



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:17 AM GMT

PDB ID : 1XQS  
Title : Crystal structure of the HspBP1 core domain complexed with the fragment of Hsp70 ATPase domain  
Authors : Shomura, Y.; Dragovic, Z.; Chang, H.C.; Tzvetkov, N.; Young, J.C.; Brodsky, J.L.; Guerriero, V.; Hartl, F.U.; Bracher, A.  
Deposited on : 2004-10-13  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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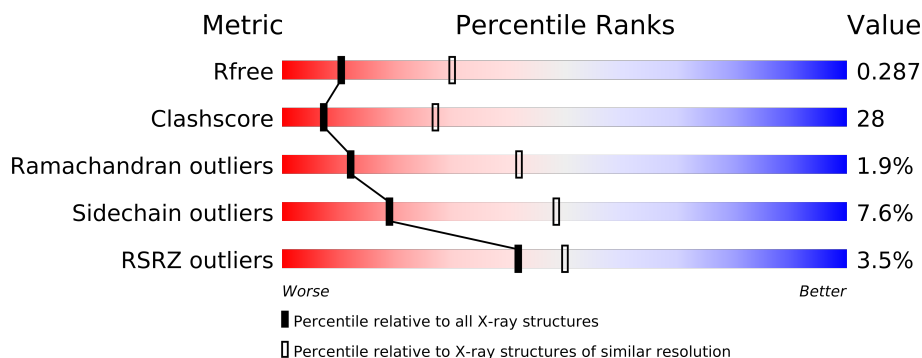
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	280	
1	B	280	
2	C	191	
2	D	191	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6795 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 HSPBP1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1278	368	380	20			
1	B	264	Total	C	N	O	S	0	0	0
			2022	1265	362	375	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLY	-	CLONING ARTIFACT	UNP Q9NZL4
A	81	SER	-	CLONING ARTIFACT	UNP Q9NZL4
A	82	HIS	-	CLONING ARTIFACT	UNP Q9NZL4
A	83	MET	-	CLONING ARTIFACT	UNP Q9NZL4
A	88	GLY	GLU	ENGINEERED	UNP Q9NZL4
B	80	GLY	-	CLONING ARTIFACT	UNP Q9NZL4
B	81	SER	-	CLONING ARTIFACT	UNP Q9NZL4
B	82	HIS	-	CLONING ARTIFACT	UNP Q9NZL4
B	83	MET	-	CLONING ARTIFACT	UNP Q9NZL4
B	88	GLY	GLU	ENGINEERED	UNP Q9NZL4

- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	165	Total	C	N	O	S	0	0	0
			1316	825	237	252	2			
2	D	165	Total	C	N	O	S	0	0	0
			1316	825	237	252	2			

There are 6 discrepancies between the modelled and reference sequences:

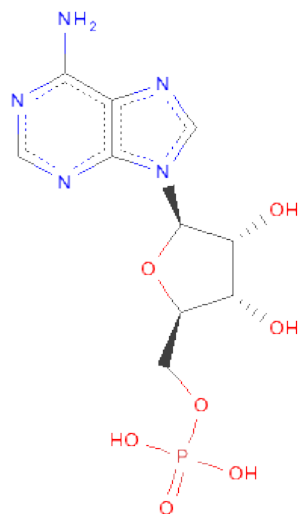
Chain	Residue	Modelled	Actual	Comment	Reference
C	181	GLY	-	CLONING ARTIFACT	UNP P08107
C	182	ALA	-	CLONING ARTIFACT	UNP P08107

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Chain	Residue	Modelled	Actual	Comment	Reference
C	183	MET	-	CLONING ARTIFACT	UNP P08107
D	181	GLY	-	CLONING ARTIFACT	UNP P08107
D	182	ALA	-	CLONING ARTIFACT	UNP P08107
D	183	MET	-	CLONING ARTIFACT	UNP P08107

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

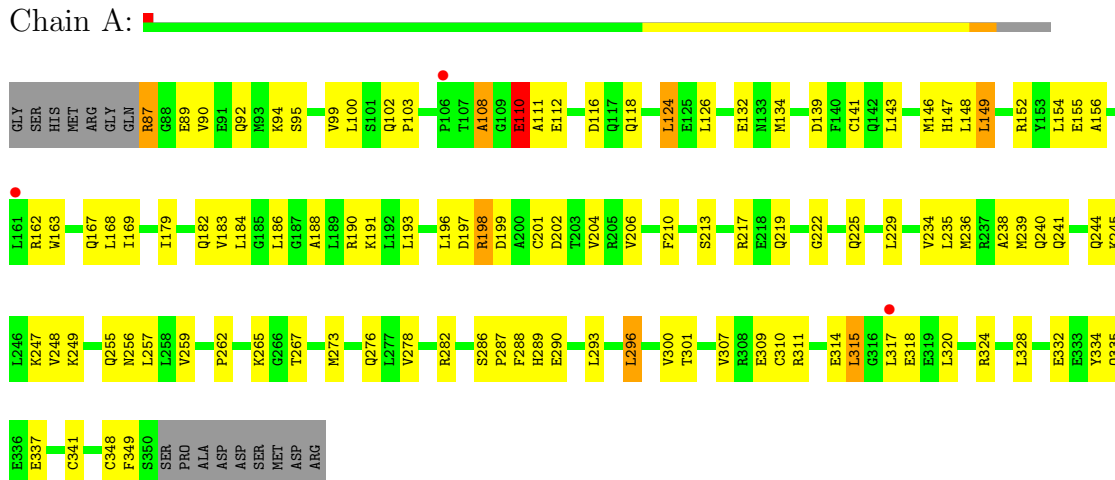
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	6	Total	O	0	0
			6	6		
4	C	18	Total	O	0	0
			18	18		
4	D	7	Total	O	0	0
			7	7		

### 3 Residue-property plots

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

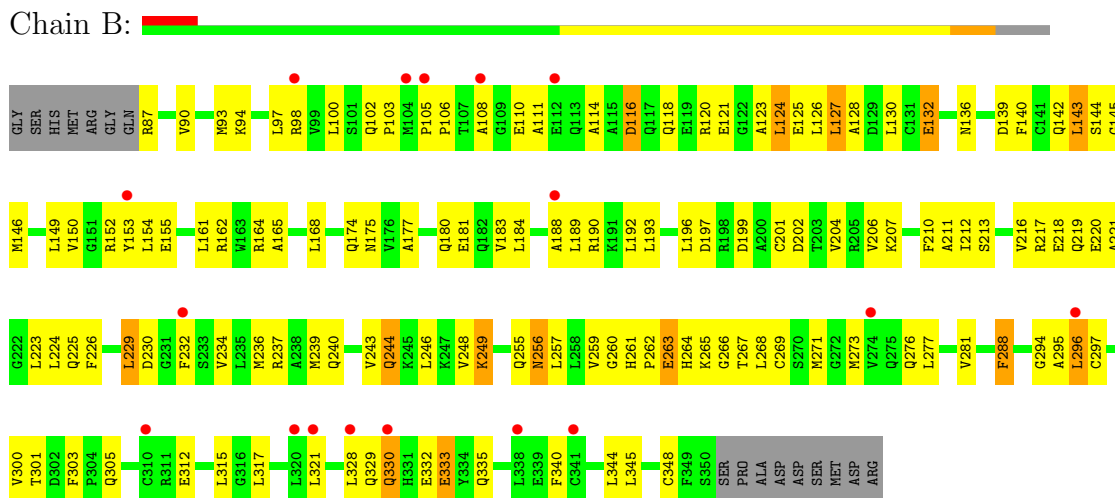
#### • Molecule 1: HSPBP1 protein

Chain A:



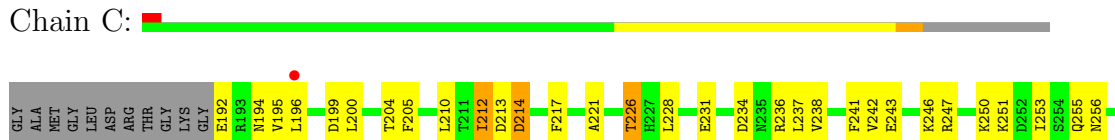
#### • Molecule 1: HSPBP1 protein

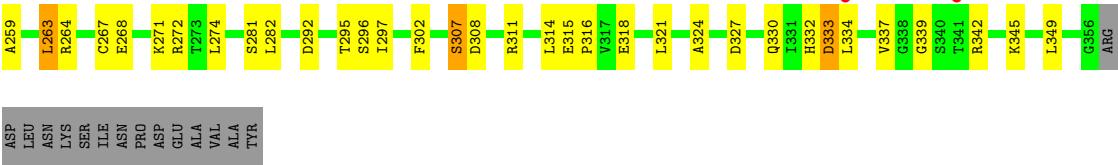
Chain B:



#### • Molecule 2: Heat shock 70 kDa protein 1

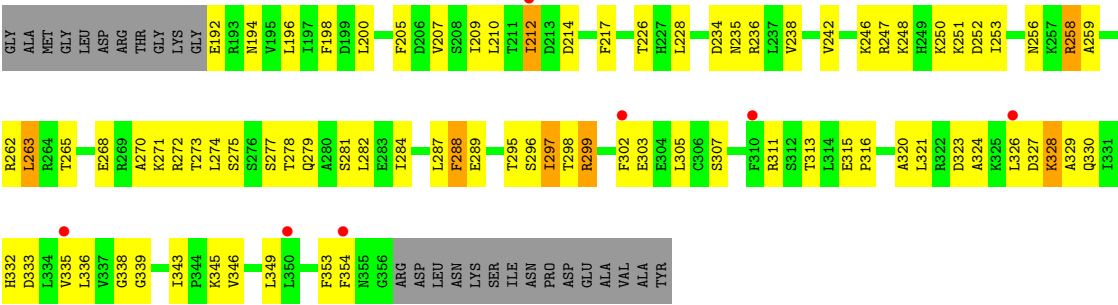
Chain C:





● Molecule 2: Heat shock 70 kDa protein 1

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.48Å 94.81Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 2.90 46.55 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.60-2.90) 99.7 (46.55-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.237 , 0.296 0.240 , 0.287	Depositor DCC
$R_{free}$ test set	1258 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.1	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 24763 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: AMP

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	0.41	0/2073	0.63	0/2793
1	B	0.35	0/2049	0.59	0/2765
2	C	0.43	0/1334	0.62	0/1790
2	D	0.40	0/1334	0.64	0/1790
All	All	0.39	0/6790	0.62	0/9138

There are no bond length outliers.

There are no bond angle outliers.

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	2046	0	2057	99	0
1	B	2022	0	2018	156	0
2	C	1316	0	1321	64	0
2	D	1316	0	1321	76	0
3	C	23	0	12	1	0
3	D	23	0	12	3	0
4	A	18	0	0	0	0
4	B	6	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	18	0	0	1	0
4	D	7	0	0	2	0
All	All	6795	0	6741	376	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (376) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:VAL:HG12	1:A:288:PHE:CG	1.85	1.11
1:A:273:MET:CE	1:A:276:GLN:HB3	1.80	1.11
1:B:94:LYS:HG2	1:B:143:LEU:HD21	1.32	1.08
1:A:103:PRO:HA	1:A:152:ARG:HH22	1.15	1.05
1:A:100:LEU:HD21	1:A:124:LEU:HD13	1.46	0.97
1:A:273:MET:HE2	1:A:276:GLN:HB3	1.45	0.96
2:C:194:ASN:H	2:C:332:HIS:HD2	1.13	0.95
1:B:94:LYS:HG2	1:B:143:LEU:CD2	2.01	0.90
1:A:248:VAL:HG12	1:A:288:PHE:CD2	2.06	0.90
1:B:100:LEU:HD21	1:B:124:LEU:HD13	1.52	0.89
2:C:194:ASN:H	2:C:332:HIS:CD2	1.91	0.88
1:A:103:PRO:HA	1:A:152:ARG:NH2	1.89	0.86
1:B:239:MET:HE2	1:B:273:MET:CE	2.05	0.86
1:A:273:MET:CE	1:A:276:GLN:CB	2.55	0.83
2:C:295:THR:HG22	2:C:296:SER:N	1.93	0.83
1:B:236:MET:HE2	1:B:273:MET:HB2	1.59	0.82
2:C:342:ARG:HD2	3:C:401:AMP:N6	1.94	0.82
1:A:248:VAL:HG12	1:A:288:PHE:CB	2.10	0.81
1:A:262:PRO:HB3	1:A:265:LYS:HE3	1.61	0.81
1:B:262:PRO:HB3	1:B:265:LYS:HE3	1.63	0.81
1:B:90:VAL:O	1:B:94:LYS:HG3	1.80	0.80
1:A:179:ILE:O	1:A:183:VAL:HG23	1.81	0.79
1:B:123:ALA:O	1:B:127:LEU:HB2	1.81	0.79
1:B:239:MET:HE1	1:B:273:MET:SD	2.23	0.78
1:B:301:THR:HA	4:B:521:HOH:O	1.83	0.78
1:B:97:LEU:HD12	1:B:143:LEU:HD22	1.66	0.78
1:A:154:LEU:HD13	1:A:169:ILE:CD1	2.14	0.78
1:B:100:LEU:HG	1:B:153:TYR:CZ	2.19	0.77
1:B:255:GLN:O	1:B:259:VAL:HG23	1.84	0.77
2:D:194:ASN:H	2:D:332:HIS:CD2	2.03	0.77
2:D:315:GLU:HB3	2:D:316:PRO:HD3	1.65	0.77
2:C:238:VAL:O	2:C:242:VAL:HG23	1.83	0.77
2:D:258:ARG:NH1	2:D:262:ARG:HD2	2.00	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:220:GLU:O	1:B:224:LEU:HD13	1.86	0.76
2:D:295:THR:HG22	2:D:296:SER:H	1.51	0.76
2:D:194:ASN:H	2:D:332:HIS:HD2	1.31	0.76
2:D:256:ASN:HD22	2:D:259:ALA:HB2	1.51	0.76
1:A:273:MET:HE1	1:A:276:GLN:HG2	1.69	0.75
2:C:295:THR:HG22	2:C:296:SER:H	1.51	0.75
1:A:100:LEU:HD21	1:A:124:LEU:CD1	2.17	0.74
1:A:273:MET:HE1	1:A:276:GLN:CG	2.17	0.74
2:C:307:SER:HB2	2:C:311:ARG:HH12	1.51	0.74
1:B:239:MET:CE	1:B:273:MET:SD	2.76	0.74
2:C:315:GLU:HB3	2:C:316:PRO:HD3	1.68	0.73
1:A:92:GLN:O	1:A:95:SER:HB3	1.89	0.73
1:B:219:GLN:NE2	1:B:221:ALA:HB3	2.03	0.73
1:B:140:PHE:HE2	1:B:146:MET:HE2	1.53	0.73
1:B:193:LEU:HD21	1:B:226:PHE:HE1	1.54	0.73
1:B:344:LEU:O	1:B:348:CYS:HB2	1.88	0.72
1:B:236:MET:HG3	1:B:273:MET:HE1	1.70	0.72
1:B:256:ASN:ND2	1:B:256:ASN:O	2.23	0.72
1:A:273:MET:HA	1:A:273:MET:HE3	1.72	0.72
1:B:177:ALA:O	1:B:181:GLU:HG3	1.90	0.72
1:B:90:VAL:HG13	1:B:94:LYS:HE3	1.73	0.71
1:B:312:GLU:HB2	1:B:315:LEU:HD13	1.72	0.70
1:B:240:GLN:HG2	1:B:276:GLN:OE1	1.90	0.70
2:C:255:GLN:HE21	2:D:323:ASP:HB3	1.56	0.70
1:B:332:GLU:HB3	1:B:335:GLN:HE21	1.56	0.70
2:D:198:PHE:HB3	2:D:336:LEU:HD23	1.72	0.70
1:A:236:MET:O	1:A:240:GLN:HG3	1.92	0.70
1:A:262:PRO:O	1:A:265:LYS:HG3	1.91	0.70
1:A:154:LEU:HD13	1:A:169:ILE:HD12	1.74	0.69
2:D:313:THR:O	2:D:316:PRO:HD2	1.93	0.69
2:C:345:LYS:O	2:C:349:LEU:HD23	1.93	0.69
1:A:273:MET:CE	1:A:273:MET:HA	2.23	0.69
1:A:307:VAL:O	1:A:311:ARG:HG3	1.93	0.69
2:D:295:THR:HG22	2:D:296:SER:N	2.07	0.68
2:D:238:VAL:HG13	2:D:263:LEU:HD13	1.75	0.68
1:B:94:LYS:CG	1:B:143:LEU:HD21	2.17	0.67
1:A:154:LEU:CD1	1:A:169:ILE:HD12	2.23	0.67
2:C:271:LYS:HG3	2:C:302:PHE:CZ	2.30	0.66
1:A:99:VAL:O	1:A:102:GLN:HG2	1.96	0.65
2:D:345:LYS:O	2:D:349:LEU:HD23	1.95	0.65
2:C:237:LEU:HD22	2:C:297:ILE:CD1	2.27	0.65
1:B:236:MET:CE	1:B:273:MET:HB2	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:295:THR:CG2	2:C:296:SER:N	2.60	0.65
1:B:217:ARG:HH21	2:D:281:SER:CB	2.09	0.64
1:A:193:LEU:HD22	1:A:234:VAL:HG21	1.79	0.64
2:C:237:LEU:CD2	2:C:297:ILE:CD1	2.75	0.64
1:A:87:ARG:N	1:A:87:ARG:HD2	2.12	0.64
1:B:207:LYS:O	1:B:210:PHE:HB3	1.96	0.64
2:D:234:ASP:OD2	2:D:271:LYS:HD3	1.97	0.64
2:D:212:ILE:C	2:D:212:ILE:HD13	2.18	0.64
1:B:142:GLN:C	1:B:144:SER:H	2.02	0.64
1:B:248:VAL:HB	1:B:288:PHE:HB2	1.80	0.63
2:C:295:THR:CG2	2:C:296:SER:H	2.11	0.63
1:B:146:MET:CE	1:B:146:MET:HA	2.28	0.63
1:A:134:MET:HG3	4:C:511:HOH:O	1.97	0.63
1:B:128:ALA:HA	1:B:168:LEU:HD13	1.81	0.63
1:A:134:MET:SD	2:C:268:GLU:OE1	2.57	0.62
2:C:241:PHE:CE1	2:C:295:THR:HG21	2.34	0.62
1:B:329:GLN:HA	1:B:329:GLN:OE1	1.99	0.62
2:C:327:ASP:H	2:C:330:GLN:NE2	1.97	0.62
1:B:232:PHE:CD1	1:B:268:LEU:HD21	2.34	0.62
1:A:310:CYS:HB3	1:A:317:LEU:HD23	1.82	0.62
2:C:255:GLN:HA	2:C:255:GLN:OE1	2.00	0.62
2:D:272:ARG:HG3	3:D:402:AMP:C6	2.35	0.62
2:C:327:ASP:HB3	2:C:330:GLN:HE21	1.65	0.61
1:B:243:VAL:HG12	1:B:246:LEU:H	1.65	0.61
2:D:238:VAL:O	2:D:242:VAL:HG23	2.00	0.61
1:A:154:LEU:O	1:A:162:ARG:HG2	2.00	0.61
1:B:175:ASN:HB3	2:D:273:THR:OG1	2.00	0.61
2:C:221:ALA:HB2	2:C:324:ALA:HB2	1.83	0.61
2:D:256:ASN:HD22	2:D:259:ALA:CB	2.14	0.60
2:C:237:LEU:CD2	2:C:297:ILE:HD13	2.32	0.60
2:D:252:ASP:HB2	4:D:529:HOH:O	2.02	0.60
1:B:294:GLY:HA2	1:B:340:PHE:CD1	2.37	0.60
2:D:209:ILE:CD1	2:D:321:LEU:HD23	2.32	0.60
1:A:154:LEU:HD13	1:A:169:ILE:HD11	1.84	0.59
1:A:248:VAL:CG1	1:A:288:PHE:CD2	2.85	0.59
2:C:241:PHE:HE1	2:C:295:THR:HG21	1.67	0.59
2:D:256:ASN:ND2	2:D:259:ALA:H	1.99	0.59
1:A:248:VAL:HG12	1:A:288:PHE:HB3	1.85	0.59
1:A:318:GLU:HB2	1:A:349:PHE:CE2	2.38	0.59
1:B:239:MET:HE2	1:B:273:MET:HE3	1.83	0.59
1:B:146:MET:O	1:B:150:VAL:HG23	2.03	0.58
1:B:116:ASP:O	1:B:120:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:221:ALA:CB	2:C:324:ALA:HB2	2.33	0.58
1:B:236:MET:O	1:B:240:GLN:HG3	2.03	0.58
2:D:209:ILE:HD11	2:D:321:LEU:HD23	1.85	0.58
2:C:250:LYS:O	2:C:251:LYS:HG3	2.04	0.58
2:D:353:PHE:HD2	2:D:354:PHE:CE1	2.22	0.57
1:A:236:MET:HG3	1:A:273:MET:CE	2.34	0.57
1:B:262:PRO:CB	1:B:265:LYS:HE3	2.33	0.57
2:C:315:GLU:CB	2:C:316:PRO:HD3	2.34	0.57
2:C:195:VAL:HG22	2:C:333:ASP:HB2	1.86	0.57
1:A:273:MET:CE	1:A:276:GLN:CG	2.83	0.57
2:C:199:ASP:HA	2:C:337:VAL:O	2.05	0.57
1:B:162:ARG:HD2	1:B:199:ASP:OD2	2.05	0.57
2:D:192:GLU:OE2	2:D:192:GLU:HA	2.05	0.57
1:B:193:LEU:HD21	1:B:226:PHE:CE1	2.36	0.57
1:A:210:PHE:HB2	1:A:249:LYS:HE3	1.86	0.56
1:B:87:ARG:HG3	1:B:90:VAL:HG23	1.87	0.56
1:B:256:ASN:C	1:B:256:ASN:HD22	2.01	0.56
1:A:108:ALA:HB1	1:A:112:GLU:CD	2.25	0.56
2:D:270:ALA:O	2:D:274:LEU:HD13	2.05	0.56
2:D:246:LYS:O	2:D:250:LYS:HA	2.05	0.56
1:B:218:GLU:OE1	2:D:277:SER:HB3	2.05	0.56
1:B:244:GLN:O	1:B:248:VAL:HG13	2.05	0.56
1:B:317:LEU:HG	1:B:321:LEU:HD11	1.87	0.56
2:C:212:ILE:HD13	2:C:212:ILE:C	2.25	0.56
1:B:300:VAL:HG12	4:B:521:HOH:O	2.05	0.55
1:B:273:MET:O	1:B:277:LEU:HG	2.07	0.55
1:A:217:ARG:HG2	1:A:256:ASN:OD1	2.06	0.55
1:A:188:ALA:O	1:A:191:LYS:N	2.39	0.55
1:A:241:GLN:O	1:A:247:LYS:NZ	2.38	0.55
2:C:200:LEU:HD13	2:C:205:PHE:CD1	2.41	0.55
2:D:287:LEU:O	2:D:288:PHE:HB2	2.07	0.55
2:D:251:LYS:HE3	2:D:289:GLU:OE2	2.07	0.54
1:B:312:GLU:CB	1:B:315:LEU:HD13	2.37	0.54
1:B:118:GLN:O	1:B:121:GLU:HB2	2.06	0.54
1:A:236:MET:HE2	1:A:273:MET:SD	2.48	0.54
2:C:236:ARG:NH2	2:C:308:ASP:OD2	2.41	0.54
1:A:248:VAL:HG23	1:A:249:LYS:N	2.23	0.54
1:B:153:TYR:O	1:B:155:GLU:N	2.40	0.54
2:D:274:LEU:O	2:D:299:ARG:NE	2.41	0.54
1:A:273:MET:HE3	1:A:276:GLN:HB3	1.81	0.54
1:B:330:GLN:O	1:B:330:GLN:HG2	2.07	0.54
1:B:102:GLN:HA	1:B:102:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:LEU:O	1:B:344:LEU:HD21	2.08	0.54
2:D:327:ASP:HB3	2:D:330:GLN:NE2	2.22	0.54
1:B:110:GLU:O	1:B:114:ALA:HB2	2.09	0.53
1:A:282:ARG:HG2	1:A:320:LEU:HD11	1.91	0.53
2:D:315:GLU:CB	2:D:316:PRO:HD3	2.34	0.53
2:C:196:LEU:HB3	2:C:334:LEU:HD23	1.90	0.53
2:C:237:LEU:HD22	2:C:297:ILE:HD13	1.88	0.53
1:B:243:VAL:HG11	1:B:246:LEU:HG	1.90	0.53
1:B:100:LEU:HG	1:B:153:TYR:OH	2.09	0.53
1:A:162:ARG:NH1	1:A:199:ASP:OD2	2.42	0.53
2:D:209:ILE:HD12	2:D:320:ALA:O	2.08	0.53
1:B:90:VAL:CG1	1:B:94:LYS:HE3	2.39	0.53
1:B:256:ASN:C	1:B:256:ASN:ND2	2.60	0.53
2:D:253:ILE:HG12	4:D:504:HOH:O	2.08	0.53
1:B:248:VAL:HA	1:B:288:PHE:CD1	2.44	0.52
1:B:143:LEU:H	1:B:143:LEU:HD12	1.74	0.52
1:A:182:GLN:O	1:A:186:LEU:HG	2.09	0.52
1:B:146:MET:SD	1:B:183:VAL:HG22	2.50	0.52
2:D:345:LYS:HE3	2:D:349:LEU:HD21	1.92	0.52
1:B:321:LEU:HB2	1:B:345:LEU:HD21	1.91	0.52
1:B:188:ALA:O	1:B:190:ARG:N	2.43	0.52
1:A:289:HIS:HD2	1:A:324:ARG:HH12	1.57	0.52
1:B:97:LEU:CD1	1:B:143:LEU:HD22	2.38	0.52
2:C:231:GLU:OE2	2:C:264:ARG:HD2	2.10	0.52
1:B:239:MET:CE	1:B:273:MET:CE	2.82	0.52
1:B:201:CYS:SG	1:B:204:VAL:HG23	2.50	0.52
2:C:194:ASN:N	2:C:332:HIS:HD2	1.95	0.52
1:B:262:PRO:O	1:B:265:LYS:HG3	2.10	0.51
1:B:100:LEU:HD13	1:B:123:ALA:HB3	1.92	0.51
1:B:268:LEU:O	1:B:271:MET:HB3	2.10	0.51
1:B:236:MET:CG	1:B:273:MET:HE1	2.40	0.51
1:B:301:THR:CA	4:B:521:HOH:O	2.48	0.51
2:D:299:ARG:O	2:D:303:GLU:HG3	2.10	0.51
1:B:239:MET:HE2	1:B:273:MET:SD	2.44	0.51
1:A:265:LYS:NZ	1:A:301:THR:O	2.43	0.51
1:A:245:LYS:O	1:A:249:LYS:HB2	2.11	0.51
1:A:293:LEU:HD23	1:A:341:CYS:HB2	1.93	0.51
1:B:220:GLU:OE1	1:B:220:GLU:HA	2.10	0.51
1:A:255:GLN:O	1:A:259:VAL:HG23	2.11	0.50
2:D:196:LEU:HD23	2:D:196:LEU:C	2.32	0.50
2:D:198:PHE:CB	2:D:336:LEU:HD23	2.39	0.50
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:212:ILE:HG13	2:C:217:PHE:CE2	2.47	0.50
2:D:271:LYS:HG3	2:D:302:PHE:CZ	2.46	0.50
2:D:279:GLN:O	2:D:279:GLN:HG2	2.12	0.50
1:B:217:ARG:C	1:B:219:GLN:N	2.65	0.50
2:D:212:ILE:HG13	2:D:217:PHE:CE2	2.47	0.50
1:B:202:ASP:O	1:B:206:VAL:HG23	2.11	0.50
1:B:188:ALA:C	1:B:190:ARG:N	2.63	0.50
2:D:236:ARG:HD2	2:D:305:LEU:O	2.11	0.50
1:B:261:HIS:N	1:B:262:PRO:HD3	2.27	0.49
1:B:266:GLY:O	1:B:268:LEU:N	2.45	0.49
1:B:97:LEU:HD21	1:B:140:PHE:CE1	2.47	0.49
1:B:219:GLN:HE22	1:B:221:ALA:HB3	1.78	0.49
1:B:269:CYS:C	1:B:271:MET:H	2.16	0.49
1:B:223:LEU:O	1:B:226:PHE:HB3	2.12	0.49
1:A:87:ARG:NH1	1:A:139:ASP:OD2	2.46	0.49
2:D:272:ARG:HG3	3:D:402:AMP:N6	2.27	0.49
1:A:110:GLU:C	1:A:112:GLU:H	2.15	0.49
2:D:282:LEU:N	2:D:282:LEU:HD12	2.28	0.49
1:B:93:MET:HB3	1:B:130:LEU:HD12	1.94	0.49
1:B:197:ASP:OD2	1:B:234:VAL:HG13	2.13	0.49
2:D:200:LEU:CD1	2:D:205:PHE:HB2	2.42	0.49
2:C:318:GLU:O	2:C:321:LEU:HB2	2.13	0.49
1:A:236:MET:HA	1:A:239:MET:HG3	1.93	0.49
1:B:132:GLU:O	2:D:265:THR:HB	2.12	0.49
1:A:134:MET:HE2	2:C:272:ARG:CZ	2.42	0.49
1:B:212:ILE:O	1:B:216:VAL:HG22	2.12	0.49
2:C:243:GLU:HA	2:C:246:LYS:HE3	1.94	0.49
1:B:192:LEU:HD13	1:B:211:ALA:HB3	1.95	0.48
1:B:332:GLU:HA	1:B:335:GLN:HG3	1.95	0.48
2:C:204:THR:HG22	2:C:226:THR:HA	1.94	0.48
2:D:338:GLY:HA2	3:D:402:AMP:O1P	2.14	0.48
1:B:213:SER:O	1:B:217:ARG:HD3	2.14	0.48
2:D:299:ARG:HG2	2:D:299:ARG:HH11	1.78	0.48
2:D:307:SER:HB2	2:D:311:ARG:HH12	1.79	0.48
1:A:245:LYS:NZ	2:C:292:ASP:OD2	2.43	0.48
2:D:295:THR:CG2	2:D:296:SER:H	2.24	0.48
1:A:94:LYS:HE2	1:A:143:LEU:HD21	1.96	0.47
2:D:284:ILE:HD12	2:D:287:LEU:HD22	1.95	0.47
2:D:297:ILE:HG13	2:D:298:THR:N	2.29	0.47
1:B:340:PHE:CD2	1:B:340:PHE:N	2.79	0.47
2:C:274:LEU:HD21	2:C:297:ILE:HG23	1.95	0.47
1:B:118:GLN:HA	1:B:121:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:CYS:HB3	1:A:204:VAL:HG23	1.95	0.47
2:D:328:LYS:HG3	2:D:329:ALA:N	2.29	0.47
2:D:343:ILE:HB	2:D:346:VAL:HG23	1.95	0.47
1:A:335:GLN:NE2	2:C:247:ARG:HD2	2.29	0.47
1:B:124:LEU:HD11	1:B:149:LEU:HD11	1.97	0.47
1:B:219:GLN:HE21	1:B:221:ALA:HB3	1.80	0.47
1:A:240:GLN:HE21	1:A:276:GLN:NE2	2.13	0.47
1:B:100:LEU:HD13	1:B:123:ALA:CB	2.44	0.47
1:A:245:LYS:HA	1:A:248:VAL:HG22	1.97	0.47
2:C:234:ASP:OD1	2:C:268:GLU:HG3	2.15	0.47
1:B:236:MET:HE1	1:B:271:MET:HG2	1.98	0.46
1:B:210:PHE:O	1:B:213:SER:HB3	2.15	0.46
2:C:212:ILE:HG13	2:C:217:PHE:CZ	2.50	0.46
1:A:146:MET:HG2	1:A:183:VAL:HG22	1.98	0.46
2:D:212:ILE:HD13	2:D:212:ILE:O	2.15	0.46
1:B:317:LEU:HG	1:B:321:LEU:CD1	2.46	0.46
1:A:332:GLU:O	1:A:335:GLN:HG3	2.15	0.46
1:A:225:GLN:O	1:A:229:LEU:HD12	2.15	0.46
1:B:94:LYS:O	1:B:98:ARG:HG3	2.15	0.46
2:C:238:VAL:HG13	2:C:263:LEU:HD13	1.98	0.46
1:A:290:GLU:HA	1:A:337:GLU:HG3	1.98	0.46
1:A:278:VAL:HG11	1:A:315:LEU:HG	1.98	0.46
1:A:108:ALA:HB1	1:A:112:GLU:HB3	1.96	0.45
1:B:300:VAL:C	4:B:521:HOH:O	2.55	0.45
1:A:202:ASP:O	1:A:206:VAL:HG23	2.16	0.45
1:B:260:GLY:O	1:B:261:HIS:ND1	2.49	0.45
1:B:121:GLU:HG2	1:B:164:ARG:HD2	1.97	0.45
2:D:295:THR:CG2	2:D:296:SER:N	2.76	0.45
1:A:213:SER:OG	1:A:217:ARG:HD3	2.16	0.45
2:C:339:GLY:O	2:C:342:ARG:HG3	2.17	0.45
2:C:243:GLU:HA	2:C:246:LYS:CE	2.46	0.45
2:D:256:ASN:ND2	2:D:259:ALA:N	2.64	0.45
1:A:198:ARG:HH11	1:A:198:ARG:CB	2.30	0.45
2:D:234:ASP:OD1	2:D:268:GLU:HG3	2.17	0.45
1:B:263:GLU:HG2	1:B:264:HIS:N	2.31	0.45
1:B:288:PHE:CD1	1:B:288:PHE:O	2.70	0.45
1:A:248:VAL:CG1	1:A:288:PHE:HB3	2.46	0.44
2:D:299:ARG:HG2	2:D:299:ARG:NH1	2.32	0.44
1:B:317:LEU:O	1:B:321:LEU:HG	2.17	0.44
1:B:281:VAL:O	1:B:281:VAL:HG12	2.16	0.44
1:A:286:SER:HB2	1:A:287:PRO:CD	2.47	0.44
1:B:217:ARG:O	1:B:219:GLN:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:CYS:HB2	1:B:305:GLN:NE2	2.32	0.44
2:C:250:LYS:C	2:C:251:LYS:HG3	2.38	0.44
1:A:244:GLN:O	1:A:247:LYS:N	2.51	0.44
2:C:256:ASN:ND2	2:C:259:ALA:HB2	2.31	0.44
2:C:263:LEU:HD22	2:C:267:CYS:SG	2.58	0.44
1:B:188:ALA:C	1:B:190:ARG:H	2.21	0.44
1:A:147:HIS:N	1:A:147:HIS:CD2	2.84	0.44
1:A:163:TRP:HB3	1:A:204:VAL:HA	2.00	0.44
1:A:100:LEU:HB3	1:A:148:LEU:HD21	2.00	0.43
2:D:196:LEU:HD21	2:D:207:VAL:HG23	2.00	0.43
1:B:248:VAL:CG2	1:B:249:LYS:N	2.80	0.43
1:A:149:LEU:HD21	1:A:168:LEU:HG	2.00	0.43
1:B:142:GLN:C	1:B:144:SER:N	2.70	0.43
1:B:295:ALA:C	1:B:297:CYS:H	2.22	0.43
1:B:140:PHE:CZ	1:B:145:GLY:HA3	2.54	0.43
1:B:132:GLU:CD	2:D:262:ARG:HG2	2.39	0.43
2:C:314:LEU:O	2:C:315:GLU:C	2.57	0.43
1:B:248:VAL:HG12	1:B:288:PHE:CG	2.53	0.43
2:C:199:ASP:HB2	2:C:337:VAL:CG2	2.48	0.43
1:A:134:MET:HE1	2:C:272:ARG:HD2	2.00	0.43
1:B:303:PHE:CE2	1:B:305:GLN:HB3	2.53	0.43
2:D:234:ASP:O	2:D:238:VAL:HG23	2.18	0.43
1:A:235:LEU:O	1:A:238:ALA:HB3	2.18	0.43
2:C:199:ASP:CB	2:C:337:VAL:HG23	2.48	0.43
1:B:217:ARG:O	1:B:218:GLU:C	2.57	0.43
1:B:161:LEU:O	1:B:165:ALA:HB2	2.19	0.43
1:A:124:LEU:HD12	1:A:168:LEU:CD2	2.49	0.43
1:B:264:HIS:O	1:B:265:LYS:C	2.56	0.43
1:B:102:GLN:CD	1:B:103:PRO:HD2	2.39	0.43
1:B:111:ALA:O	1:B:114:ALA:HB3	2.19	0.43
1:B:333:GLU:HB3	2:D:247:ARG:O	2.19	0.43
1:B:301:THR:N	4:B:521:HOH:O	2.51	0.42
1:B:237:ARG:HH11	1:B:237:ARG:HG3	1.84	0.42
1:A:134:MET:CE	2:C:272:ARG:CZ	2.97	0.42
1:A:328:LEU:HD22	1:A:334:TYR:HB3	2.01	0.42
2:C:255:GLN:NE2	2:D:323:ASP:HB3	2.30	0.42
1:B:136:ASN:O	1:B:139:ASP:HB2	2.19	0.42
2:D:272:ARG:O	2:D:275:SER:HB2	2.19	0.42
1:A:219:GLN:HE21	1:A:222:GLY:H	1.67	0.42
1:A:139:ASP:O	1:A:143:LEU:HD12	2.20	0.42
1:A:110:GLU:O	1:A:112:GLU:N	2.53	0.42
1:B:317:LEU:HG	1:B:321:LEU:CG	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:230:ASP:O	1:B:234:VAL:HG23	2.20	0.42
1:B:105:PRO:HB2	1:B:108:ALA:HB2	2.00	0.42
1:B:146:MET:HA	1:B:146:MET:HE1	2.00	0.42
1:B:87:ARG:HE	1:B:90:VAL:CG2	2.32	0.42
1:B:236:MET:CE	1:B:271:MET:HG2	2.50	0.42
1:A:154:LEU:HD11	1:A:169:ILE:HD12	1.99	0.42
1:B:100:LEU:CD1	1:B:123:ALA:HB3	2.49	0.42
2:D:209:ILE:HD13	2:D:321:LEU:HD23	2.02	0.42
1:A:141:CYS:HB3	1:A:182:GLN:HE22	1.85	0.42
2:D:324:ALA:O	2:D:326:LEU:HD13	2.20	0.42
1:B:269:CYS:C	1:B:271:MET:N	2.73	0.42
1:B:180:GLN:O	1:B:184:LEU:HG	2.20	0.42
1:B:175:ASN:HB3	2:D:273:THR:HG1	1.85	0.41
1:B:124:LEU:HA	1:B:124:LEU:HD12	1.86	0.41
1:B:248:VAL:HG12	1:B:288:PHE:CD2	2.55	0.41
2:D:343:ILE:HB	2:D:346:VAL:CG2	2.50	0.41
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.88	0.41
1:B:262:PRO:CA	1:B:265:LYS:HE3	2.50	0.41
1:B:128:ALA:CA	1:B:168:LEU:HD13	2.49	0.41
1:A:286:SER:HB2	1:A:287:PRO:HD2	2.02	0.41
2:D:207:VAL:HG11	2:D:316:PRO:HB2	2.01	0.41
2:C:242:VAL:HG13	2:C:253:ILE:HG12	2.02	0.41
1:B:333:GLU:CB	2:D:248:LYS:HA	2.50	0.41
1:B:193:LEU:HD12	1:B:229:LEU:HD13	2.02	0.41
1:A:134:MET:HE2	2:C:272:ARG:NH1	2.36	0.41
2:C:345:LYS:HE3	2:C:349:LEU:HD21	2.03	0.41
1:B:105:PRO:O	1:B:106:PRO:C	2.59	0.41
1:A:236:MET:HG3	1:A:273:MET:HE1	2.02	0.41
1:B:120:ARG:O	1:B:124:LEU:HB2	2.20	0.41
1:B:260:GLY:C	1:B:261:HIS:ND1	2.74	0.41
1:B:217:ARG:HH21	2:D:281:SER:HB2	1.85	0.41
1:A:307:VAL:HG13	1:A:348:CYS:SG	2.61	0.41
2:D:212:ILE:HG13	2:D:217:PHE:CZ	2.56	0.41
2:C:213:ASP:OD1	2:C:214:ASP:HB2	2.21	0.41
1:B:125:GLU:O	1:B:126:LEU:C	2.60	0.41
1:A:87:ARG:HH11	1:A:90:VAL:CG2	2.34	0.41
2:D:200:LEU:HD13	2:D:205:PHE:HB2	2.02	0.41
1:A:184:LEU:HA	1:A:184:LEU:HD23	1.87	0.41
2:C:237:LEU:HD21	2:C:297:ILE:HD13	2.01	0.40
1:B:139:ASP:O	1:B:142:GLN:HB2	2.20	0.40
1:A:314:GLU:HG3	1:A:314:GLU:H	1.56	0.40
1:B:87:ARG:CG	1:B:90:VAL:HG23	2.48	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:87:ARG:C	1:A:89:GLU:H	2.23	0.40
1:B:142:GLN:HA	1:B:142:GLN:OE1	2.21	0.40
1:B:219:GLN:HG3	1:B:219:GLN:O	2.20	0.40
1:A:110:GLU:C	1:A:112:GLU:N	2.74	0.40
2:C:200:LEU:HA	2:C:200:LEU:HD12	1.89	0.40
1:B:132:GLU:CD	2:D:262:ARG:HE	2.24	0.40
2:C:281:SER:C	2:C:282:LEU:HD12	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/280 (94%)	234 (89%)	24 (9%)	4 (2%)	15	50
1	B	262/280 (94%)	218 (83%)	36 (14%)	8 (3%)	7	26
2	C	163/191 (85%)	149 (91%)	13 (8%)	1 (1%)	33	76
2	D	163/191 (85%)	147 (90%)	13 (8%)	3 (2%)	13	44
All	All	850/942 (90%)	748 (88%)	86 (10%)	16 (2%)	12	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	B	154	LEU
1	B	267	THR
2	D	328	LYS
1	A	156	ALA
1	B	143	LEU
1	B	296	LEU
2	D	288	PHE
1	A	108	ALA
1	A	110	GLU
1	B	189	LEU

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Mol	Chain	Res	Type
1	B	116	ASP
2	C	307	SER
1	B	225	GLN
1	B	333	GLU
2	D	339	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	219/235 (93%)	200 (91%)	19 (9%)	15	41
1	B	214/235 (91%)	199 (93%)	15 (7%)	21	53
2	C	144/163 (88%)	136 (94%)	8 (6%)	30	66
2	D	144/163 (88%)	131 (91%)	13 (9%)	14	39
All	All	721/796 (91%)	666 (92%)	55 (8%)	19	48

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	110	GLU
1	A	116	ASP
1	A	118	GLN
1	A	124	LEU
1	A	126	LEU
1	A	132	GLU
1	A	149	LEU
1	A	155	GLU
1	A	167	GLN
1	A	190	ARG
1	A	196	LEU
1	A	197	ASP
1	A	198	ARG
1	A	257	LEU
1	A	267	THR
1	A	296	LEU

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Mol	Chain	Res	Type
1	A	300	VAL
1	A	315	LEU
1	B	124	LEU
1	B	127	LEU
1	B	132	GLU
1	B	152	ARG
1	B	174	GLN
1	B	196	LEU
1	B	229	LEU
1	B	244	GLN
1	B	249	LYS
1	B	256	ASN
1	B	257	LEU
1	B	263	GLU
1	B	288	PHE
1	B	328	LEU
1	B	330	GLN
2	C	192	GLU
2	C	210	LEU
2	C	212	ILE
2	C	214	ASP
2	C	226	THR
2	C	228	LEU
2	C	263	LEU
2	C	333	ASP
2	D	210	LEU
2	D	212	ILE
2	D	214	ASP
2	D	226	THR
2	D	228	LEU
2	D	235	ASN
2	D	258	ARG
2	D	263	LEU
2	D	278	THR
2	D	297	ILE
2	D	299	ARG
2	D	333	ASP
2	D	335	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	118	GLN
1	A	136	ASN
1	A	147	HIS
1	A	182	GLN
1	A	219	GLN
1	A	255	GLN
1	A	276	GLN
1	A	289	HIS
1	A	335	GLN
1	B	102	GLN
1	B	117	GLN
1	B	136	ASN
1	B	147	HIS
1	B	219	GLN
1	B	240	GLN
1	B	255	GLN
1	B	276	GLN
1	B	289	HIS
1	B	305	GLN
1	B	331	HIS
1	B	335	GLN
2	C	239	ASN
2	C	330	GLN
2	C	332	HIS
2	D	239	ASN
2	D	249	HIS
2	D	256	ASN
2	D	330	GLN
2	D	332	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	AMP	C	401	-	25,25,25	2.15	6 (24%)	38,38,38	1.49	7 (18%)
3	AMP	D	402	-	25,25,25	2.11	6 (24%)	38,38,38	1.44	5 (13%)

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	AMP	C	401	-	-	0/10/26/26	0/1/3/3
3	AMP	D	402	-	-	0/10/26/26	0/1/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	AMP	C4-N3	5.98	1.44	1.35
3	D	402	AMP	C4-N3	5.64	1.44	1.35
3	C	401	AMP	P-O3P	4.07	1.69	1.54
3	D	402	AMP	P-O3P	4.03	1.69	1.54
3	C	401	AMP	C8-N7	-3.67	1.27	1.34
3	D	402	AMP	C8-N7	-3.62	1.27	1.34
3	D	402	AMP	C2-N3	3.33	1.38	1.32
3	C	401	AMP	C2'-C1'	-3.01	1.49	1.53
3	C	401	AMP	C2-N3	2.89	1.37	1.32
3	D	402	AMP	C2'-C1'	-2.84	1.49	1.53
3	C	401	AMP	C2-N1	2.69	1.39	1.33
3	D	402	AMP	C2-N1	2.63	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	AMP	N3-C2-N1	-5.15	124.40	128.71
3	D	402	AMP	N3-C2-N1	-4.97	124.55	128.71
3	D	402	AMP	C8-N9-C4	-2.75	104.80	106.90
3	C	401	AMP	C8-N9-C4	-2.68	104.85	106.90
3	D	402	AMP	C3'-C2'-C1'	2.67	105.09	100.91
3	C	401	AMP	O4'-C1'-N9	2.56	110.82	108.44
3	C	401	AMP	C4-C5-N7	2.40	111.58	109.52
3	D	402	AMP	C4-C5-N7	2.39	111.57	109.52
3	C	401	AMP	O4'-C1'-C2'	-2.24	103.33	106.77
3	C	401	AMP	P-O5'-C5'	2.14	124.38	118.19
3	D	402	AMP	O2P-P-O1P	2.08	117.24	110.44
3	C	401	AMP	C8-N9-C1'	2.02	130.37	126.38

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/280 (94%)	0.01	3 (1%) 77 84	31, 54, 88, 116	0
1	B	264/280 (94%)	0.42	17 (6%) 19 23	53, 85, 114, 143	0
2	C	165/191 (86%)	0.27	3 (1%) 65 74	29, 62, 79, 83	0
2	D	165/191 (86%)	0.33	7 (4%) 35 41	50, 67, 83, 93	0
All	All	858/942 (91%)	0.25	30 (3%) 42 50	29, 67, 102, 143	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ALA	3.4
1	B	341	CYS	3.3
1	B	330	GLN	2.9
2	C	334	LEU	2.8
1	B	296	LEU	2.7
1	B	104	MET	2.7
2	D	350	LEU	2.7
1	B	105	PRO	2.7
2	D	354	PHE	2.7
2	C	341	THR	2.6
2	D	302	PHE	2.6
1	B	310	CYS	2.5
1	B	321	LEU	2.5
1	B	232	PHE	2.4
1	B	338	LEU	2.4
1	A	161	LEU	2.3
1	B	188	ALA	2.3
2	D	335	VAL	2.3
1	B	328	LEU	2.2
2	D	326	LEU	2.2
1	B	274	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	196	LEU	2.2
1	B	153	TYR	2.1
1	A	106	PRO	2.1
1	B	320	LEU	2.1
2	D	212	ILE	2.1
1	B	112	GLU	2.0
2	D	310	PHE	2.0
1	B	98	ARG	2.0
1	A	317	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	AMP	D	402	23/23	0.20	0.16	76,81,88,90	0
3	AMP	C	401	23/23	0.21	-0.22	77,85,99,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.