Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:37 AM GMT

PDB ID	:	2B3Z
Title	:	Crystal structure of a bifunctional deaminase and reductase involved in riboflavin biosynthesis
Authors	:	Chen, S.J.; Chang, Y.C.; Liaw, S.H.
Deposited on	:	2005-09-22
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

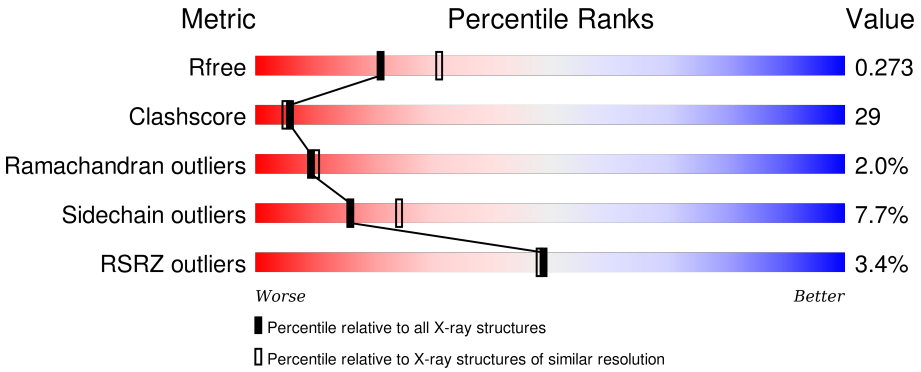
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	373	63% 30%
1	B	373	3% 53% 38% 5%
1	C	373	2% 54% 36% 5%
1	D	373	7% 50% 39% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11267 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 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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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 water.

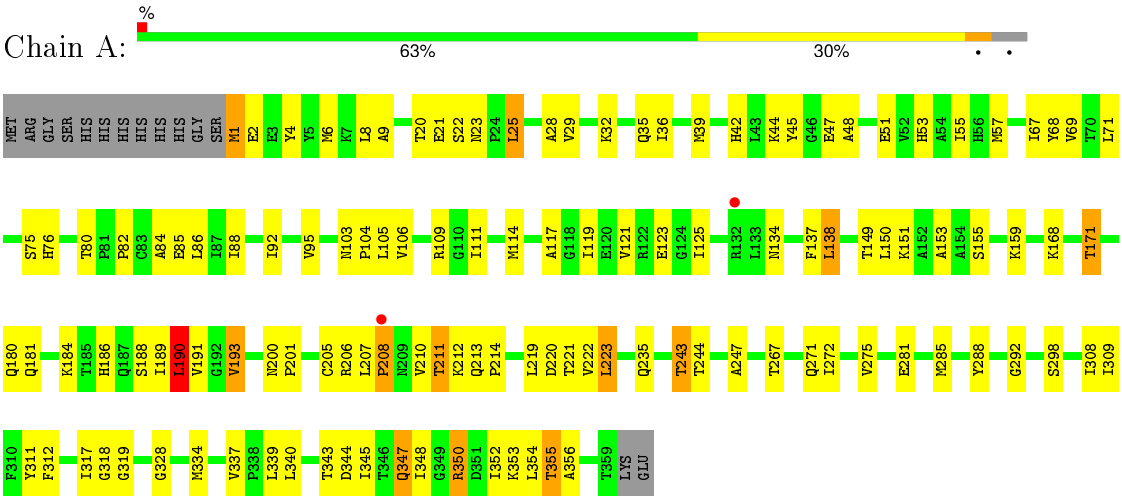
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	88	Total O 88 88	0	0
3	B	75	Total O 75 75	0	0
3	C	74	Total O 74 74	0	0
3	D	56	Total O 56 56	0	0

3 Residue-property plots (i)

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.

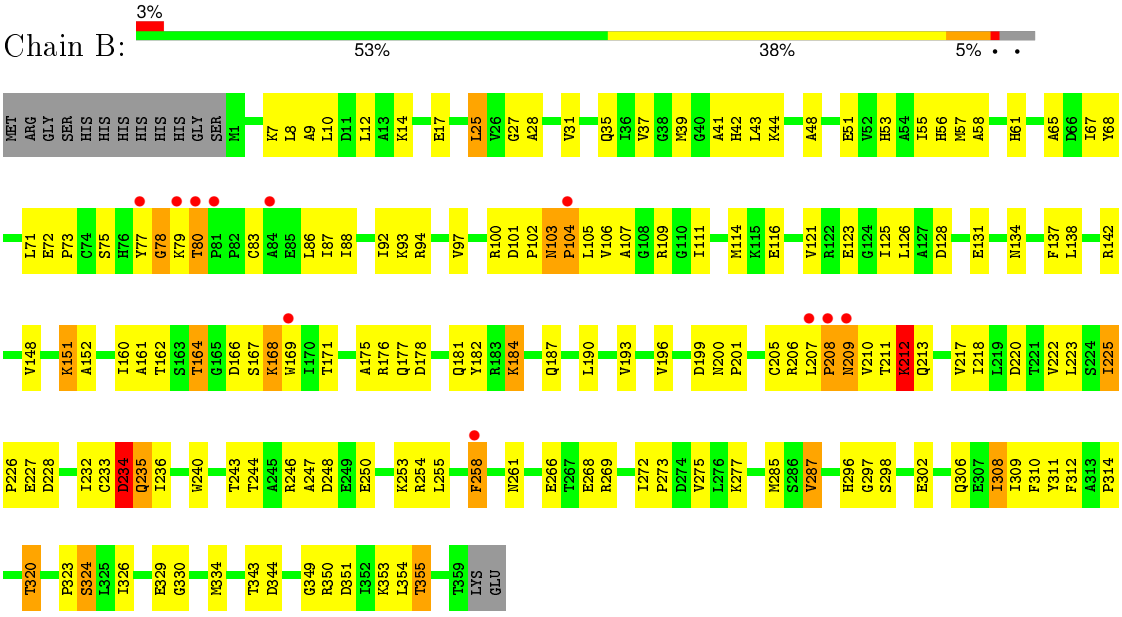
- Molecule 1: Riboflavin biosynthesis protein ribD

Chain A:



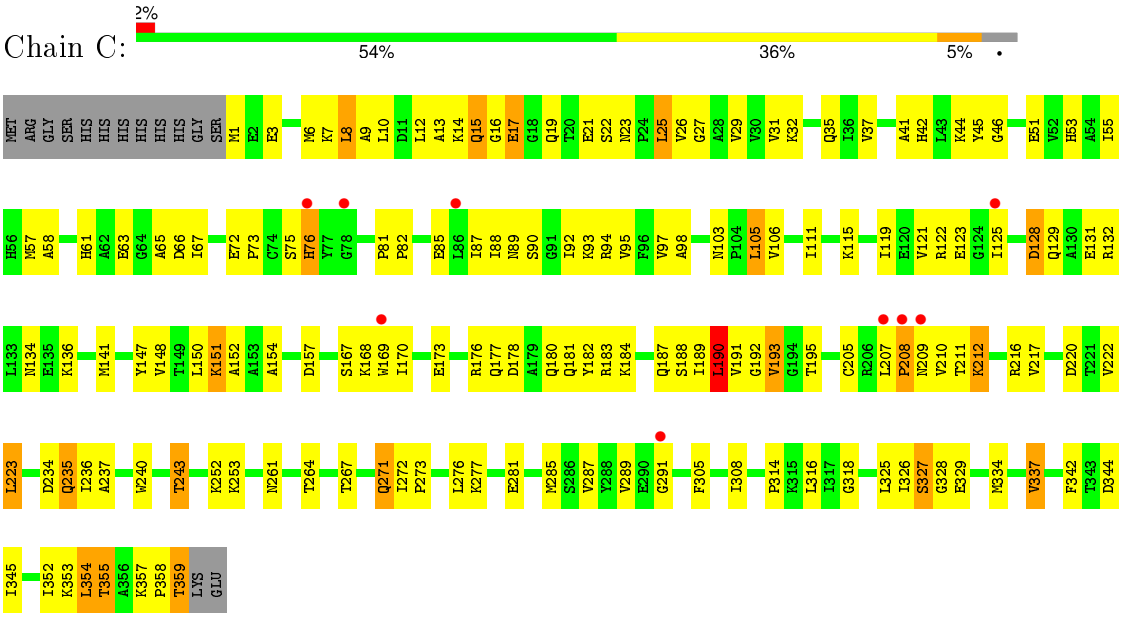
- Molecule 1: Riboflavin biosynthesis protein ribD

Chain B:



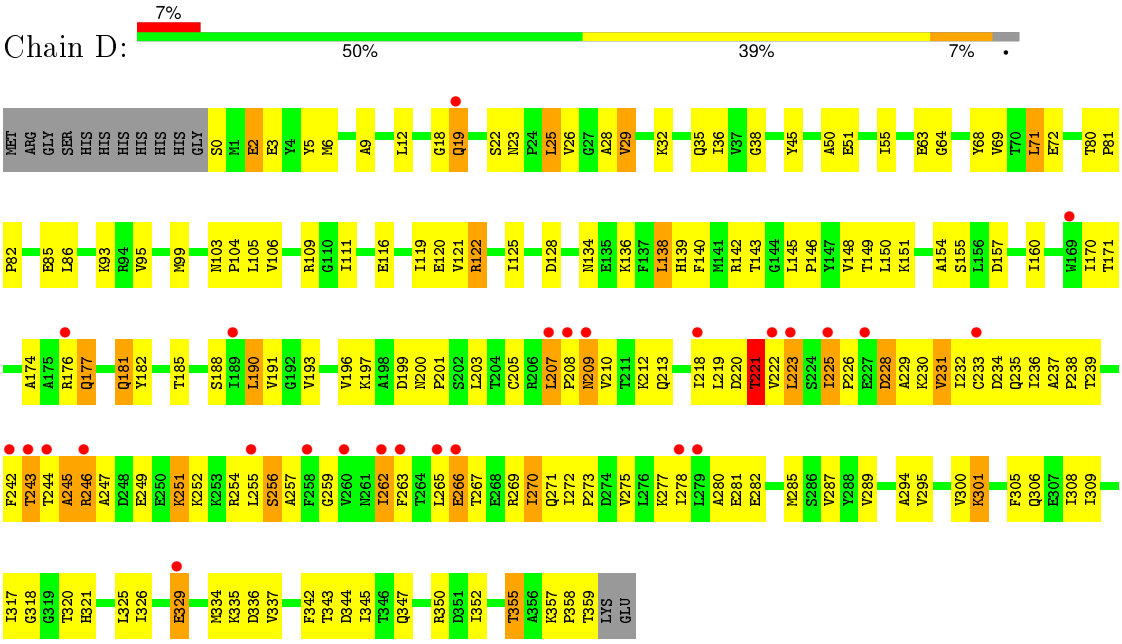
- Molecule 1: Riboflavin biosynthesis protein ribD

Chain C:



• Molecule 1: Riboflavin biosynthesis protein ribD

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.32Å 108.45Å 186.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.41 46.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.41) 97.2 (46.91-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.277 0.223 , 0.273	Depositor DCC
R_{free} test set	6818 reflections (10.10%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 67690 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11267	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/2792	0.75	2/3778 (0.1%)
1	B	0.44	0/2792	0.66	0/3778
1	C	0.45	0/2792	0.68	2/3778 (0.1%)
1	D	0.43	0/2798	0.66	0/3786
All	All	0.46	0/11174	0.69	4/15120 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	LEU	CA-CB-CG	6.86	131.08	115.30
1	C	190	LEU	CA-CB-CG	6.44	130.12	115.30
1	C	291	GLY	N-CA-C	5.84	127.69	113.10
1	A	319	GLY	N-CA-C	5.52	126.91	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2741	0	2782	132	0
1	B	2741	0	2782	181	0
1	C	2741	0	2782	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2747	0	2787	194	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	A	88	0	0	22	0
3	B	75	0	0	27	0
3	C	74	0	0	29	0
3	D	56	0	0	30	0
All	All	11267	0	11133	636	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:HG21	3:B:1401:HOH:O	1.20	1.31
1:D:0:SER:HA	3:D:1408:HOH:O	1.35	1.26
1:A:211:THR:HG22	3:A:1441:HOH:O	1.37	1.21
1:D:245:ALA:HA	3:D:1405:HOH:O	1.38	1.19
1:C:271:GLN:HG3	3:C:1385:HOH:O	1.50	1.10
1:C:176:ARG:HD3	3:C:1381:HOH:O	1.51	1.09
1:D:320:THR:HA	3:D:1376:HOH:O	1.49	1.09
1:D:270:ILE:H	1:D:270:ILE:HD13	1.18	1.08
1:B:184:LYS:HZ1	1:B:207:LEU:HB2	1.21	1.03
1:C:329:GLU:HA	3:C:1390:HOH:O	1.63	0.99
1:D:320:THR:CA	3:D:1376:HOH:O	2.07	0.99
1:C:85:GLU:HG2	1:C:89:ASN:HD21	1.24	0.98
1:A:318:GLY:HA3	1:B:330:GLY:CA	1.93	0.97
1:D:223:LEU:HD22	1:D:251:LYS:HE3	1.45	0.96
1:D:160:ILE:HD11	1:D:325:LEU:HD23	1.48	0.95
3:C:1393:HOH:O	1:D:334:MET:HG2	1.68	0.93
1:D:201:PRO:HG2	1:D:203:LEU:HD21	1.52	0.91
1:C:168:LYS:HB2	3:C:1393:HOH:O	1.70	0.91
1:D:148:VAL:H	1:D:306:GLN:NE2	1.68	0.91
1:A:205:CYS:H	1:A:213:GLN:HE22	1.19	0.91
1:D:99:MET:HE2	1:D:138:LEU:HD11	1.54	0.89
1:D:245:ALA:CA	3:D:1405:HOH:O	2.07	0.88
1:C:37:VAL:HG21	1:C:61:HIS:HB2	1.55	0.88
1:B:125:ILE:HD12	1:B:125:ILE:H	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LYS:O	1:D:234:ASP:HB3	1.74	0.87
1:D:271:GLN:HG2	1:D:273:PRO:HD2	1.54	0.87
1:B:171:THR:HA	3:B:1391:HOH:O	1.73	0.87
1:A:25:LEU:H	1:A:134:ASN:HD21	1.20	0.86
1:A:350:ARG:CD	3:A:1376:HOH:O	2.22	0.86
1:A:318:GLY:HA3	1:B:330:GLY:HA3	1.56	0.86
1:B:193:VAL:HG11	1:B:220:ASP:CG	1.96	0.86
1:B:227:GLU:HG2	1:B:255:LEU:HD21	1.56	0.85
1:B:37:VAL:HG11	1:B:61:HIS:HB2	1.59	0.85
1:C:169:TRP:N	3:C:1393:HOH:O	2.05	0.84
1:B:148:VAL:H	1:B:306:GLN:HE21	1.25	0.84
1:A:344:ASP:HB3	1:A:355:THR:HG23	1.59	0.84
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.08	0.83
1:A:318:GLY:HA3	1:B:330:GLY:HA2	1.56	0.83
1:A:221:THR:O	1:A:243:THR:HG22	1.79	0.83
1:A:88:ILE:HD11	1:A:114:MET:HA	1.59	0.83
1:B:171:THR:CB	3:B:1391:HOH:O	2.27	0.83
1:C:37:VAL:HG22	1:C:58:ALA:HA	1.62	0.82
1:D:148:VAL:H	1:D:306:GLN:HE21	1.23	0.82
1:C:111:ILE:HG23	1:C:121:VAL:HG11	1.60	0.82
1:B:243:THR:HG22	1:B:244:THR:H	1.43	0.81
1:D:270:ILE:CD1	1:D:270:ILE:H	1.93	0.81
1:B:166:ASP:OD1	1:B:168:LYS:HB2	1.80	0.81
1:C:31:VAL:HG11	3:C:1362:HOH:O	1.81	0.80
1:C:168:LYS:CA	3:C:1393:HOH:O	2.30	0.79
1:C:85:GLU:HG2	1:C:89:ASN:ND2	1.99	0.78
1:B:75:SER:CB	1:B:109:ARG:HD2	2.14	0.78
1:D:334:MET:O	1:D:337:VAL:HG12	1.83	0.77
1:D:150:LEU:HD12	1:D:308:ILE:HD11	1.67	0.77
1:A:32:LYS:NZ	3:A:1434:HOH:O	2.15	0.77
1:A:207:LEU:HB3	1:A:208:PRO:HD2	1.67	0.77
1:A:271:GLN:CG	3:A:1423:HOH:O	2.31	0.76
1:D:321:HIS:N	3:D:1376:HOH:O	2.15	0.76
1:D:270:ILE:HD13	1:D:270:ILE:N	1.99	0.76
1:B:269:ARG:NE	3:B:1428:HOH:O	2.17	0.76
1:D:320:THR:CG2	3:D:1376:HOH:O	2.33	0.76
1:B:177:GLN:HG2	3:B:1397:HOH:O	1.84	0.76
1:B:51:GLU:OE2	3:B:1363:HOH:O	2.04	0.76
1:C:344:ASP:HB3	1:C:355:THR:HG23	1.67	0.75
1:A:243:THR:HG21	1:A:247:ALA:HB2	1.67	0.75
1:C:271:GLN:HA	1:C:271:GLN:HE21	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:O	1:A:243:THR:HG23	1.87	0.75
1:B:349:GLY:HA3	3:B:1383:HOH:O	1.86	0.75
1:C:168:LYS:CB	3:C:1393:HOH:O	2.32	0.74
1:B:75:SER:HB3	1:B:109:ARG:HD2	1.67	0.74
1:D:301:LYS:HE2	1:D:301:LYS:O	1.87	0.74
1:B:171:THR:CA	3:B:1391:HOH:O	2.32	0.74
1:A:271:GLN:HG3	3:A:1423:HOH:O	1.86	0.74
1:D:3:GLU:OE2	3:D:1408:HOH:O	2.05	0.74
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.70	0.73
1:B:184:LYS:NZ	1:B:184:LYS:HB2	2.03	0.73
1:A:159:LYS:HE2	3:A:1366:HOH:O	1.88	0.73
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.19	0.72
1:C:76:HIS:O	1:C:82:PRO:HG3	1.88	0.72
1:D:221:THR:HG23	1:D:270:ILE:HD12	1.71	0.72
1:D:116:GLU:OE1	3:D:1384:HOH:O	2.08	0.72
1:C:329:GLU:CA	3:C:1390:HOH:O	2.28	0.72
1:D:103:ASN:OD1	3:D:1407:HOH:O	2.07	0.71
1:C:329:GLU:O	3:C:1390:HOH:O	2.08	0.71
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.73	0.71
1:A:68:TYR:OH	3:A:1402:HOH:O	2.08	0.71
1:D:64:GLY:HA2	1:D:93:LYS:HG2	1.72	0.71
1:B:125:ILE:HG22	1:B:126:LEU:HD13	1.73	0.71
1:D:320:THR:O	3:D:1367:HOH:O	2.09	0.71
1:B:37:VAL:HG12	1:B:58:ALA:HA	1.72	0.71
1:A:75:SER:OG	1:A:109:ARG:HD2	1.90	0.71
1:A:88:ILE:HD12	1:A:117:ALA:CB	2.21	0.70
1:C:168:LYS:O	3:C:1415:HOH:O	2.09	0.70
1:A:207:LEU:HB3	1:A:208:PRO:CD	2.21	0.70
1:D:249:GLU:O	3:D:1383:HOH:O	2.10	0.70
1:D:295:VAL:HG23	3:D:1375:HOH:O	1.90	0.70
1:B:37:VAL:HG11	1:B:61:HIS:CB	2.22	0.69
1:A:39:MET:HE1	1:C:15:GLN:HG2	1.74	0.69
1:D:245:ALA:O	3:D:1409:HOH:O	2.10	0.69
1:B:344:ASP:HB3	1:B:355:THR:HG23	1.74	0.69
1:C:103:ASN:HA	1:C:141:MET:HG3	1.73	0.69
1:C:272:ILE:HB	1:C:273:PRO:HD3	1.75	0.69
1:D:266:GLU:CD	1:D:266:GLU:H	1.96	0.69
1:D:32:LYS:HE2	1:D:63:GLU:O	1.92	0.69
1:A:29:VAL:HG22	1:A:68:TYR:HB2	1.73	0.69
1:A:123:GLU:OE1	3:A:1396:HOH:O	2.11	0.68
1:B:243:THR:HG22	1:B:244:THR:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLU:OE1	1:D:111:ILE:HG12	1.93	0.68
1:C:191:VAL:CG1	1:C:195:THR:HB	2.23	0.68
1:D:243:THR:HG22	1:D:244:THR:H	1.59	0.68
1:B:184:LYS:HZ1	1:B:207:LEU:CB	2.04	0.68
1:A:328:GLY:H	1:B:320:THR:HG22	1.59	0.68
1:D:146:PRO:HD3	1:D:280:ALA:HB2	1.75	0.68
1:A:80:THR:O	3:A:1419:HOH:O	2.12	0.67
1:B:171:THR:HB	3:B:1391:HOH:O	1.92	0.67
1:D:247:ALA:HB3	3:D:1409:HOH:O	1.93	0.67
1:B:51:GLU:O	1:B:55:ILE:HG12	1.94	0.67
1:B:25:LEU:H	1:B:134:ASN:HD21	1.42	0.67
1:A:155:SER:HB3	1:A:317:ILE:HD12	1.75	0.67
1:B:344:ASP:OD2	3:B:1372:HOH:O	2.12	0.67
1:C:216:ARG:HD2	1:C:237:ALA:HB3	1.76	0.67
1:D:104:PRO:HG2	3:D:1407:HOH:O	1.95	0.66
1:C:181:GLN:HG3	1:C:182:TYR:N	2.09	0.66
1:B:184:LYS:HZ3	1:B:184:LYS:HB2	1.59	0.66
1:D:6:MET:HG2	1:D:125:ILE:HG22	1.76	0.66
1:B:167:SER:O	1:B:169:TRP:N	2.29	0.66
1:A:334:MET:HB2	1:B:168:LYS:HB3	1.78	0.66
1:B:177:GLN:NE2	3:B:1397:HOH:O	2.15	0.66
1:D:200:ASN:HD21	1:D:230:LYS:HG2	1.59	0.66
1:D:104:PRO:CD	3:D:1407:HOH:O	2.43	0.66
1:C:23:ASN:ND2	1:C:45:TYR:HD2	1.94	0.66
1:D:171:THR:HG21	3:D:1391:HOH:O	1.94	0.66
1:A:21:GLU:N	3:A:1440:HOH:O	2.10	0.66
1:D:252:LYS:HG2	1:D:262:ILE:HD12	1.78	0.66
1:B:151:LYS:HD2	1:B:152:ALA:N	2.11	0.66
1:D:308:ILE:C	1:D:309:ILE:HD12	2.16	0.65
1:C:187:GLN:OE1	1:C:285:MET:HB2	1.96	0.65
1:C:168:LYS:N	3:C:1393:HOH:O	2.30	0.65
1:B:243:THR:HG21	1:B:247:ALA:HB2	1.77	0.65
1:C:31:VAL:CG1	1:C:66:ASP:HB2	2.26	0.65
1:B:103:ASN:ND2	1:B:105:LEU:HD13	2.12	0.65
1:B:57:MET:O	3:B:1399:HOH:O	2.14	0.65
1:B:329:GLU:HG3	3:B:1377:HOH:O	1.96	0.65
1:B:55:ILE:HG13	1:B:86:LEU:CD1	2.27	0.65
1:D:230:LYS:O	1:D:232:ILE:N	2.31	0.64
1:C:193:VAL:HG13	1:C:220:ASP:HB2	1.78	0.64
1:C:93:LYS:NZ	1:C:93:LYS:HB3	2.13	0.64
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:PRO:HG2	1:D:203:LEU:CD2	2.26	0.64
1:A:84:ALA:O	1:A:88:ILE:HG12	1.98	0.64
1:A:88:ILE:HD13	1:A:119:ILE:HD12	1.81	0.63
1:A:153:ALA:HB1	1:A:171:THR:HG23	1.80	0.63
1:A:151:LYS:HD2	1:A:288:TYR:OH	1.98	0.63
1:D:150:LEU:HD12	1:D:308:ILE:CD1	2.27	0.63
1:C:223:LEU:HG	1:C:243:THR:HG21	1.79	0.63
1:C:37:VAL:HG21	1:C:61:HIS:CB	2.28	0.63
1:C:111:ILE:HG22	1:C:115:LYS:HD2	1.81	0.63
1:B:103:ASN:HD21	1:B:105:LEU:HD13	1.63	0.63
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.19	0.63
1:B:269:ARG:CD	3:B:1428:HOH:O	2.46	0.62
1:B:79:LYS:O	1:B:80:THR:HG23	1.98	0.62
1:C:105:LEU:H	1:C:105:LEU:HD23	1.64	0.62
1:D:221:THR:CG2	1:D:270:ILE:HD12	2.29	0.62
1:B:312:PHE:HE2	1:B:354:LEU:HD12	1.65	0.62
1:A:22:SER:HA	1:A:285:MET:CE	2.30	0.62
1:D:208:PRO:O	1:D:209:ASN:HB2	2.00	0.62
1:D:320:THR:O	1:D:321:HIS:HB2	2.00	0.61
1:D:120:GLU:OE1	3:D:1392:HOH:O	2.16	0.61
1:B:220:ASP:O	1:B:243:THR:HG23	1.99	0.61
1:C:95:VAL:CG1	1:C:121:VAL:HG22	2.29	0.61
1:D:207:LEU:HD23	1:D:208:PRO:HD2	1.80	0.61
1:A:25:LEU:H	1:A:134:ASN:ND2	1.94	0.61
1:C:51:GLU:O	1:C:55:ILE:HD13	2.00	0.61
1:C:211:THR:O	1:C:212:LYS:HB2	2.00	0.61
1:C:328:GLY:HA3	3:C:1409:HOH:O	2.01	0.61
1:C:21:GLU:HG3	1:C:22:SER:H	1.64	0.61
1:D:170:ILE:HG23	1:D:171:THR:N	2.16	0.61
1:A:193:VAL:HG22	1:A:219:LEU:O	2.01	0.61
1:A:88:ILE:HD12	1:A:117:ALA:HB3	1.81	0.61
1:C:352:ILE:HG22	1:C:354:LEU:CD2	2.31	0.60
1:C:42:HIS:N	3:C:1378:HOH:O	2.32	0.60
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.65	0.60
1:C:354:LEU:HD23	1:C:354:LEU:N	2.16	0.60
1:D:245:ALA:O	1:D:247:ALA:N	2.33	0.60
1:C:87:ILE:HG23	1:C:92:ILE:HG13	1.84	0.60
1:B:56:HIS:HE1	3:B:1382:HOH:O	1.84	0.60
1:D:148:VAL:HB	1:D:305:PHE:HA	1.84	0.60
1:C:6:MET:HG3	1:C:125:ILE:HB	1.83	0.60
1:C:326:ILE:HB	1:D:318:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:HG2	1:D:182:TYR:N	2.17	0.59
1:B:234:ASP:C	1:B:234:ASP:OD2	2.41	0.59
1:D:223:LEU:HD23	1:D:225:ILE:HG22	1.83	0.59
1:D:218:ILE:N	1:D:218:ILE:HD12	2.18	0.59
1:B:222:VAL:HG12	1:B:222:VAL:O	2.02	0.59
1:D:267:THR:HG22	1:D:269:ARG:H	1.67	0.58
1:C:191:VAL:HG13	1:C:195:THR:HB	1.83	0.58
1:D:188:SER:OG	1:D:287:VAL:HG22	2.02	0.58
1:B:35:GLN:NE2	1:D:19:GLN:HB2	2.17	0.58
1:B:225:ILE:HD13	1:B:226:PRO:N	2.18	0.58
1:B:75:SER:HB2	1:B:109:ARG:HD2	1.85	0.58
1:C:318:GLY:HA2	1:D:326:ILE:HG22	1.85	0.58
1:A:184:LYS:NZ	3:A:1448:HOH:O	2.36	0.58
1:A:318:GLY:CA	1:B:330:GLY:HA3	2.29	0.58
1:C:220:ASP:O	1:C:243:THR:HG22	2.04	0.58
1:C:271:GLN:CG	3:C:1385:HOH:O	2.26	0.58
1:D:222:VAL:O	1:D:222:VAL:HG22	2.01	0.58
1:C:176:ARG:CD	3:C:1381:HOH:O	2.29	0.57
1:D:295:VAL:N	3:D:1375:HOH:O	2.16	0.57
1:D:5:TYR:CE1	1:D:36:ILE:HD11	2.38	0.57
1:B:266:GLU:OE2	3:B:1408:HOH:O	2.17	0.57
1:A:95:VAL:HG23	1:A:119:ILE:HG21	1.86	0.57
1:B:314:PRO:HG3	1:B:350:ARG:O	2.05	0.57
1:C:240:TRP:CD1	1:C:261:ASN:HB2	2.39	0.57
1:B:55:ILE:HG13	1:B:86:LEU:HD11	1.87	0.57
1:A:21:GLU:HB2	1:A:45:TYR:CD1	2.40	0.57
1:B:7:LYS:HA	1:B:10:LEU:HD12	1.85	0.57
1:D:329:GLU:HB3	3:D:1379:HOH:O	2.03	0.57
1:B:151:LYS:C	1:B:151:LYS:HD2	2.25	0.57
1:D:245:ALA:C	1:D:247:ALA:H	2.07	0.57
1:D:25:LEU:HB2	1:D:134:ASN:HD21	1.69	0.57
1:D:344:ASP:O	1:D:345:ILE:HD13	2.04	0.57
1:D:111:ILE:HD12	1:D:121:VAL:HG11	1.87	0.57
1:A:21:GLU:CA	3:A:1440:HOH:O	2.52	0.56
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.70	0.56
1:B:308:ILE:HD11	1:B:310:PHE:CZ	2.40	0.56
1:B:184:LYS:HE3	1:B:210:VAL:HG12	1.86	0.56
1:A:28:ALA:HA	1:A:68:TYR:O	2.06	0.56
1:D:320:THR:HG23	3:D:1376:HOH:O	2.00	0.56
1:B:166:ASP:OD1	1:B:168:LYS:CB	2.53	0.56
1:B:308:ILE:HD11	1:B:310:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:O	1:B:212:LYS:HB2	2.06	0.56
1:C:267:THR:HG21	3:C:1385:HOH:O	2.04	0.56
1:D:104:PRO:HD2	3:D:1407:HOH:O	2.04	0.56
1:B:35:GLN:NE2	1:D:19:GLN:CB	2.69	0.56
1:D:190:LEU:HB3	1:D:289:VAL:HG22	1.87	0.56
1:C:188:SER:C	1:C:189:ILE:HD13	2.26	0.55
1:B:254:ARG:HG3	1:B:254:ARG:HH11	1.71	0.55
1:C:122:ARG:HD2	3:C:1418:HOH:O	2.05	0.55
1:D:138:LEU:O	1:D:142:ARG:HD2	2.06	0.55
1:D:149:THR:HG23	1:D:309:ILE:HD13	1.89	0.55
1:C:178:ASP:O	1:C:181:GLN:HG2	2.05	0.55
1:A:51:GLU:O	1:A:55:ILE:HG12	2.05	0.55
1:B:44:LYS:NZ	1:D:35:GLN:OE1	2.35	0.55
1:B:209:ASN:ND2	3:B:1401:HOH:O	2.40	0.55
1:C:167:SER:HA	1:D:334:MET:HE2	1.89	0.55
1:B:344:ASP:HB3	1:B:355:THR:CG2	2.37	0.55
1:B:246:ARG:HG3	1:B:246:ARG:NH1	2.21	0.55
1:B:53:HIS:HE1	3:B:1378:HOH:O	1.89	0.55
1:B:324:SER:OG	3:B:1364:HOH:O	2.18	0.55
1:C:6:MET:CE	1:C:98:ALA:HB2	2.37	0.55
1:C:167:SER:HA	1:D:334:MET:CE	2.37	0.55
1:D:344:ASP:HB3	1:D:355:THR:HG23	1.90	0.55
1:B:67:ILE:HD13	1:B:87:ILE:CD1	2.37	0.55
1:D:28:ALA:HA	1:D:68:TYR:O	2.07	0.54
1:B:220:ASP:OD2	1:B:225:ILE:HB	2.07	0.54
1:D:80:THR:HB	1:D:81:PRO:HD2	1.89	0.54
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.89	0.54
1:B:355:THR:HG22	3:B:1372:HOH:O	2.06	0.54
1:C:55:ILE:HD11	1:C:67:ILE:HD12	1.88	0.54
1:D:122:ARG:NH1	1:D:122:ARG:HA	2.22	0.54
1:D:139:HIS:O	1:D:143:THR:HG23	2.08	0.54
3:C:1393:HOH:O	1:D:334:MET:CB	2.55	0.54
1:B:100:ARG:NH1	1:B:123:GLU:OE1	2.41	0.54
1:B:272:ILE:HA	1:B:275:VAL:HG22	1.90	0.54
1:D:200:ASN:ND2	1:D:230:LYS:HG2	2.22	0.54
1:C:169:TRP:H	1:D:334:MET:HG2	1.72	0.54
1:D:271:GLN:CG	1:D:273:PRO:HD2	2.35	0.54
1:C:103:ASN:CA	1:C:141:MET:HG3	2.38	0.54
1:C:277:LYS:NZ	1:C:281:GLU:OE2	2.41	0.54
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.90	0.53
1:A:339:LEU:HD11	1:B:350:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HB	1:A:23:ASN:HB2	1.91	0.53
1:B:88:ILE:HD11	1:B:114:MET:HA	1.90	0.53
1:A:309:ILE:HG12	1:A:355:THR:HB	1.89	0.53
1:A:171:THR:HG23	3:A:1372:HOH:O	2.08	0.53
1:B:83:CYS:O	1:B:87:ILE:HG12	2.08	0.53
1:A:271:GLN:OE1	3:A:1421:HOH:O	2.19	0.53
1:A:21:GLU:HA	3:A:1440:HOH:O	2.09	0.53
1:B:234:ASP:O	1:B:236:ILE:HG12	2.09	0.53
1:D:106:VAL:HG22	1:D:109:ARG:NH2	2.24	0.53
1:C:191:VAL:HG11	1:C:195:THR:HB	1.91	0.53
1:C:81:PRO:HB3	1:C:85:GLU:OE1	2.08	0.53
1:D:225:ILE:O	1:D:225:ILE:HG23	2.08	0.53
1:C:23:ASN:HD21	1:C:45:TYR:HD2	1.56	0.53
1:C:344:ASP:HB3	1:C:355:THR:HG21	1.90	0.53
1:A:271:GLN:CD	3:A:1423:HOH:O	2.47	0.53
1:B:269:ARG:HD2	3:B:1428:HOH:O	2.09	0.53
1:A:181:GLN:HA	1:A:207:LEU:HD11	1.91	0.53
1:B:131:GLU:OE1	1:B:142:ARG:NH2	2.38	0.52
1:C:90:SER:OG	1:C:92:ILE:HG12	2.08	0.52
1:D:265:LEU:HD12	1:D:265:LEU:N	2.24	0.52
1:B:41:ALA:O	1:B:43:LEU:HD22	2.08	0.52
1:B:297:GLY:HA2	1:B:326:ILE:HG23	1.90	0.52
1:A:171:THR:HG21	3:A:1380:HOH:O	2.09	0.52
1:D:193:VAL:HG11	1:D:220:ASP:CG	2.29	0.52
1:D:205:CYS:H	1:D:213:GLN:NE2	2.08	0.52
1:B:14:LYS:HE3	1:B:17:GLU:OE2	2.10	0.52
1:A:348:ILE:HD12	1:A:348:ILE:N	2.24	0.52
1:D:247:ALA:O	3:D:1409:HOH:O	2.19	0.52
1:C:66:ASP:OD2	1:C:93:LYS:NZ	2.42	0.52
1:A:272:ILE:O	1:A:275:VAL:HG22	2.10	0.52
1:D:232:ILE:HG22	1:D:233:CYS:N	2.25	0.52
1:A:350:ARG:HD3	3:A:1376:HOH:O	2.01	0.52
1:D:335:LYS:HG3	1:D:336:ASP:OD1	2.09	0.52
1:D:193:VAL:O	1:D:197:LYS:HG2	2.10	0.52
1:A:8:LEU:HD21	1:A:39:MET:HE3	1.92	0.52
1:A:134:ASN:HB2	1:A:138:LEU:HD22	1.91	0.51
1:D:104:PRO:CG	3:D:1407:HOH:O	2.53	0.51
1:D:143:THR:OG1	1:D:145:LEU:HB2	2.09	0.51
1:A:42:HIS:HD2	1:A:48:ALA:O	1.93	0.51
1:C:252:LYS:HE2	3:C:1388:HOH:O	2.09	0.51
1:A:235:GLN:HA	1:A:235:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:GLU:C	3:C:1390:HOH:O	2.43	0.51
1:D:344:ASP:C	1:D:345:ILE:HD13	2.30	0.51
1:C:23:ASN:ND2	1:C:42:HIS:HE1	2.09	0.51
1:A:57:MET:HG3	1:C:53:HIS:CD2	2.45	0.51
1:A:22:SER:HA	1:A:285:MET:HE2	1.93	0.51
1:A:308:ILE:HG22	1:A:356:ALA:O	2.11	0.51
1:B:355:THR:CG2	3:B:1372:HOH:O	2.58	0.51
1:A:125:ILE:HD12	1:A:125:ILE:N	2.26	0.51
1:B:160:ILE:O	1:B:161:ALA:HB2	2.09	0.51
1:D:337:VAL:HG13	1:D:337:VAL:O	2.11	0.51
1:C:353:LYS:C	1:C:354:LEU:HD23	2.31	0.51
1:A:44:LYS:NZ	1:C:35:GLN:NE2	2.58	0.51
1:D:294:ALA:HB3	3:D:1375:HOH:O	2.11	0.51
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.92	0.50
1:D:320:THR:O	1:D:321:HIS:CB	2.59	0.50
1:B:272:ILE:HB	1:B:273:PRO:HD3	1.94	0.50
1:C:345:ILE:HD13	1:D:352:ILE:HD12	1.93	0.50
1:A:312:PHE:HE2	1:A:354:LEU:HD12	1.76	0.50
1:A:350:ARG:HD2	3:A:1376:HOH:O	1.97	0.50
1:D:122:ARG:HH11	1:D:122:ARG:HA	1.75	0.50
1:A:205:CYS:SG	1:A:210:VAL:HG12	2.52	0.50
1:C:191:VAL:HG12	1:C:192:GLY:O	2.11	0.50
1:A:345:ILE:HG23	1:A:354:LEU:CD2	2.42	0.50
1:B:272:ILE:O	1:B:275:VAL:HG22	2.11	0.50
1:C:234:ASP:OD2	1:C:235:GLN:N	2.45	0.50
1:C:132:ARG:HH22	1:C:357:LYS:HZ2	1.60	0.50
1:B:42:HIS:HD2	1:B:48:ALA:O	1.94	0.50
1:B:125:ILE:H	1:B:125:ILE:CD1	2.15	0.50
1:D:145:LEU:HD21	1:D:277:LYS:HE3	1.93	0.50
1:D:255:LEU:C	1:D:257:ALA:H	2.15	0.50
1:D:105:LEU:N	3:D:1407:HOH:O	2.45	0.50
1:C:6:MET:HE1	1:C:98:ALA:HB2	1.94	0.49
1:D:246:ARG:HH11	1:D:246:ARG:HG3	1.77	0.49
1:D:278:ILE:O	1:D:281:GLU:HB2	2.11	0.49
1:A:2:GLU:N	1:A:2:GLU:OE2	2.46	0.49
1:D:230:LYS:C	1:D:234:ASP:HB3	2.33	0.49
1:A:21:GLU:HG3	1:A:45:TYR:CG	2.47	0.49
1:C:1:MET:N	3:C:1369:HOH:O	2.01	0.49
1:D:26:VAL:HG23	1:D:50:ALA:HB2	1.94	0.49
1:C:352:ILE:HG22	1:C:354:LEU:HD21	1.94	0.49
1:B:93:LYS:HG3	1:B:94:ARG:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:C	1:A:189:ILE:HD13	2.33	0.49
1:D:242:PHE:CE2	1:D:275:VAL:HG13	2.48	0.49
1:C:111:ILE:HD12	1:C:121:VAL:HG11	1.94	0.49
1:D:255:LEU:C	1:D:257:ALA:N	2.65	0.49
1:A:105:LEU:O	1:A:105:LEU:HD12	2.13	0.49
1:A:243:THR:HG22	1:A:244:THR:H	1.78	0.49
1:D:128:ASP:HB2	3:D:1401:HOH:O	2.13	0.49
1:B:187:GLN:HE22	1:B:285:MET:HE2	1.77	0.49
1:C:31:VAL:HG13	1:C:66:ASP:HB2	1.93	0.49
1:C:211:THR:HG22	1:C:211:THR:O	2.12	0.49
1:B:184:LYS:HZ3	1:B:207:LEU:HD12	1.78	0.49
1:A:125:ILE:HD12	1:A:125:ILE:H	1.77	0.49
1:B:71:LEU:HD22	1:B:72:GLU:H	1.77	0.49
1:C:173:GLU:O	1:C:177:GLN:HB2	2.13	0.48
1:D:99:MET:CE	1:D:138:LEU:HD11	2.37	0.48
1:D:229:ALA:HA	1:D:233:CYS:SG	2.53	0.48
1:D:234:ASP:OD1	1:D:234:ASP:O	2.31	0.48
1:D:149:THR:CG2	1:D:309:ILE:HD13	2.43	0.48
1:B:77:TYR:O	1:B:78:GLY:O	2.31	0.48
1:D:251:LYS:HA	1:D:254:ARG:HB3	1.94	0.48
1:C:66:ASP:OD2	1:C:94:ARG:HG2	2.12	0.48
1:B:210:VAL:HG21	1:B:213:GLN:HE21	1.77	0.48
1:D:223:LEU:HD22	1:D:251:LYS:CE	2.32	0.48
1:A:150:LEU:HB2	1:A:308:ILE:HD12	1.96	0.48
1:C:180:GLN:NE2	1:C:183:ARG:HD2	2.29	0.48
1:B:258:PHE:N	1:B:258:PHE:CD1	2.81	0.48
1:D:140:PHE:HA	1:D:145:LEU:O	2.14	0.48
1:A:82:PRO:HG2	1:A:85:GLU:HB2	1.94	0.48
1:C:173:GLU:HA	3:C:1381:HOH:O	2.12	0.48
1:B:184:LYS:NZ	1:B:207:LEU:HD12	2.28	0.48
1:C:352:ILE:HD13	1:D:345:ILE:HD12	1.94	0.48
1:D:19:GLN:O	1:D:19:GLN:OE1	2.31	0.48
1:D:82:PRO:HG2	1:D:85:GLU:HB2	1.96	0.48
1:A:1:MET:HE2	1:A:4:TYR:HB3	1.96	0.48
1:C:190:LEU:HD22	1:C:217:VAL:CG1	2.43	0.48
1:D:22:SER:HA	1:D:285:MET:HE1	1.95	0.48
1:A:111:ILE:HG23	1:A:121:VAL:HG11	1.96	0.48
1:C:119:ILE:HD12	1:C:119:ILE:N	2.28	0.48
1:C:37:VAL:HG22	1:C:58:ALA:CA	2.38	0.48
1:B:125:ILE:HD12	1:B:125:ILE:N	2.20	0.48
1:A:88:ILE:HD13	1:A:119:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:HG12	1:B:355:THR:HB	1.95	0.48
1:D:255:LEU:O	1:D:257:ALA:N	2.47	0.48
1:A:222:VAL:HG13	1:A:222:VAL:O	2.13	0.48
1:C:31:VAL:CG1	3:C:1362:HOH:O	2.52	0.47
1:B:73:PRO:HA	3:B:1363:HOH:O	2.12	0.47
1:C:154:ALA:HB2	1:C:325:LEU:HD21	1.95	0.47
1:B:148:VAL:H	1:B:306:GLN:NE2	2.03	0.47
1:B:312:PHE:CE2	1:B:354:LEU:HD12	2.48	0.47
1:B:240:TRP:CD1	1:B:261:ASN:HB2	2.49	0.47
1:C:236:ILE:HG22	1:C:236:ILE:O	2.13	0.47
1:D:234:ASP:O	1:D:236:ILE:N	2.46	0.47
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.96	0.47
1:A:190:LEU:HD12	1:A:191:VAL:N	2.28	0.47
1:C:26:VAL:O	1:C:41:ALA:HA	2.15	0.47
1:D:200:ASN:ND2	1:D:230:LYS:CG	2.78	0.47
1:D:193:VAL:CG1	1:D:220:ASP:HA	2.45	0.47
1:D:23:ASN:OD1	1:D:45:TYR:CD1	2.67	0.47
3:C:1393:HOH:O	1:D:334:MET:CG	2.41	0.47
1:C:93:LYS:HZ2	1:C:93:LYS:HB3	1.80	0.47
1:B:106:VAL:HG22	1:B:109:ARG:HH21	1.79	0.47
1:D:151:LYS:HA	1:D:309:ILE:O	2.14	0.47
1:D:105:LEU:HD13	1:D:105:LEU:O	2.15	0.47
1:D:170:ILE:HG23	1:D:171:THR:H	1.80	0.47
1:D:190:LEU:CB	1:D:289:VAL:HG22	2.44	0.47
1:A:272:ILE:HD13	1:A:298:SER:HB3	1.97	0.47
1:B:93:LYS:HG3	1:B:94:ARG:HG3	1.97	0.47
1:C:150:LEU:HD23	1:C:289:VAL:HB	1.97	0.47
1:D:300:VAL:HG21	1:D:326:ILE:CD1	2.42	0.47
1:B:268:GLU:CD	1:B:268:GLU:H	2.16	0.47
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.76	0.47
1:C:97:VAL:O	1:C:123:GLU:HA	2.15	0.47
1:C:37:VAL:O	1:C:37:VAL:HG22	2.15	0.47
1:C:31:VAL:HG12	1:C:66:ASP:HB2	1.95	0.47
1:D:193:VAL:HG13	1:D:219:LEU:O	2.15	0.47
1:B:8:LEU:O	1:B:12:LEU:HD13	2.15	0.47
1:B:71:LEU:HD22	1:B:72:GLU:N	2.30	0.47
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.44	0.46
1:C:9:ALA:O	1:C:27:GLY:HA3	2.15	0.46
1:A:149:THR:OG1	1:A:186:HIS:HE1	1.98	0.46
1:C:105:LEU:H	1:C:105:LEU:CD2	2.23	0.46
1:B:258:PHE:N	1:B:258:PHE:HD1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TYR:C	1:B:184:LYS:N	2.69	0.46
1:B:126:LEU:HD12	1:B:126:LEU:N	2.31	0.46
1:B:97:VAL:O	1:B:123:GLU:HA	2.16	0.46
1:B:142:ARG:HG3	1:B:142:ARG:NH1	2.29	0.46
1:A:308:ILE:O	1:A:308:ILE:HG23	2.15	0.46
1:C:151:LYS:C	1:C:151:LYS:HD2	2.36	0.46
1:B:137:PHE:HD1	1:B:138:LEU:HD12	1.79	0.46
1:A:344:ASP:HB3	1:A:355:THR:CG2	2.39	0.46
1:C:42:HIS:HB3	3:C:1378:HOH:O	2.13	0.46
1:A:67:ILE:HG22	1:A:92:ILE:HG21	1.98	0.46
1:C:191:VAL:CG1	1:C:192:GLY:O	2.64	0.46
1:D:252:LYS:O	1:D:262:ILE:HD13	2.16	0.46
1:B:101:ASP:OD2	1:B:102:PRO:HD2	2.16	0.46
1:B:105:LEU:N	1:B:105:LEU:HD12	2.30	0.46
1:B:329:GLU:CB	3:B:1377:HOH:O	2.63	0.46
1:B:222:VAL:CG1	1:B:222:VAL:O	2.62	0.46
1:C:188:SER:O	1:C:189:ILE:HD13	2.16	0.46
1:B:102:PRO:O	1:B:104:PRO:HD3	2.16	0.46
1:A:212:LYS:N	3:A:1441:HOH:O	2.49	0.45
1:D:270:ILE:O	1:D:270:ILE:HG12	2.15	0.45
1:B:220:ASP:CG	1:B:223:LEU:HA	2.36	0.45
1:A:155:SER:HB3	1:A:317:ILE:CD1	2.45	0.45
1:C:37:VAL:CG2	1:C:58:ALA:HA	2.41	0.45
1:C:252:LYS:NZ	1:C:264:THR:OG1	2.46	0.45
1:D:196:VAL:HG11	1:D:225:ILE:HG12	1.99	0.45
1:B:31:VAL:O	1:B:65:ALA:HB1	2.17	0.45
1:D:236:ILE:O	1:D:237:ALA:HB2	2.16	0.45
1:C:342:PHE:CE2	1:D:352:ILE:HG12	2.51	0.45
1:D:226:PRO:C	1:D:228:ASP:H	2.19	0.45
1:D:358:PRO:O	1:D:359:THR:C	2.55	0.45
1:C:207:LEU:HA	1:C:208:PRO:HD3	1.82	0.45
1:A:207:LEU:N	1:A:210:VAL:HG11	2.32	0.45
1:C:150:LEU:CD2	1:C:289:VAL:HB	2.47	0.45
1:B:196:VAL:HG21	1:B:218:ILE:HD13	1.97	0.45
1:C:157:ASP:OD1	1:C:316:LEU:HA	2.17	0.45
1:A:211:THR:HG22	1:A:212:LYS:N	2.32	0.45
1:B:125:ILE:CG2	1:B:126:LEU:HD13	2.43	0.45
1:B:177:GLN:CG	3:B:1397:HOH:O	2.54	0.45
1:D:347:GLN:HG3	1:D:352:ILE:HD13	1.98	0.45
1:D:343:THR:HG21	1:D:357:LYS:HD2	1.99	0.45
1:B:223:LEU:HD22	1:B:247:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:HA	1:D:207:LEU:HD12	1.99	0.45
1:A:44:LYS:HZ2	1:C:35:GLN:HE22	1.64	0.45
1:B:272:ILE:O	1:B:275:VAL:CG2	2.64	0.45
1:A:207:LEU:H	1:A:210:VAL:HG11	1.82	0.45
1:A:88:ILE:CD1	1:A:114:MET:HA	2.38	0.45
1:D:193:VAL:HG13	1:D:220:ASP:HA	1.98	0.45
1:B:164:THR:O	1:B:164:THR:CG2	2.64	0.45
1:C:105:LEU:HG	1:C:106:VAL:H	1.82	0.45
1:C:181:GLN:CG	1:C:182:TYR:N	2.78	0.44
1:D:256:SER:HB2	1:D:262:ILE:HD13	1.98	0.44
1:A:22:SER:HA	1:A:285:MET:HE1	1.99	0.44
1:C:32:LYS:HD3	1:C:65:ALA:HB2	1.99	0.44
1:C:334:MET:HA	1:C:337:VAL:HG13	1.99	0.44
1:C:358:PRO:C	1:C:359:THR:HG23	2.37	0.44
1:D:177:GLN:HB3	1:D:177:GLN:HE21	1.61	0.44
1:B:181:GLN:O	1:B:184:LYS:HB3	2.17	0.44
1:A:350:ARG:NE	3:A:1376:HOH:O	2.47	0.44
1:B:243:THR:CG2	1:B:244:THR:H	2.21	0.44
1:D:71:LEU:HD22	1:D:72:GLU:H	1.83	0.44
1:D:226:PRO:C	1:D:228:ASP:N	2.70	0.44
1:A:8:LEU:HD11	1:A:39:MET:CE	2.47	0.44
1:C:223:LEU:CG	1:C:243:THR:HG21	2.47	0.44
1:A:222:VAL:CG1	1:A:222:VAL:O	2.65	0.44
1:A:347:GLN:HG2	1:A:352:ILE:HG12	2.00	0.44
1:C:17:GLU:O	1:C:19:GLN:HG3	2.18	0.44
1:B:298:SER:O	1:B:302:GLU:HG2	2.18	0.44
1:A:47:GLU:OE2	1:C:61:HIS:HE1	2.01	0.44
1:A:190:LEU:C	1:A:190:LEU:HD12	2.38	0.44
1:B:9:ALA:O	1:B:27:GLY:HA3	2.17	0.44
1:B:134:ASN:O	1:B:138:LEU:HD13	2.18	0.44
1:D:26:VAL:HG23	1:D:50:ALA:CB	2.48	0.44
1:B:311:TYR:CE1	1:B:353:LYS:HD2	2.53	0.44
1:B:206:ARG:HB2	1:B:206:ARG:NH1	2.32	0.44
1:D:252:LYS:HB2	1:D:252:LYS:NZ	2.32	0.44
1:C:25:LEU:H	1:C:134:ASN:HD21	1.66	0.44
1:C:136:LYS:HG2	1:C:147:TYR:CG	2.53	0.44
1:D:231:VAL:HB	1:D:239:THR:HG21	2.00	0.44
1:C:88:ILE:HG13	1:C:89:ASN:N	2.32	0.44
1:D:223:LEU:CD2	1:D:225:ILE:HG22	2.47	0.44
1:A:243:THR:CG2	1:A:247:ALA:HB2	2.43	0.44
1:C:23:ASN:HD21	1:C:46:GLY:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HB	1:B:92:ILE:HD13	1.99	0.44
1:A:188:SER:O	1:A:189:ILE:HD13	2.18	0.44
1:C:180:GLN:HE22	1:C:183:ARG:HD2	1.83	0.44
1:C:14:LYS:O	1:C:17:GLU:HB2	2.17	0.44
1:B:184:LYS:NZ	1:B:207:LEU:HB2	2.09	0.43
1:A:25:LEU:N	1:A:134:ASN:HD21	2.01	0.43
1:B:148:VAL:HG22	1:B:287:VAL:HG13	1.99	0.43
1:B:105:LEU:N	1:B:105:LEU:CD1	2.81	0.43
1:D:155:SER:HB3	1:D:317:ILE:HG13	2.00	0.43
1:B:233:CYS:O	1:B:235:GLN:N	2.51	0.43
1:B:164:THR:O	1:B:164:THR:HG23	2.18	0.43
1:D:95:VAL:HG23	1:D:119:ILE:HG21	1.99	0.43
1:D:22:SER:HA	1:D:285:MET:CE	2.48	0.43
1:B:268:GLU:CD	1:B:268:GLU:N	2.72	0.43
1:B:184:LYS:O	1:B:184:LYS:HG3	2.19	0.43
1:B:206:ARG:CZ	1:B:206:ARG:HB2	2.48	0.43
1:A:180:GLN:OE1	1:A:206:ARG:N	2.43	0.43
1:C:8:LEU:O	1:C:12:LEU:HD13	2.19	0.43
1:B:199:ASP:O	1:B:200:ASN:C	2.56	0.43
1:A:137:PHE:HD1	1:A:138:LEU:HD13	1.83	0.43
1:D:256:SER:HB2	1:D:262:ILE:CD1	2.49	0.43
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.18	0.43
1:A:53:HIS:HB3	1:C:57:MET:CE	2.48	0.43
1:A:213:GLN:NE2	1:A:214:PRO:HD2	2.33	0.43
1:D:350:ARG:NH1	3:D:1411:HOH:O	2.48	0.43
1:D:231:VAL:O	1:D:239:THR:HG21	2.19	0.43
1:B:205:CYS:HB3	1:B:213:GLN:HE22	1.83	0.43
1:C:95:VAL:HG12	1:C:121:VAL:HG22	1.99	0.43
1:D:190:LEU:HD11	1:D:219:LEU:HG	2.00	0.43
1:B:43:LEU:HD22	1:B:43:LEU:N	2.34	0.43
1:A:35:GLN:OE1	1:C:44:LYS:NZ	2.43	0.43
1:A:223:LEU:HB2	1:A:243:THR:HG21	2.00	0.43
1:D:174:ALA:O	1:D:177:GLN:HB3	2.18	0.43
1:A:76:HIS:O	1:A:82:PRO:HB3	2.19	0.42
1:C:148:VAL:HB	1:C:305:PHE:HA	2.00	0.42
1:A:292:GLY:CA	3:A:1377:HOH:O	2.67	0.42
1:A:6:MET:O	1:A:9:ALA:HB3	2.19	0.42
1:D:9:ALA:HA	1:D:12:LEU:HD12	2.01	0.42
1:C:7:LYS:HD2	1:C:7:LYS:HA	1.84	0.42
1:B:182:TYR:C	1:B:184:LYS:H	2.21	0.42
1:D:230:LYS:C	1:D:232:ILE:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TYR:OH	1:A:353:LYS:HE2	2.19	0.42
1:D:170:ILE:CG2	1:D:171:THR:N	2.80	0.42
1:B:250:GLU:O	1:B:254:ARG:HB2	2.20	0.42
1:C:10:LEU:O	1:C:13:ALA:HB3	2.19	0.42
1:D:237:ALA:HB1	1:D:238:PRO:CD	2.49	0.42
1:B:232:ILE:HD12	1:B:255:LEU:HD22	2.01	0.42
1:A:53:HIS:HB3	1:C:57:MET:HE3	2.02	0.42
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.79	0.42
1:D:181:GLN:CG	1:D:182:TYR:N	2.82	0.42
1:C:151:LYS:HD2	1:C:152:ALA:N	2.33	0.42
1:B:162:THR:C	1:B:164:THR:H	2.22	0.42
1:D:51:GLU:O	1:D:55:ILE:HG13	2.20	0.42
1:D:309:ILE:HD12	1:D:309:ILE:N	2.35	0.42
1:A:106:VAL:O	1:A:109:ARG:HB2	2.19	0.42
1:B:296:HIS:HB3	1:B:326:ILE:CD1	2.50	0.42
1:A:36:ILE:CD1	1:C:15:GLN:HG3	2.50	0.42
1:B:178:ASP:O	1:B:181:GLN:HG2	2.20	0.42
1:A:95:VAL:HG23	1:A:119:ILE:CG2	2.50	0.42
1:C:72:GLU:HA	1:C:73:PRO:HD3	1.92	0.42
1:A:168:LYS:O	1:B:334:MET:HG3	2.20	0.42
1:D:225:ILE:C	1:D:225:ILE:HD13	2.40	0.41
1:B:111:ILE:HD12	1:B:123:GLU:OE1	2.20	0.41
1:B:103:ASN:C	1:B:105:LEU:H	2.23	0.41
1:B:329:GLU:HB3	3:B:1377:HOH:O	2.20	0.41
1:C:253:LYS:HE3	1:C:253:LYS:HB2	1.91	0.41
1:B:28:ALA:HA	1:B:68:TYR:O	2.20	0.41
1:D:222:VAL:O	1:D:223:LEU:C	2.59	0.41
1:C:205:CYS:HB3	1:C:210:VAL:HG11	2.01	0.41
1:B:205:CYS:O	1:B:210:VAL:HG11	2.21	0.41
1:B:223:LEU:HB2	1:B:243:THR:HG21	2.03	0.41
1:A:44:LYS:HZ3	1:C:35:GLN:NE2	2.17	0.41
1:C:75:SER:HA	1:C:82:PRO:HB3	2.02	0.41
1:B:200:ASN:N	1:B:201:PRO:CD	2.84	0.41
1:A:317:ILE:HG22	1:A:318:GLY:O	2.21	0.41
1:D:154:ALA:HB2	1:D:160:ILE:HD13	2.03	0.41
1:C:327:SER:HB3	1:C:328:GLY:H	1.63	0.41
1:B:171:THR:OG1	1:B:175:ALA:HB3	2.21	0.41
1:D:208:PRO:O	1:D:209:ASN:CB	2.67	0.41
1:D:29:VAL:HA	1:D:38:GLY:O	2.20	0.41
1:A:103:ASN:HA	1:A:104:PRO:HD3	1.91	0.41
1:D:136:LYS:HE3	1:D:185:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:O	1:C:37:VAL:CG2	2.69	0.41
1:B:190:LEU:HA	1:B:217:VAL:O	2.20	0.41
1:C:76:HIS:C	1:C:82:PRO:HG3	2.41	0.41
1:B:103:ASN:O	1:B:105:LEU:N	2.53	0.41
1:B:65:ALA:O	1:B:92:ILE:HG23	2.20	0.41
1:B:12:LEU:CD2	1:B:39:MET:HB3	2.51	0.41
1:D:263:PHE:N	1:D:263:PHE:CD1	2.88	0.41
1:D:210:VAL:O	1:D:210:VAL:HG23	2.20	0.41
1:B:253:LYS:HE2	1:B:253:LYS:HB3	1.90	0.41
1:C:276:LEU:HD23	1:C:276:LEU:HA	1.91	0.41
1:C:128:ASP:O	1:C:131:GLU:HB3	2.21	0.41
1:D:230:LYS:C	1:D:232:ILE:H	2.24	0.41
1:C:42:HIS:CA	3:C:1378:HOH:O	2.69	0.41
1:D:122:ARG:NH1	3:D:1365:HOH:O	2.53	0.41
1:D:143:THR:C	1:D:145:LEU:N	2.74	0.41
1:D:2:GLU:H	1:D:2:GLU:HG2	1.53	0.41
1:C:169:TRP:HZ3	1:D:335:LYS:N	2.19	0.40
1:A:29:VAL:HG23	1:A:29:VAL:O	2.20	0.40
1:C:326:ILE:HG12	1:D:157:ASP:HB2	2.03	0.40
1:A:312:PHE:CE2	1:A:354:LEU:HD12	2.54	0.40
1:A:1:MET:HE2	1:A:4:TYR:CB	2.52	0.40
1:D:201:PRO:C	1:D:203:LEU:HD22	2.42	0.40
1:B:161:ALA:HB3	1:B:323:PRO:HG3	2.02	0.40
1:A:1:MET:HA	1:A:1:MET:CE	2.51	0.40
1:D:176:ARG:HB3	1:D:176:ARG:HE	1.63	0.40
1:D:245:ALA:C	1:D:247:ALA:N	2.73	0.40
1:C:37:VAL:HG23	3:C:1372:HOH:O	2.20	0.40
1:A:125:ILE:CD1	1:A:125:ILE:H	2.34	0.40
1:A:345:ILE:HG23	1:A:354:LEU:HD23	2.02	0.40
1:C:29:VAL:HG22	1:C:29:VAL:O	2.20	0.40
1:C:90:SER:HG	1:C:92:ILE:HG12	1.87	0.40
1:B:314:PRO:HD3	1:B:351:ASP:OD2	2.22	0.40
1:C:16:GLY:O	1:C:17:GLU:C	2.60	0.40
1:A:200:ASN:N	1:A:201:PRO:CD	2.84	0.40
1:B:244:THR:HB	3:B:1404:HOH:O	2.20	0.40
1:C:223:LEU:HA	1:C:223:LEU:HD23	1.89	0.40
1:C:314:PRO:HG3	1:D:342:PHE:CD2	2.57	0.40
1:C:184:LYS:NZ	1:C:184:LYS:CB	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	336 (94%)	19 (5%)	2 (1%)	30 41
1	B	357/373 (96%)	320 (90%)	28 (8%)	9 (2%)	7 6
1	C	357/373 (96%)	332 (93%)	21 (6%)	4 (1%)	17 24
1	D	358/373 (96%)	310 (87%)	35 (10%)	13 (4%)	4 3
All	All	1429/1492 (96%)	1298 (91%)	103 (7%)	28 (2%)	9 10

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
1	B	78	GLY
1	B	168	LYS
1	B	234	ASP
1	B	235	GLN
1	C	212	LYS
1	D	235	GLN
1	D	246	ARG
1	B	208	PRO
1	B	212	LYS
1	C	170	ILE
1	D	231	VAL
1	D	329	GLU
1	A	211	THR
1	B	209	ASN
1	C	17	GLU
1	D	259	GLY
1	D	282	GLU
1	B	107	ALA
1	D	209	ASN
1	D	212	LYS
1	D	256	SER

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Mol	Chain	Res	Type
1	C	208	PRO
1	D	221	THR
1	D	245	ALA
1	D	18	GLY
1	D	262	ILE
1	B	104	PRO

5.3.2 Protein sidechains (i)

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%)	274 (94%)	19 (6%)	21	32
1	B	293/305 (96%)	272 (93%)	21 (7%)	18	27
1	C	293/305 (96%)	268 (92%)	25 (8%)	13	19
1	D	294/305 (96%)	269 (92%)	25 (8%)	13	19
All	All	1173/1220 (96%)	1083 (92%)	90 (8%)	16	24

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	25	LEU
1	A	69	VAL
1	A	71	LEU
1	A	86	LEU
1	A	138	LEU
1	A	171	THR
1	A	190	LEU
1	A	193	VAL
1	A	223	LEU
1	A	243	THR
1	A	267	THR
1	A	281	GLU
1	A	337	VAL
1	A	340	LEU

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Mol	Chain	Res	Type
1	A	343	THR
1	A	347	GLN
1	A	350	ARG
1	A	355	THR
1	B	25	LEU
1	B	80	THR
1	B	103	ASN
1	B	116	GLU
1	B	128	ASP
1	B	151	LYS
1	B	164	THR
1	B	176	ARG
1	B	184	LYS
1	B	212	LYS
1	B	225	ILE
1	B	228	ASP
1	B	234	ASP
1	B	248	ASP
1	B	258	PHE
1	B	287	VAL
1	B	308	ILE
1	B	320	THR
1	B	324	SER
1	B	343	THR
1	B	355	THR
1	C	3	GLU
1	C	8	LEU
1	C	15	GLN
1	C	25	LEU
1	C	63	GLU
1	C	76	HIS
1	C	105	LEU
1	C	128	ASP
1	C	129	GLN
1	C	151	LYS
1	C	190	LEU
1	C	193	VAL
1	C	209	ASN
1	C	222	VAL
1	C	223	LEU
1	C	235	GLN
1	C	243	THR

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Mol	Chain	Res	Type
1	C	271	GLN
1	C	287	VAL
1	C	308	ILE
1	C	327	SER
1	C	337	VAL
1	C	354	LEU
1	C	355	THR
1	C	359	THR
1	D	2	GLU
1	D	19	GLN
1	D	25	LEU
1	D	29	VAL
1	D	69	VAL
1	D	71	LEU
1	D	86	LEU
1	D	122	ARG
1	D	138	LEU
1	D	177	GLN
1	D	181	GLN
1	D	190	LEU
1	D	191	VAL
1	D	199	ASP
1	D	207	LEU
1	D	221	THR
1	D	223	LEU
1	D	225	ILE
1	D	228	ASP
1	D	243	THR
1	D	251	LYS
1	D	266	GLU
1	D	270	ILE
1	D	301	LYS
1	D	355	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	42	HIS
1	A	53	HIS
1	A	134	ASN
1	A	139	HIS

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Mol	Chain	Res	Type
1	A	186	HIS
1	A	209	ASN
1	A	213	GLN
1	A	235	GLN
1	A	296	HIS
1	A	341	GLN
1	B	23	ASN
1	B	42	HIS
1	B	103	ASN
1	B	134	ASN
1	B	186	HIS
1	B	271	GLN
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	42	HIS
1	C	53	HIS
1	C	56	HIS
1	C	61	HIS
1	C	89	ASN
1	C	180	GLN
1	C	186	HIS
1	C	209	ASN
1	C	271	GLN
1	C	332	GLN
1	C	341	GLN
1	D	53	HIS
1	D	89	ASN
1	D	134	ASN
1	D	177	GLN
1	D	180	GLN
1	D	186	HIS
1	D	213	GLN
1	D	306	GLN
1	D	347	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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%)	-0.06	2 (0%)	90	90	18, 36, 57, 71	0
1	B	359/373 (96%)	0.17	11 (3%)	52	51	22, 45, 72, 95	0
1	C	359/373 (96%)	0.19	9 (2%)	61	60	25, 45, 69, 93	0
1	D	360/373 (96%)	0.37	27 (7%)	17	16	25, 50, 92, 99	0
All	All	1437/1492 (96%)	0.17	49 (3%)	49	48	18, 43, 80, 99	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	PRO	5.6
1	D	207	LEU	5.4
1	D	222	VAL	5.3
1	B	208	PRO	4.9
1	D	262	ILE	4.5
1	C	208	PRO	4.4
1	D	255	LEU	4.2
1	D	209	ASN	4.2
1	C	209	ASN	4.0
1	D	242	PHE	3.9
1	B	81	PRO	3.8
1	B	77	TYR	3.4
1	D	223	LEU	3.3
1	C	169	TRP	3.2
1	D	279	LEU	3.2
1	D	243	THR	3.1
1	C	78	GLY	2.9
1	D	266	GLU	2.9
1	D	260	VAL	2.8
1	D	258	PHE	2.7
1	C	207	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	2.7
1	D	233	CYS	2.6
1	B	79	LYS	2.6
1	B	209	ASN	2.6
1	B	80	THR	2.6
1	D	218	ILE	2.5
1	B	258	PHE	2.5
1	D	246	ARG	2.5
1	D	278	ILE	2.5
1	C	86	LEU	2.5
1	C	125	ILE	2.5
1	D	225	ILE	2.5
1	C	291	GLY	2.5
1	B	169	TRP	2.5
1	D	19	GLN	2.5
1	D	176	ARG	2.3
1	D	265	LEU	2.3
1	D	263	PHE	2.3
1	B	207	LEU	2.3
1	A	208	PRO	2.3
1	A	132	ARG	2.3
1	D	169	TRP	2.3
1	B	104	PRO	2.3
1	D	227	GLU	2.1
1	C	76	HIS	2.1
1	D	244	THR	2.1
1	D	329	GLU	2.1
1	D	189	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	1360	1/1	0.99	0.15	-	31,31,31,31	0
2	ZN	D	1360	1/1	0.99	0.18	-	41,41,41,41	0
2	ZN	B	1360	1/1	0.99	0.09	-	44,44,44,44	0
2	ZN	C	1360	1/1	0.94	0.09	-	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.