,52,52	1.37	7 (13%)	80,80,80	1.22	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	381	-	-	0/35/77/77	0/3/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	381	NDP	C6N-C5N	3.54	1.40	1.33
3	B	381	NDP	C4N-C5N	-3.52	1.41	1.49
3	B	381	NDP	C4N-C3N	-3.35	1.43	1.50
3	B	381	NDP	C2N-C3N	2.88	1.40	1.34
3	B	381	NDP	C1D-N1N	2.59	1.51	1.46
3	B	381	NDP	C4A-N9A	-2.45	1.34	1.37
3	B	381	NDP	C2A-N3A	2.17	1.36	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	381	NDP	PN-O3-PA	4.06	143.58	131.68
3	B	381	NDP	N3A-C2A-N1A	-3.13	126.09	128.71
3	B	381	NDP	O4B-C1B-C2B	-2.95	104.19	106.95
3	B	381	NDP	C1D-N1N-C2N	-2.67	116.47	121.02
3	B	381	NDP	C4A-C5A-N7A	2.61	111.76	109.52
3	B	381	NDP	C5N-C4N-C3N	2.57	119.56	112.60
3	B	381	NDP	C8A-N9A-C4A	-2.35	105.11	106.90
3	B	381	NDP	P2B-O2B-C2B	2.07	126.32	121.96
3	B	381	NDP	C4N-C3N-C2N	-2.03	119.21	121.68

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	A	359/373 (96%)	0.05	3 (0%) 83 38	37, 58, 78, 99	0
1	B	359/373 (96%)	0.35	17 (4%) 30 13	45, 66, 98, 128	0
1	C	359/373 (96%)	0.40	24 (6%) 17 8	41, 70, 99, 122	0
1	D	360/373 (96%)	0.26	13 (3%) 41 17	44, 66, 110, 123	0
All	All	1437/1492 (96%)	0.27	57 (3%) 36 15	37, 64, 99, 128	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ASN	9.1
1	B	209	ASN	6.2
1	C	208	PRO	6.2
1	D	209	ASN	5.7
1	B	208	PRO	5.1
1	C	86	LEU	4.8
1	C	169	TRP	3.9
1	B	207	LEU	3.8
1	D	169	TRP	3.6
1	D	310	PHE	3.5
1	C	105	LEU	3.4
1	C	29	VAL	3.4
1	B	92	ILE	3.3
1	C	77	TYR	3.0
1	C	5	TYR	3.0
1	D	309	ILE	2.9
1	D	354	LEU	2.9
1	D	311	TYR	2.8
1	C	43	LEU	2.8
1	B	316	LEU	2.7
1	C	67	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	71	LEU	2.7
1	C	81	PRO	2.7
1	D	242	PHE	2.6
1	C	12	LEU	2.5
1	D	312	PHE	2.5
1	B	257	ALA	2.5
1	D	241	ILE	2.5
1	D	219	LEU	2.5
1	C	113	MET	2.5
1	B	132	ARG	2.4
1	C	114	MET	2.4
1	B	212	LYS	2.4
1	C	92	ILE	2.3
1	D	262	ILE	2.3
1	C	68	TYR	2.3
1	A	209	ASN	2.3
1	B	93	LYS	2.3
1	B	352	ILE	2.3
1	B	30	VAL	2.2
1	B	260	VAL	2.1
1	C	69	VAL	2.1
1	C	316	LEU	2.1
1	B	259	GLY	2.1
1	C	123	GLU	2.1
1	C	133	LEU	2.1
1	C	119	ILE	2.1
1	B	342	PHE	2.1
1	B	114	MET	2.0
1	D	208	PRO	2.0
1	A	348	ILE	2.0
1	C	130	ALA	2.0
1	A	114	MET	2.0
1	C	28	ALA	2.0
1	B	205	CYS	2.0
1	C	30	VAL	2.0
1	D	207	LEU	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
3	NDP	B	381	48/48	0.22	0.44	76,85,88,91	0
2	ZN	A	1360	1/1	0.19	0.25	73,73,73,73	0
2	ZN	D	1360	1/1	0.14	-1.02	78,78,78,78	0
2	ZN	B	1360	1/1	0.10	-1.26	63,63,63,63	0
2	ZN	C	1360	1/1	0.10	-2.30	92,92,92,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.