



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:43 am GMT

PDB ID : 1AYR  
Title : ARRESTIN FROM BOVINE ROD OUTER SEGMENTS  
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Deposited on : 1997-11-10  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

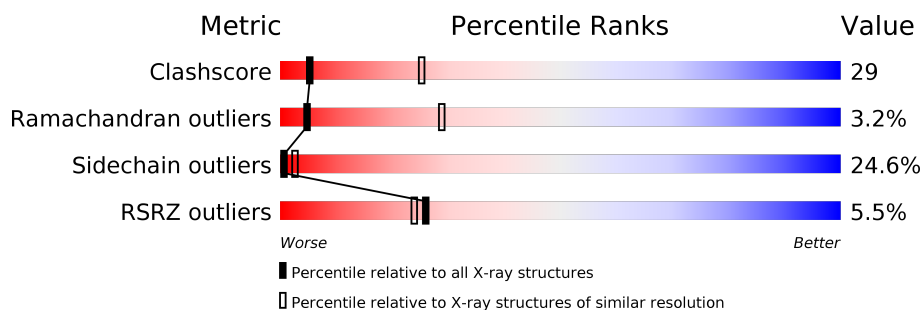
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	<div> <div>5%</div> <div>40% 45% 14%</div> <div>.</div> </div>
1	B	368	<div> <div>5%</div> <div>43% 40% 15%</div> <div>..</div> </div>
1	C	368	<div> <div>5%</div> <div>41% 45% 13%</div> <div>.</div> </div>
1	D	368	<div> <div>7%</div> <div>42% 42% 15%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11743 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 ARRESTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2882	1841	488	543	10			
1	B	363	Total	C	N	O	S	0	0	0
			2847	1821	482	534	10			
1	C	368	Total	C	N	O	S	0	0	0
			2882	1841	488	543	10			
1	D	363	Total	C	N	O	S	0	0	0
			2847	1821	482	534	10			

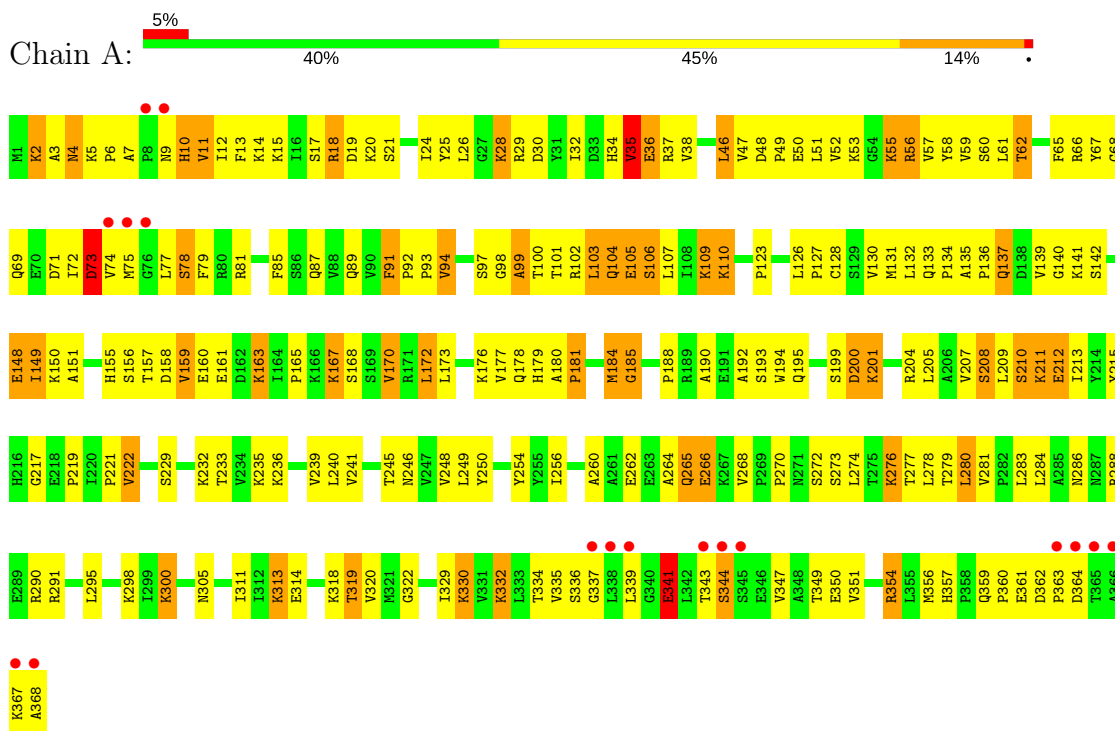
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	46	Total	O	0	0
			46	46		
2	C	78	Total	O	0	0
			78	78		
2	D	62	Total	O	0	0
			62	62		

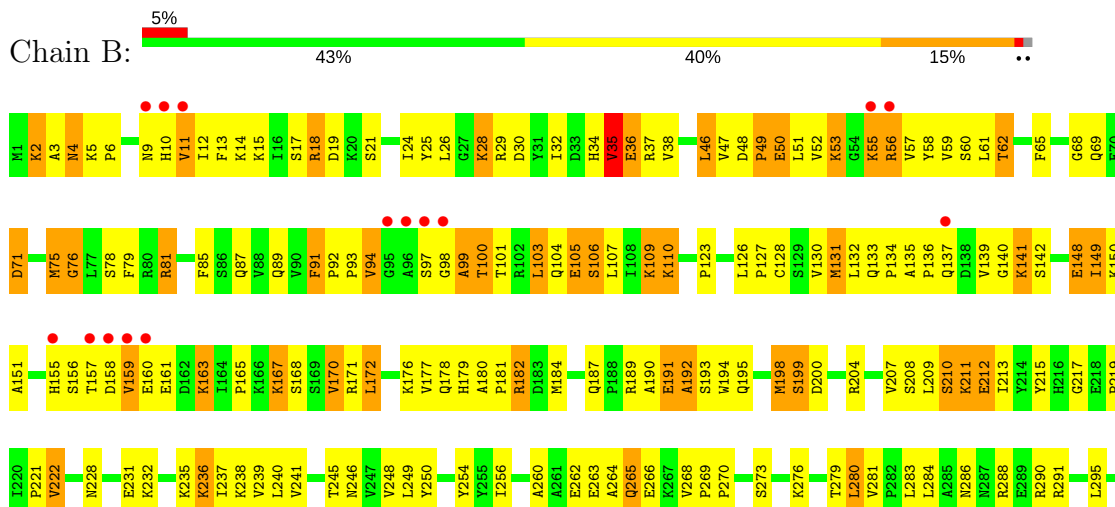
### 3 Residue-property plots

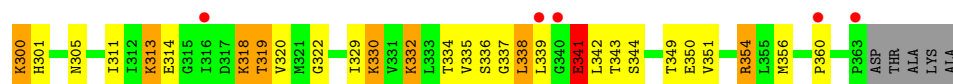
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: ARRESTIN

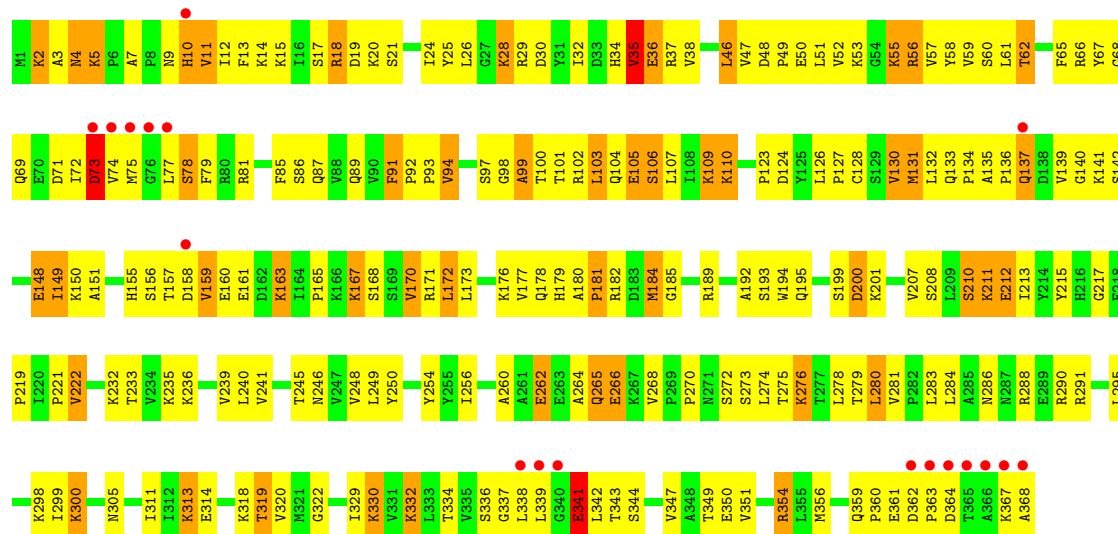


#### • Molecule 1: ARRESTIN

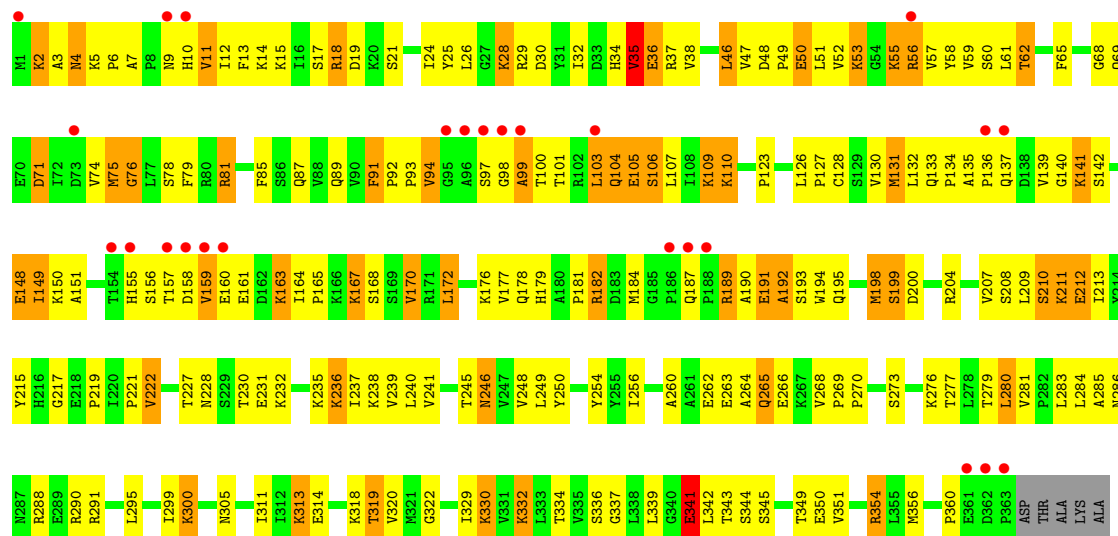




• Molecule 1: ARRESTIN



• Molecule 1: ARRESTIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.17Å 185.53Å 90.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.00 – 3.30 26.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (130.00-3.30) 41.9 (26.98-3.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.37 (at 3.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.254 , 0.316 0.248 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.31	0/2940	0.57	3/3987 (0.1%)
1	B	0.30	0/2905	0.57	1/3941 (0.0%)
1	C	0.30	0/2940	0.57	3/3987 (0.1%)
1	D	0.30	0/2905	0.57	2/3941 (0.1%)
All	All	0.30	0/11690	0.57	9/15856 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	ASN	N-CA-C	-7.17	91.65	111.00
1	A	9	ASN	N-CA-C	-7.05	91.97	111.00
1	C	9	ASN	N-CA-C	-6.86	92.47	111.00
1	B	9	ASN	N-CA-C	-6.86	92.48	111.00
1	A	7	ALA	N-CA-C	-5.22	96.90	111.00
1	C	7	ALA	N-CA-C	-5.19	96.99	111.00
1	C	10	HIS	N-CA-C	-5.10	97.23	111.00
1	A	10	HIS	N-CA-C	-5.09	97.24	111.00
1	D	7	ALA	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2882	0	2971	190	0
1	B	2847	0	2937	164	0
1	C	2882	0	2971	174	0
1	D	2847	0	2937	166	0
2	A	99	0	0	17	0
2	B	46	0	0	8	0
2	C	78	0	0	14	0
2	D	62	0	0	11	0
All	All	11743	0	11816	680	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 (680) 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:10:HIS:O	1:B:11:VAL:HG23	1.68	0.94
1:A:2:LYS:HG2	1:A:29:ARG:HH11	1.36	0.90
1:D:2:LYS:HG2	1:D:29:ARG:HH11	1.37	0.89
1:B:2:LYS:HG2	1:B:29:ARG:HH11	1.35	0.88
1:B:91:PHE:HB3	1:B:92:PRO:HD3	1.56	0.88
1:D:10:HIS:O	1:D:11:VAL:HG23	1.72	0.87
1:D:91:PHE:HB3	1:D:92:PRO:HD3	1.56	0.86
1:A:10:HIS:O	1:A:11:VAL:HG23	1.75	0.86
1:A:91:PHE:HB3	1:A:92:PRO:HD3	1.56	0.86
1:C:157:THR:HA	2:C:385:HOH:O	1.76	0.86
1:A:336:SER:HA	1:A:343:THR:HA	1.58	0.86
1:D:336:SER:HA	1:D:343:THR:HA	1.58	0.85
1:B:81:ARG:HG2	1:C:195:GLN:HB3	1.59	0.84
1:C:91:PHE:HB3	1:C:92:PRO:HD3	1.58	0.84
1:C:10:HIS:O	1:C:11:VAL:HG23	1.77	0.84
1:B:151:ALA:HB3	1:B:170:VAL:HG23	1.61	0.83
1:A:151:ALA:HB3	1:A:170:VAL:HG23	1.61	0.83
1:B:336:SER:HA	1:B:343:THR:HA	1.58	0.83
1:C:2:LYS:HG2	1:C:29:ARG:HH11	1.43	0.82
1:C:151:ALA:HB3	1:C:170:VAL:HG23	1.61	0.81
1:C:336:SER:HA	1:C:343:THR:HA	1.60	0.81
1:D:151:ALA:HB3	1:D:170:VAL:HG23	1.61	0.80
1:A:264:ALA:HB2	1:A:278:LEU:HD21	1.63	0.80
1:A:195:GLN:HB3	1:D:81:ARG:HG2	1.63	0.79
1:C:219:PRO:HA	1:C:281:VAL:HG22	1.64	0.79
1:B:89:GLN:HE21	1:B:94:VAL:HG22	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HE2	1:B:342:LEU:HG	1.65	0.79
1:A:89:GLN:HE21	1:A:94:VAL:HG22	1.47	0.78
1:C:264:ALA:HB2	1:C:278:LEU:HD21	1.65	0.78
1:D:74:VAL:HA	2:D:410:HOH:O	1.83	0.78
1:A:192:ALA:HB2	1:A:349:THR:HG21	1.66	0.78
1:A:233:THR:OG1	1:A:270:PRO:HD3	1.83	0.77
1:B:219:PRO:HA	1:B:281:VAL:HG22	1.64	0.77
1:D:89:GLN:HE21	1:D:94:VAL:HG22	1.50	0.77
1:A:219:PRO:HA	1:A:281:VAL:HG22	1.65	0.77
1:D:219:PRO:HA	1:D:281:VAL:HG22	1.65	0.76
1:A:260:ALA:HB1	2:A:452:HOH:O	1.84	0.75
1:B:182:ARG:HG2	1:B:360:PRO:HD2	1.69	0.75
1:B:2:LYS:HG2	1:B:29:ARG:NH1	2.02	0.74
1:D:182:ARG:HG2	1:D:360:PRO:HD2	1.68	0.74
1:D:2:LYS:HG2	1:D:29:ARG:NH1	2.02	0.74
1:B:338:LEU:HA	2:B:386:HOH:O	1.86	0.74
1:B:238:LYS:HG3	1:B:263:GLU:HB3	1.67	0.74
1:B:68:GLY:O	1:B:71:ASP:HB2	1.89	0.73
1:D:135:ALA:HB1	1:D:136:PRO:HD2	1.71	0.73
1:D:238:LYS:HG3	1:D:263:GLU:HB3	1.70	0.73
1:D:68:GLY:O	1:D:71:ASP:HB2	1.89	0.73
1:D:181:PRO:HG2	1:D:184:MET:HG2	1.71	0.73
1:A:34:HIS:O	1:A:36:GLU:N	2.22	0.73
1:B:34:HIS:O	1:B:36:GLU:N	2.22	0.72
1:C:89:GLN:HE21	1:C:94:VAL:HG22	1.54	0.72
1:C:184:MET:HB3	1:C:213:ILE:HD12	1.69	0.72
1:D:13:PHE:HE2	1:D:28:LYS:HA	1.55	0.72
1:A:194:TRP:CE2	1:A:347:VAL:HB	2.25	0.72
1:A:135:ALA:HB1	1:A:136:PRO:HD2	1.72	0.72
1:D:34:HIS:O	1:D:36:GLU:N	2.22	0.72
1:B:181:PRO:HG2	1:B:184:MET:HG2	1.71	0.71
1:C:34:HIS:O	1:C:36:GLU:N	2.23	0.71
1:D:157:THR:HG21	1:D:163:LYS:HD2	1.70	0.71
1:B:157:THR:HG21	1:B:163:LYS:HD2	1.72	0.71
1:B:13:PHE:HE2	1:B:28:LYS:HA	1.54	0.70
1:D:195:GLN:HG2	1:D:204:ARG:HG2	1.73	0.70
1:A:2:LYS:HG2	1:A:29:ARG:NH1	2.05	0.70
1:C:13:PHE:HE2	1:C:28:LYS:HA	1.55	0.70
1:A:13:PHE:HE2	1:A:28:LYS:HA	1.56	0.70
1:B:135:ALA:HB1	1:B:136:PRO:HD2	1.71	0.70
1:C:135:ALA:HB1	1:C:136:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ILE:HD13	1:B:107:LEU:HD11	1.74	0.69
1:D:190:ALA:HB3	1:D:209:LEU:HB2	1.74	0.69
1:A:204:ARG:HD2	2:A:432:HOH:O	1.93	0.69
1:B:190:ALA:HB3	1:B:209:LEU:HB2	1.74	0.69
1:A:157:THR:HG21	1:A:163:LYS:HD2	1.76	0.68
1:A:12:ILE:HD13	1:A:107:LEU:HD11	1.74	0.68
1:C:12:ILE:HD13	1:C:107:LEU:HD11	1.75	0.68
1:D:12:ILE:HD13	1:D:107:LEU:HD11	1.75	0.68
1:D:204:ARG:HD3	2:D:387:HOH:O	1.92	0.68
1:B:195:GLN:HG2	1:B:204:ARG:HG2	1.75	0.68
1:A:18:ARG:HD3	2:A:428:HOH:O	1.92	0.68
1:A:184:MET:HB3	1:A:213:ILE:HD12	1.74	0.68
1:A:91:PHE:HB3	1:A:92:PRO:CD	2.24	0.68
1:B:91:PHE:HB3	1:B:92:PRO:CD	2.24	0.68
1:C:330:LYS:HG2	1:C:350:GLU:HG3	1.77	0.67
1:A:337:GLY:H	1:A:343:THR:HA	1.60	0.66
1:B:18:ARG:HH12	1:C:137:GLN:HB2	1.58	0.66
1:A:66:ARG:NH2	2:A:398:HOH:O	2.29	0.66
1:C:157:THR:HG21	1:C:163:LYS:HD2	1.77	0.66
1:D:48:ASP:HB3	1:D:51:LEU:HB2	1.77	0.66
1:A:361:GLU:C	1:A:363:PRO:HD3	2.16	0.66
1:A:344:SER:HA	2:A:458:HOH:O	1.95	0.66
1:C:2:LYS:HG2	1:C:29:ARG:NH1	2.09	0.66
1:A:330:LYS:HG2	1:A:350:GLU:HG3	1.77	0.66
1:C:361:GLU:C	1:C:363:PRO:HD3	2.16	0.66
1:B:48:ASP:HB3	1:B:51:LEU:HB2	1.77	0.65
1:D:91:PHE:HB3	1:D:92:PRO:CD	2.24	0.65
1:D:330:LYS:HG2	1:D:350:GLU:HG3	1.77	0.65
1:A:102:ARG:NH1	1:A:368:ALA:HB3	2.10	0.65
1:C:91:PHE:HB3	1:C:92:PRO:CD	2.26	0.65
1:A:48:ASP:HB3	1:A:51:LEU:HB2	1.78	0.65
1:B:330:LYS:HG2	1:B:350:GLU:HG3	1.77	0.65
1:D:337:GLY:H	1:D:343:THR:HA	1.62	0.65
1:C:299:ILE:HB	2:C:426:HOH:O	1.95	0.65
1:C:35:VAL:HG13	1:C:181:PRO:HB3	1.78	0.64
1:C:264:ALA:HB1	1:C:276:LYS:HD3	1.79	0.64
1:A:300:LYS:H	1:A:300:LYS:HE2	1.63	0.64
1:A:73:ASP:OD2	1:A:77:LEU:HD13	1.98	0.63
1:C:48:ASP:HB3	1:C:51:LEU:HB2	1.78	0.63
1:C:337:GLY:H	1:C:343:THR:HA	1.62	0.63
1:B:17:SER:HB2	1:B:167:LYS:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLY:H	1:B:343:THR:HA	1.64	0.63
1:B:100:THR:HA	2:B:411:HOH:O	1.99	0.63
1:D:300:LYS:H	1:D:300:LYS:HE2	1.64	0.63
1:C:73:ASP:OD2	1:C:77:LEU:HD13	1.99	0.62
1:B:300:LYS:H	1:B:300:LYS:HE2	1.63	0.62
1:D:217:GLY:HA2	1:D:283:LEU:HD21	1.82	0.62
1:A:17:SER:HB2	1:A:167:LYS:O	1.99	0.62
1:C:217:GLY:HA2	1:C:283:LEU:HD21	1.81	0.62
1:D:17:SER:HB2	1:D:167:LYS:O	1.99	0.62
1:D:236:LYS:HG2	1:D:264:ALA:O	2.00	0.62
1:B:49:PRO:HA	2:B:413:HOH:O	1.98	0.62
1:C:300:LYS:H	1:C:300:LYS:HE2	1.64	0.62
1:D:60:SER:HB3	1:D:87:GLN:HG3	1.82	0.62
1:A:192:ALA:CB	1:A:349:THR:HG21	2.30	0.61
1:A:20:LYS:NZ	2:A:400:HOH:O	2.33	0.61
1:A:217:GLY:HA2	1:A:283:LEU:HD21	1.82	0.61
1:C:342:LEU:HD12	2:C:417:HOH:O	2.00	0.61
1:B:60:SER:HB3	1:B:87:GLN:HG3	1.82	0.61
1:C:192:ALA:HB2	1:C:349:THR:HG21	1.82	0.61
1:C:264:ALA:HB1	1:C:276:LYS:CD	2.31	0.61
1:D:235:LYS:HE2	1:D:336:SER:HB3	1.82	0.61
1:A:60:SER:HB3	1:A:87:GLN:HG3	1.83	0.61
1:C:60:SER:HB3	1:C:87:GLN:HG3	1.83	0.61
1:C:235:LYS:HE2	1:C:336:SER:HB3	1.82	0.60
1:D:285:ALA:HA	2:D:418:HOH:O	2.02	0.60
1:D:13:PHE:CE2	1:D:28:LYS:HA	2.36	0.60
1:B:235:LYS:HE2	1:B:336:SER:HB3	1.83	0.60
1:C:13:PHE:CE2	1:C:28:LYS:HA	2.37	0.60
1:D:311:ILE:HG22	1:D:313:LYS:HE3	1.84	0.60
1:B:71:ASP:OD2	1:B:141:LYS:HB3	2.02	0.60
1:B:236:LYS:HG2	1:B:264:ALA:O	2.01	0.60
1:C:311:ILE:HG22	1:C:313:LYS:HE3	1.83	0.60
1:D:14:LYS:NZ	2:D:428:HOH:O	2.33	0.60
1:B:217:GLY:HA2	1:B:283:LEU:HD21	1.82	0.60
1:C:330:LYS:HD2	1:C:332:LYS:HE2	1.84	0.60
1:C:17:SER:HB2	1:C:167:LYS:O	2.01	0.60
1:C:134:PRO:HD2	1:C:142:SER:HB3	1.84	0.59
1:D:105:GLU:O	1:D:109:LYS:HG2	2.03	0.59
1:D:91:PHE:CB	1:D:92:PRO:HD3	2.31	0.59
1:A:344:SER:OG	2:A:434:HOH:O	2.16	0.59
1:B:148:GLU:O	1:B:148:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLU:O	1:C:109:LYS:HG2	2.03	0.59
1:A:148:GLU:O	1:A:148:GLU:HG3	2.02	0.59
1:A:311:ILE:HG22	1:A:313:LYS:HE3	1.84	0.59
1:B:228:ASN:ND2	1:B:268:VAL:O	2.31	0.59
1:A:277:THR:O	1:B:341:GLU:HB3	2.03	0.59
1:A:105:GLU:O	1:A:109:LYS:HG2	2.03	0.59
1:A:35:VAL:HG13	1:A:181:PRO:HB3	1.84	0.59
1:A:66:ARG:HB2	1:A:71:ASP:OD1	2.03	0.59
1:A:178:GLN:HG3	2:A:440:HOH:O	2.03	0.59
1:B:311:ILE:HG22	1:B:313:LYS:HE3	1.84	0.59
1:B:91:PHE:CB	1:B:92:PRO:HD3	2.32	0.59
1:C:239:VAL:HG12	1:C:280:LEU:HD11	1.86	0.58
1:A:19:ASP:OD2	1:A:168:SER:HB3	2.04	0.58
1:B:13:PHE:CE2	1:B:28:LYS:HA	2.36	0.58
1:A:213:ILE:HG12	1:A:354:ARG:HB2	1.86	0.58
1:B:330:LYS:HD2	1:B:332:LYS:HE2	1.85	0.58
1:D:191:GLU:O	1:D:192:ALA:HB2	2.04	0.58
1:D:239:VAL:HG12	1:D:280:LEU:HD11	1.86	0.58
1:A:134:PRO:HD2	1:A:142:SER:HB3	1.86	0.58
1:B:239:VAL:HG12	1:B:280:LEU:HD11	1.86	0.58
1:D:10:HIS:O	1:D:11:VAL:CG2	2.49	0.58
1:D:237:ILE:HD12	1:D:266:GLU:HG3	1.86	0.58
1:D:249:LEU:HD22	1:D:322:GLY:HA2	1.86	0.58
1:D:330:LYS:HD2	1:D:332:LYS:HE2	1.85	0.58
1:A:13:PHE:CE2	1:A:28:LYS:HA	2.37	0.58
1:B:10:HIS:O	1:B:11:VAL:CG2	2.49	0.58
1:A:330:LYS:HD2	1:A:332:LYS:HE2	1.84	0.58
1:A:56:ARG:HD3	1:A:58:TYR:OH	2.04	0.58
1:B:105:GLU:O	1:B:109:LYS:HG2	2.03	0.58
1:B:167:LYS:HE3	2:B:391:HOH:O	2.04	0.58
1:C:213:ILE:HG12	1:C:354:ARG:HB2	1.86	0.58
1:C:184:MET:HE2	1:C:213:ILE:HB	1.85	0.57
1:C:249:LEU:HD22	1:C:322:GLY:HA2	1.87	0.57
1:D:136:PRO:HA	2:D:377:HOH:O	2.04	0.57
1:B:254:TYR:CE2	1:B:256:ILE:HD11	2.40	0.57
1:A:239:VAL:HG12	1:A:280:LEU:HD11	1.85	0.57
1:B:237:ILE:HD12	1:B:266:GLU:HG3	1.85	0.57
1:D:148:GLU:O	1:D:148:GLU:HG3	2.03	0.57
1:D:56:ARG:HD3	1:D:58:TYR:OH	2.04	0.57
1:A:249:LEU:HD22	1:A:322:GLY:HA2	1.87	0.57
1:A:67:TYR:O	1:A:78:SER:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ALA:HB1	1:D:194:TRP:CH2	2.39	0.57
1:D:19:ASP:OD2	1:D:168:SER:HB3	2.05	0.57
1:C:128:CYS:SG	1:C:178:GLN:HG2	2.44	0.57
1:C:19:ASP:OD2	1:C:168:SER:HB3	2.04	0.57
1:C:56:ARG:HD3	1:C:58:TYR:OH	2.05	0.57
1:A:10:HIS:O	1:A:11:VAL:CG2	2.51	0.57
1:B:19:ASP:OD2	1:B:168:SER:HB3	2.05	0.56
1:B:191:GLU:O	1:B:192:ALA:HB2	2.04	0.56
1:C:148:GLU:O	1:C:148:GLU:HG3	2.04	0.56
1:D:213:ILE:HG12	1:D:354:ARG:HB2	1.86	0.56
1:C:67:TYR:O	1:C:78:SER:HB3	2.04	0.56
1:D:222:VAL:HG11	1:D:329:ILE:HG21	1.87	0.56
1:B:213:ILE:HG12	1:B:354:ARG:HB2	1.86	0.56
1:B:56:ARG:HD3	1:B:58:TYR:OH	2.05	0.56
1:A:201:LYS:HB3	1:A:229:SER:O	2.06	0.56
1:A:201:LYS:HG2	1:A:229:SER:O	2.05	0.56
1:A:222:VAL:HG11	1:A:329:ILE:HG21	1.88	0.56
1:C:254:TYR:CE2	1:C:256:ILE:HD11	2.41	0.56
1:C:91:PHE:CB	1:C:92:PRO:HD3	2.33	0.56
1:A:232:LYS:HD2	2:A:385:HOH:O	2.04	0.56
1:B:192:ALA:HB1	1:B:194:TRP:CH2	2.40	0.56
1:B:128:CYS:SG	1:B:178:GLN:HG2	2.44	0.56
1:C:124:ASP:HB3	2:C:437:HOH:O	2.06	0.56
1:D:134:PRO:HD2	1:D:142:SER:HB3	1.88	0.56
1:D:228:ASN:ND2	1:D:268:VAL:O	2.32	0.56
1:D:254:TYR:CE2	1:D:256:ILE:HD11	2.41	0.56
1:B:222:VAL:HG11	1:B:329:ILE:HG21	1.88	0.55
1:A:265:GLN:HA	1:A:265:GLN:NE2	2.21	0.55
1:C:10:HIS:O	1:C:11:VAL:CG2	2.50	0.55
1:C:275:THR:O	1:D:345:SER:HA	2.06	0.55
1:C:222:VAL:HG11	1:C:329:ILE:HG21	1.87	0.55
1:A:254:TYR:CE2	1:A:256:ILE:HD11	2.41	0.55
1:A:235:LYS:HE2	1:A:336:SER:HB3	1.89	0.55
1:A:47:VAL:HB	1:A:52:VAL:HG21	1.88	0.55
1:A:18:ARG:HD2	1:A:167:LYS:HB2	1.89	0.55
1:A:72:ILE:HD11	1:A:298:LYS:HE2	1.87	0.55
1:B:2:LYS:HE3	1:B:29:ARG:CD	2.37	0.55
1:C:5:LYS:HE2	2:C:440:HOH:O	2.06	0.55
1:A:128:CYS:SG	1:A:178:GLN:HG2	2.47	0.55
1:B:249:LEU:HD22	1:B:322:GLY:HA2	1.87	0.55
1:A:91:PHE:CB	1:A:92:PRO:HD3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PRO:HD2	1:B:142:SER:HB3	1.87	0.54
1:B:136:PRO:HD3	1:B:291:ARG:NH1	2.22	0.54
1:C:66:ARG:HB2	1:C:71:ASP:OD1	2.06	0.54
1:C:72:ILE:HD11	1:C:298:LYS:HE2	1.88	0.54
1:B:2:LYS:HE3	1:B:29:ARG:HD3	1.90	0.54
1:D:18:ARG:HD2	1:D:167:LYS:HB2	1.90	0.54
1:D:277:THR:HG23	2:D:413:HOH:O	2.06	0.54
1:C:130:VAL:HG21	2:C:421:HOH:O	2.07	0.54
1:D:160:GLU:OE1	1:D:160:GLU:HA	2.08	0.54
1:D:189:ARG:HG2	2:D:378:HOH:O	2.08	0.54
1:D:238:LYS:HD3	2:D:372:HOH:O	2.07	0.54
1:A:79:PHE:CD2	1:A:250:TYR:HB2	2.43	0.54
1:B:160:GLU:HA	1:B:160:GLU:OE1	2.08	0.54
1:D:212:GLU:HG3	1:D:213:ILE:HG13	1.89	0.54
1:B:127:PRO:O	1:B:176:LYS:HE2	2.08	0.54
1:C:127:PRO:O	1:C:176:LYS:HE2	2.07	0.54
1:C:265:GLN:NE2	1:C:265:GLN:HA	2.22	0.54
1:A:2:LYS:HE3	1:A:29:ARG:CD	2.37	0.54
1:C:212:GLU:HG3	1:C:213:ILE:HG13	1.90	0.54
1:C:35:VAL:CG1	1:C:181:PRO:HB3	2.37	0.54
1:C:276:LYS:HE2	1:D:342:LEU:HG	1.90	0.53
1:C:192:ALA:CB	1:C:349:THR:HG21	2.39	0.53
1:A:127:PRO:O	1:A:176:LYS:HE2	2.08	0.53
1:A:136:PRO:HD3	1:A:291:ARG:NH1	2.23	0.53
1:D:136:PRO:HD3	1:D:291:ARG:NH1	2.24	0.53
1:C:182:ARG:HD2	2:C:394:HOH:O	2.08	0.53
1:C:233:THR:OG1	1:C:270:PRO:HD3	2.08	0.53
1:D:128:CYS:SG	1:D:178:GLN:HG2	2.48	0.53
1:D:236:LYS:HZ3	1:D:263:GLU:CD	2.12	0.53
1:B:249:LEU:HD13	1:B:319:THR:O	2.09	0.53
1:A:212:GLU:HG3	1:A:213:ILE:HG13	1.91	0.53
1:C:110:LYS:HG3	2:C:439:HOH:O	2.07	0.53
1:C:136:PRO:HD3	1:C:291:ARG:NH1	2.23	0.53
1:D:123:PRO:HG2	1:D:126:LEU:HG	1.91	0.53
1:D:231:GLU:C	1:D:270:PRO:HG3	2.29	0.53
1:A:265:GLN:C	1:A:266:GLU:HG2	2.29	0.53
1:B:18:ARG:HD2	1:B:167:LYS:HB2	1.90	0.53
1:C:123:PRO:HG2	1:C:126:LEU:HG	1.91	0.53
1:C:160:GLU:OE1	1:C:160:GLU:HA	2.08	0.53
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.09	0.52
1:C:311:ILE:O	1:C:311:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:HIS:HD2	2:B:408:HOH:O	1.92	0.52
1:D:127:PRO:O	1:D:176:LYS:HE2	2.08	0.52
1:A:268:VAL:HG13	1:A:274:LEU:HB2	1.91	0.52
1:B:212:GLU:HG3	1:B:213:ILE:HG13	1.91	0.52
1:D:249:LEU:HD13	1:D:319:THR:O	2.09	0.52
1:A:3:ALA:O	1:A:4:ASN:HB2	2.08	0.52
1:A:123:PRO:HG2	1:A:126:LEU:HG	1.91	0.52
1:A:249:LEU:HD13	1:A:319:THR:O	2.09	0.52
1:C:59:VAL:HA	1:C:150:LYS:O	2.10	0.52
1:D:71:ASP:OD2	1:D:141:LYS:HB3	2.09	0.52
1:B:254:TYR:HE2	1:B:256:ILE:HD11	1.74	0.52
1:D:254:TYR:HE2	1:D:256:ILE:HD11	1.75	0.52
1:A:59:VAL:HA	1:A:150:LYS:O	2.10	0.52
1:A:264:ALA:HB1	1:A:276:LYS:CD	2.40	0.52
1:B:59:VAL:HA	1:B:150:LYS:O	2.10	0.52
1:C:249:LEU:HD13	1:C:319:THR:O	2.10	0.52
1:A:68:GLY:HA3	1:A:78:SER:HB2	1.91	0.52
1:C:20:LYS:HE3	2:C:380:HOH:O	2.10	0.52
1:D:32:ILE:HG23	1:D:179:HIS:CD2	2.45	0.52
1:A:32:ILE:HG23	1:A:179:HIS:CD2	2.46	0.51
1:C:265:GLN:C	1:C:266:GLU:HG2	2.29	0.51
1:C:354:ARG:NH1	1:C:354:ARG:HG3	2.25	0.51
1:C:48:ASP:O	1:C:52:VAL:HG22	2.10	0.51
1:B:211:LYS:HD3	1:B:213:ILE:O	2.10	0.51
1:B:48:ASP:O	1:B:52:VAL:HG22	2.10	0.51
1:C:5:LYS:NZ	2:C:410:HOH:O	2.43	0.51
1:A:354:ARG:HG3	1:A:354:ARG:NH1	2.25	0.51
1:D:91:PHE:O	1:D:93:PRO:HD3	2.10	0.51
1:B:231:GLU:C	1:B:270:PRO:HG3	2.31	0.51
1:B:311:ILE:HG22	1:B:311:ILE:O	2.10	0.51
1:C:134:PRO:HG3	1:C:140:GLY:O	2.10	0.51
1:C:18:ARG:HD2	1:C:167:LYS:HB2	1.90	0.51
1:D:59:VAL:HA	1:D:150:LYS:O	2.10	0.51
1:D:211:LYS:HD3	1:D:213:ILE:O	2.10	0.51
1:C:211:LYS:HD3	1:C:213:ILE:O	2.10	0.51
1:C:102:ARG:NH1	1:C:368:ALA:HB3	2.24	0.51
1:A:188:PRO:HB2	1:A:209:LEU:HB2	1.93	0.51
1:A:344:SER:HB3	2:A:405:HOH:O	2.11	0.51
1:C:276:LYS:HZ1	1:D:342:LEU:HD12	1.74	0.51
1:A:190:ALA:HB2	1:A:351:VAL:HG22	1.92	0.51
1:A:211:LYS:HD3	1:A:213:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:HG3	1:A:140:GLY:O	2.11	0.51
1:B:329:ILE:O	1:B:350:GLU:HA	2.11	0.51
1:B:25:TYR:HE2	1:B:46:LEU:HB2	1.76	0.51
1:C:32:ILE:HG23	1:C:179:HIS:CD2	2.45	0.51
1:D:2:LYS:HE3	1:D:29:ARG:CD	2.40	0.51
1:D:311:ILE:HG22	1:D:311:ILE:O	2.11	0.51
1:D:329:ILE:O	1:D:350:GLU:HA	2.10	0.51
1:A:48:ASP:O	1:A:52:VAL:HG22	2.11	0.51
1:B:106:SER:O	1:B:110:LYS:HB2	2.11	0.51
1:B:123:PRO:HG2	1:B:126:LEU:HG	1.92	0.51
1:B:236:LYS:HZ3	1:B:263:GLU:CD	2.14	0.51
1:C:106:SER:O	1:C:110:LYS:HB2	2.11	0.51
1:C:254:TYR:HE2	1:C:256:ILE:HD11	1.76	0.51
1:D:194:TRP:CD2	1:D:349:THR:HG21	2.46	0.51
1:A:106:SER:O	1:A:110:LYS:HB2	2.11	0.50
1:D:354:ARG:HG3	1:D:354:ARG:NH1	2.26	0.50
1:A:336:SER:HB2	1:A:343:THR:OG1	2.11	0.50
1:A:329:ILE:O	1:A:350:GLU:HA	2.11	0.50
1:C:248:VAL:O	1:C:319:THR:HG22	2.12	0.50
1:C:25:TYR:HE2	1:C:46:LEU:HB2	1.76	0.50
1:D:25:TYR:HE2	1:D:46:LEU:HB2	1.76	0.50
1:C:68:GLY:HA3	1:C:78:SER:HB2	1.92	0.50
1:C:184:MET:CE	1:C:213:ILE:HB	2.41	0.50
1:A:103:LEU:HD22	1:A:107:LEU:HD12	1.94	0.50
1:A:341:GLU:HB3	2:A:405:HOH:O	2.11	0.50
1:B:354:ARG:NH2	2:B:376:HOH:O	2.45	0.50
1:D:132:LEU:HD23	1:D:133:GLN:N	2.27	0.50
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.77	0.50
1:C:329:ILE:O	1:C:350:GLU:HA	2.12	0.50
1:C:3:ALA:O	1:C:4:ASN:HB2	2.11	0.50
1:D:48:ASP:O	1:D:52:VAL:HG22	2.11	0.50
1:B:75:MET:O	1:B:76:GLY:C	2.50	0.50
1:C:103:LEU:HD22	1:C:107:LEU:HD12	1.94	0.50
1:D:299:ILE:HG22	2:D:420:HOH:O	2.11	0.50
1:A:254:TYR:HE2	1:A:256:ILE:HD11	1.75	0.50
1:B:32:ILE:HG23	1:B:179:HIS:CD2	2.46	0.50
1:B:248:VAL:O	1:B:319:THR:HG22	2.12	0.50
1:D:106:SER:O	1:D:110:LYS:HB2	2.11	0.50
1:D:55:LYS:HB3	1:D:155:HIS:HB3	1.94	0.50
1:A:25:TYR:HE2	1:A:46:LEU:HB2	1.76	0.49
1:B:132:LEU:HD23	1:B:133:GLN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HD23	1:C:133:GLN:N	2.27	0.49
1:A:248:VAL:O	1:A:319:THR:HG22	2.12	0.49
1:A:4:ASN:ND2	2:A:426:HOH:O	2.45	0.49
1:D:283:LEU:O	1:D:286:ASN:HB2	2.12	0.49
1:D:248:VAL:O	1:D:319:THR:HG22	2.12	0.49
1:A:311:ILE:HG22	1:A:311:ILE:O	2.11	0.49
1:B:283:LEU:O	1:B:286:ASN:HB2	2.12	0.49
1:C:354:ARG:HH11	1:C:354:ARG:HG3	1.77	0.49
1:D:134:PRO:HG3	1:D:140:GLY:O	2.12	0.49
1:D:336:SER:HB2	1:D:343:THR:OG1	2.12	0.49
1:A:300:LYS:HE2	1:A:300:LYS:N	2.28	0.49
1:B:354:ARG:HG3	1:B:354:ARG:NH1	2.27	0.49
1:A:35:VAL:CG1	1:A:181:PRO:HB3	2.41	0.49
1:B:103:LEU:HD22	1:B:107:LEU:HD12	1.94	0.49
1:A:15:LYS:NZ	2:A:388:HOH:O	2.45	0.49
1:A:276:LYS:HZ1	1:B:342:LEU:HD12	1.78	0.49
1:A:283:LEU:O	1:A:286:ASN:HB2	2.12	0.49
1:B:238:LYS:HG3	1:B:263:GLU:CB	2.40	0.49
1:D:246:ASN:ND2	2:D:430:HOH:O	2.45	0.49
1:C:362:ASP:N	1:C:363:PRO:HD3	2.28	0.49
1:A:132:LEU:HD23	1:A:133:GLN:N	2.28	0.49
1:B:295:LEU:HD12	1:B:295:LEU:N	2.28	0.49
1:C:283:LEU:O	1:C:286:ASN:HB2	2.12	0.49
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.78	0.49
1:D:75:MET:O	1:D:76:GLY:C	2.50	0.49
1:A:55:LYS:HB3	1:A:155:HIS:HB3	1.95	0.48
1:A:91:PHE:CB	1:A:92:PRO:CD	2.90	0.48
1:C:342:LEU:CD1	2:C:417:HOH:O	2.58	0.48
1:B:134:PRO:HG3	1:B:140:GLY:O	2.12	0.48
1:B:55:LYS:HB3	1:B:155:HIS:HB3	1.95	0.48
1:A:362:ASP:N	1:A:363:PRO:HD3	2.28	0.48
1:C:55:LYS:HB3	1:C:155:HIS:HB3	1.95	0.48
1:A:72:ILE:HG23	1:A:173:LEU:HD11	1.95	0.48
1:B:199:SER:O	1:B:200:ASP:HB2	2.13	0.48
1:C:195:GLN:HE21	1:C:200:ASP:HA	1.78	0.48
1:A:184:MET:HB2	1:A:212:GLU:CG	2.43	0.48
1:C:91:PHE:O	1:C:93:PRO:HD3	2.14	0.48
1:B:91:PHE:O	1:B:93:PRO:HD3	2.13	0.48
1:D:91:PHE:CB	1:D:92:PRO:CD	2.90	0.48
1:C:79:PHE:CD2	1:C:250:TYR:HB2	2.48	0.48
1:D:103:LEU:HD22	1:D:107:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:NH2	2:B:384:HOH:O	2.47	0.48
1:C:12:ILE:HD12	1:C:107:LEU:HD21	1.96	0.48
1:B:194:TRP:CD2	1:B:349:THR:HG21	2.49	0.47
1:B:61:LEU:HD13	1:B:149:ILE:HD12	1.96	0.47
1:A:295:LEU:HD12	1:A:295:LEU:N	2.29	0.47
1:A:12:ILE:HD12	1:A:107:LEU:HD21	1.96	0.47
1:A:195:GLN:HE21	1:A:200:ASP:HA	1.79	0.47
1:C:336:SER:HB2	1:C:343:THR:OG1	2.13	0.47
1:C:61:LEU:HD13	1:C:149:ILE:HD12	1.97	0.47
1:A:61:LEU:HD13	1:A:149:ILE:HD12	1.97	0.47
1:B:336:SER:HB2	1:B:343:THR:OG1	2.14	0.47
1:D:164:ILE:HB	2:D:393:HOH:O	2.15	0.47
1:D:295:LEU:HD12	1:D:295:LEU:N	2.29	0.47
1:D:300:LYS:N	1:D:300:LYS:HE2	2.29	0.47
1:D:21:SER:HB3	1:D:51:LEU:HB3	1.96	0.47
1:D:57:VAL:HB	1:D:91:PHE:HB2	1.96	0.47
1:B:91:PHE:CB	1:B:92:PRO:CD	2.91	0.47
1:A:212:GLU:OE2	1:A:354:ARG:NH1	2.48	0.47
1:A:21:SER:HB3	1:A:51:LEU:HB3	1.97	0.47
1:C:91:PHE:CB	1:C:92:PRO:CD	2.91	0.47
1:D:61:LEU:HD13	1:D:149:ILE:HD12	1.97	0.47
1:D:265:GLN:CD	1:D:265:GLN:H	2.18	0.47
1:A:19:ASP:OD1	1:A:167:LYS:HE2	2.15	0.47
1:B:231:GLU:HA	1:B:270:PRO:HG3	1.97	0.47
1:B:65:PHE:CD2	1:B:249:LEU:HD23	2.50	0.47
1:C:2:LYS:HE3	1:C:29:ARG:CD	2.44	0.47
1:B:135:ALA:HA	1:B:291:ARG:HB3	1.96	0.47
1:C:212:GLU:OE2	1:C:354:ARG:NH1	2.48	0.47
1:D:199:SER:O	1:D:200:ASP:HB2	2.14	0.47
1:A:2:LYS:HE3	1:A:29:ARG:HD2	1.96	0.47
1:C:74:VAL:O	1:C:74:VAL:HG22	2.15	0.47
1:C:135:ALA:HA	1:C:291:ARG:HB3	1.97	0.46
1:C:295:LEU:HD12	1:C:295:LEU:N	2.29	0.46
1:D:337:GLY:H	1:D:343:THR:CA	2.28	0.46
1:A:337:GLY:N	1:A:343:THR:HA	2.28	0.46
1:A:276:LYS:CE	1:B:342:LEU:HG	2.42	0.46
1:C:47:VAL:HB	1:C:52:VAL:HG21	1.96	0.46
1:A:232:LYS:HG2	1:A:337:GLY:CA	2.46	0.46
1:C:194:TRP:CE2	1:C:347:VAL:HB	2.51	0.46
1:D:12:ILE:HD12	1:D:107:LEU:HD21	1.97	0.46
1:B:21:SER:HB3	1:B:51:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:HB	1:B:91:PHE:HB2	1.96	0.46
1:B:35:VAL:CG2	1:B:36:GLU:N	2.79	0.46
1:C:35:VAL:CG2	1:C:36:GLU:N	2.79	0.46
1:D:212:GLU:OE2	1:D:354:ARG:NH1	2.49	0.46
1:D:65:PHE:CE2	1:D:249:LEU:HB3	2.51	0.46
1:A:65:PHE:CE2	1:A:249:LEU:HB3	2.51	0.46
1:A:74:VAL:HG22	1:A:74:VAL:O	2.16	0.46
1:B:157:THR:CG2	1:B:163:LYS:HD2	2.44	0.46
1:A:337:GLY:H	1:A:343:THR:CA	2.26	0.46
1:B:265:GLN:H	1:B:265:GLN:CD	2.18	0.46
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.79	0.46
1:C:86:SER:HA	2:C:424:HOH:O	2.16	0.46
1:A:65:PHE:CD2	1:A:249:LEU:HD23	2.50	0.46
1:D:47:VAL:HB	1:D:52:VAL:HG21	1.96	0.46
1:B:65:PHE:CE2	1:B:249:LEU:HB3	2.50	0.46
1:B:300:LYS:N	1:B:300:LYS:HE2	2.29	0.46
1:C:65:PHE:CD2	1:C:249:LEU:HD23	2.51	0.46
1:A:184:MET:HB3	1:A:213:ILE:CD1	2.46	0.45
1:B:4:ASN:O	1:B:13:PHE:HB3	2.15	0.45
1:B:50:GLU:HA	1:B:53:LYS:HB2	1.98	0.45
1:C:337:GLY:N	1:C:343:THR:HA	2.30	0.45
1:D:238:LYS:HG3	1:D:263:GLU:CB	2.43	0.45
1:D:50:GLU:HA	1:D:53:LYS:HB2	1.98	0.45
1:A:335:VAL:HG12	1:A:336:SER:N	2.32	0.45
1:B:12:ILE:HD12	1:B:107:LEU:HD21	1.97	0.45
1:A:184:MET:HE2	1:A:213:ILE:HB	1.97	0.45
1:C:131:MET:HB2	1:C:131:MET:HE3	1.83	0.45
1:D:28:LYS:HD3	1:D:30:ASP:O	2.16	0.45
1:D:35:VAL:CG2	1:D:36:GLU:N	2.79	0.45
1:A:65:PHE:CG	1:A:249:LEU:HD23	2.51	0.45
1:C:207:VAL:HB	1:C:351:VAL:HG21	1.98	0.45
1:D:149:ILE:HG22	1:D:172:LEU:HB2	1.98	0.45
1:D:337:GLY:N	1:D:343:THR:HA	2.30	0.45
1:B:232:LYS:HG2	1:B:337:GLY:CA	2.46	0.45
1:A:57:VAL:HB	1:A:91:PHE:HB2	1.97	0.45
1:C:19:ASP:HB2	1:C:167:LYS:C	2.37	0.45
1:C:19:ASP:OD1	1:C:167:LYS:HE2	2.17	0.45
1:C:28:LYS:HD3	1:C:30:ASP:O	2.17	0.45
1:B:149:ILE:HG22	1:B:172:LEU:HB2	1.98	0.45
1:B:249:LEU:HA	1:B:249:LEU:HD12	1.83	0.45
1:D:19:ASP:HB2	1:D:167:LYS:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:LYS:HE3	1:D:29:ARG:HD3	1.98	0.45
1:A:184:MET:CE	1:A:213:ILE:HB	2.46	0.45
1:A:194:TRP:NE1	1:A:347:VAL:HB	2.31	0.45
1:A:35:VAL:CG2	1:A:36:GLU:N	2.79	0.45
1:B:28:LYS:HD3	1:B:30:ASP:O	2.16	0.45
1:C:65:PHE:CE2	1:C:249:LEU:HB3	2.51	0.45
1:D:269:PRO:HB2	1:D:270:PRO:HD2	1.98	0.45
1:D:231:GLU:HA	1:D:270:PRO:HG3	1.98	0.45
1:B:269:PRO:HB2	1:B:270:PRO:HD2	1.98	0.45
1:B:212:GLU:OE2	1:B:354:ARG:NH1	2.50	0.45
1:C:155:HIS:HE1	1:C:165:PRO:HG2	1.81	0.45
1:C:102:ARG:NH2	2:C:438:HOH:O	2.36	0.45
1:C:98:GLY:O	1:C:99:ALA:C	2.55	0.45
1:A:264:ALA:HB1	1:A:276:LYS:HD3	1.98	0.44
1:A:276:LYS:HZ3	1:B:342:LEU:HA	1.82	0.44
1:D:65:PHE:CG	1:D:249:LEU:HD23	2.52	0.44
1:D:65:PHE:CD2	1:D:249:LEU:HD23	2.51	0.44
1:A:201:LYS:NZ	2:A:416:HOH:O	2.49	0.44
1:B:131:MET:HE3	1:B:131:MET:HB2	1.83	0.44
1:B:19:ASP:HB2	1:B:167:LYS:C	2.37	0.44
1:C:149:ILE:HG22	1:C:172:LEU:HB2	1.99	0.44
1:A:135:ALA:HA	1:A:291:ARG:HB3	1.99	0.44
1:A:167:LYS:HG2	1:A:168:SER:N	2.33	0.44
1:A:98:GLY:O	1:A:99:ALA:C	2.55	0.44
1:B:337:GLY:N	1:B:343:THR:HA	2.32	0.44
1:D:155:HIS:HE1	1:D:165:PRO:HG2	1.82	0.44
1:D:13:PHE:HE1	1:D:29:ARG:HH21	1.65	0.44
1:D:232:LYS:HG2	1:D:337:GLY:CA	2.47	0.44
1:B:19:ASP:OD1	1:B:167:LYS:HE2	2.17	0.44
1:C:341:GLU:N	2:C:417:HOH:O	2.49	0.44
1:A:360:PRO:HB2	1:A:362:ASP:OD1	2.18	0.44
1:B:210:SER:OG	1:B:221:PRO:HG2	2.17	0.44
1:B:98:GLY:O	1:B:99:ALA:C	2.56	0.44
1:A:157:THR:CG2	1:A:163:LYS:HD2	2.46	0.44
1:A:207:VAL:HB	1:A:351:VAL:HG21	2.00	0.44
1:B:155:HIS:HE1	1:B:165:PRO:HG2	1.82	0.44
1:B:167:LYS:HG2	1:B:168:SER:N	2.33	0.44
1:C:337:GLY:H	1:C:343:THR:CA	2.28	0.44
1:C:65:PHE:CG	1:C:249:LEU:HD23	2.52	0.44
1:D:207:VAL:HB	1:D:351:VAL:HG21	2.00	0.44
1:D:98:GLY:O	1:D:99:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:O	1:A:92:PRO:C	2.55	0.44
1:B:65:PHE:CG	1:B:249:LEU:HD23	2.52	0.44
1:B:320:VAL:O	1:B:320:VAL:HG12	2.18	0.44
1:D:19:ASP:OD1	1:D:167:LYS:HE2	2.17	0.44
1:B:11:VAL:O	1:B:11:VAL:HG12	2.17	0.44
1:D:131:MET:HE3	1:D:131:MET:HB2	1.87	0.44
1:D:167:LYS:HG2	1:D:168:SER:N	2.32	0.44
1:A:149:ILE:HG22	1:A:172:LEU:HB2	2.00	0.44
1:D:2:LYS:HE3	1:D:29:ARG:HD2	2.00	0.44
1:A:137:GLN:H	1:A:137:GLN:HG3	1.51	0.43
1:B:3:ALA:O	1:B:4:ASN:HB2	2.18	0.43
1:C:137:GLN:H	1:C:137:GLN:HG3	1.51	0.43
1:C:167:LYS:HG2	1:C:168:SER:N	2.32	0.43
1:B:75:MET:HG2	1:C:189:ARG:HB2	2.00	0.43
1:D:15:LYS:O	1:D:170:VAL:HG11	2.18	0.43
1:D:157:THR:CG2	1:D:163:LYS:HD2	2.43	0.43
1:B:15:LYS:O	1:B:170:VAL:HG11	2.17	0.43
1:C:210:SER:OG	1:C:221:PRO:HG2	2.17	0.43
1:C:262:GLU:HB2	1:C:280:LEU:HD21	1.99	0.43
1:C:363:PRO:O	1:C:364:ASP:HB3	2.18	0.43
1:A:195:GLN:CB	1:D:81:ARG:HG2	2.43	0.43
1:B:195:GLN:HE21	1:B:204:ARG:HH11	1.65	0.43
1:D:135:ALA:HA	1:D:291:ARG:HB3	1.98	0.43
1:A:155:HIS:HE1	1:A:165:PRO:HG2	1.82	0.43
1:B:207:VAL:HB	1:B:351:VAL:HG21	1.99	0.43
1:C:91:PHE:O	1:C:92:PRO:C	2.55	0.43
1:A:19:ASP:HB2	1:A:167:LYS:C	2.38	0.43
1:A:185:GLY:N	1:A:212:GLU:HG2	2.34	0.43
1:A:194:TRP:HH2	1:A:205:LEU:HD23	1.83	0.43
1:A:2:LYS:HE3	1:A:29:ARG:HD3	1.98	0.43
1:C:2:LYS:HE3	1:C:29:ARG:HD2	2.00	0.43
1:D:91:PHE:O	1:D:93:PRO:CD	2.67	0.43
1:A:200:ASP:HB3	2:A:396:HOH:O	2.19	0.43
1:A:363:PRO:O	1:A:364:ASP:HB3	2.18	0.43
1:C:21:SER:HB3	1:C:51:LEU:HB3	2.00	0.43
1:D:194:TRP:CZ2	1:D:349:THR:HB	2.53	0.43
1:D:211:LYS:H	1:D:211:LYS:HG3	1.73	0.43
1:D:3:ALA:O	1:D:4:ASN:HB2	2.19	0.43
1:B:133:GLN:HA	1:B:134:PRO:HD2	1.90	0.43
1:B:195:GLN:NE2	1:B:204:ARG:HH11	2.16	0.43
1:B:57:VAL:H	1:B:91:PHE:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LYS:H	1:C:211:LYS:HG3	1.72	0.43
1:C:266:GLU:CD	1:C:276:LYS:HD2	2.39	0.43
1:D:158:ASP:C	1:D:160:GLU:H	2.22	0.43
1:D:210:SER:OG	1:D:221:PRO:HG2	2.19	0.43
1:C:360:PRO:HB2	1:C:362:ASP:OD1	2.18	0.43
1:A:184:MET:HB2	1:A:212:GLU:HG3	2.01	0.43
1:A:6:PRO:HA	1:A:12:ILE:O	2.19	0.43
1:D:104:GLN:H	1:D:104:GLN:HG2	1.61	0.43
1:D:57:VAL:H	1:D:91:PHE:HB3	1.84	0.43
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.34	0.43
1:C:300:LYS:N	1:C:300:LYS:HE2	2.29	0.43
1:D:300:LYS:NZ	1:D:300:LYS:HB3	2.34	0.43
1:B:47:VAL:HB	1:B:52:VAL:HG21	1.99	0.42
1:D:198:MET:O	1:D:199:SER:HB2	2.19	0.42
1:A:137:GLN:O	1:D:18:ARG:NH1	2.52	0.42
1:A:177:VAL:HG23	1:A:179:HIS:CD2	2.55	0.42
1:A:91:PHE:O	1:A:93:PRO:HD3	2.17	0.42
1:B:300:LYS:NZ	1:B:300:LYS:HB3	2.33	0.42
1:C:268:VAL:HG13	1:C:274:LEU:HB2	2.00	0.42
1:D:14:LYS:HA	1:D:24:ILE:O	2.20	0.42
1:A:28:LYS:HD3	1:A:30:ASP:O	2.18	0.42
1:A:357:HIS:HE1	2:A:442:HOH:O	2.02	0.42
1:A:4:ASN:O	1:A:13:PHE:HB3	2.20	0.42
1:B:337:GLY:H	1:B:343:THR:CA	2.30	0.42
1:C:15:LYS:O	1:C:170:VAL:HG11	2.19	0.42
1:C:262:GLU:HB3	1:C:278:LEU:HD23	2.00	0.42
1:D:4:ASN:O	1:D:13:PHE:HB3	2.20	0.42
1:A:284:LEU:HD11	1:A:290:ARG:HG2	2.01	0.42
1:A:190:ALA:CB	1:A:351:VAL:HG22	2.49	0.42
1:B:341:GLU:C	1:B:343:THR:H	2.23	0.42
1:B:62:THR:HG23	1:B:85:PHE:HD1	1.84	0.42
1:C:284:LEU:HD11	1:C:290:ARG:HG2	2.01	0.42
1:D:177:VAL:HG23	1:D:179:HIS:CD2	2.55	0.42
1:D:62:THR:HG23	1:D:85:PHE:HD1	1.84	0.42
1:A:184:MET:HE1	1:A:213:ILE:H	1.85	0.42
1:C:184:MET:HB3	1:C:213:ILE:CD1	2.42	0.42
1:C:320:VAL:HG12	1:C:320:VAL:O	2.20	0.42
1:A:184:MET:HB2	1:A:212:GLU:HG2	2.02	0.42
1:A:232:LYS:HG2	1:A:337:GLY:HA2	2.02	0.42
1:B:14:LYS:HA	1:B:24:ILE:O	2.19	0.42
1:C:184:MET:HB2	1:C:212:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PHE:O	1:C:93:PRO:N	2.53	0.42
1:D:195:GLN:HE21	1:D:204:ARG:HH11	1.67	0.42
1:B:158:ASP:C	1:B:160:GLU:H	2.22	0.42
1:B:284:LEU:HD11	1:B:290:ARG:HG2	2.01	0.42
1:C:132:LEU:HD12	1:C:245:THR:HG21	2.01	0.42
1:C:4:ASN:O	1:C:13:PHE:HB3	2.20	0.42
1:D:284:LEU:HD11	1:D:290:ARG:HG2	2.01	0.42
1:A:15:LYS:O	1:A:170:VAL:HG11	2.19	0.42
1:B:198:MET:O	1:B:199:SER:HB2	2.19	0.42
1:C:14:LYS:HA	1:C:24:ILE:O	2.20	0.42
1:C:158:ASP:C	1:C:160:GLU:H	2.23	0.42
1:C:180:ALA:HB2	1:C:215:TYR:HE1	1.85	0.42
1:D:241:VAL:HB	1:D:260:ALA:HB3	2.02	0.42
1:D:91:PHE:O	1:D:92:PRO:C	2.58	0.42
1:A:208:SER:HB2	2:A:394:HOH:O	2.20	0.42
1:A:210:SER:OG	1:A:221:PRO:HG2	2.20	0.42
1:A:3:ALA:O	1:A:4:ASN:CB	2.68	0.42
1:B:241:VAL:HB	1:B:260:ALA:HB3	2.02	0.42
1:D:231:GLU:O	1:D:270:PRO:HG3	2.20	0.42
1:D:281:VAL:HG12	1:D:283:LEU:HG	2.02	0.42
1:D:6:PRO:HA	1:D:12:ILE:O	2.20	0.42
1:A:132:LEU:HD12	1:A:245:THR:HG21	2.02	0.41
1:B:194:TRP:CZ2	1:B:349:THR:HB	2.55	0.41
1:C:266:GLU:OE2	1:C:276:LYS:HE2	2.20	0.41
1:C:13:PHE:HE1	1:C:29:ARG:HH21	1.64	0.41
1:C:300:LYS:NZ	1:C:300:LYS:HB3	2.34	0.41
1:A:62:THR:HG23	1:A:85:PHE:HD1	1.85	0.41
1:B:48:ASP:HA	1:B:49:PRO:HD2	1.84	0.41
1:B:6:PRO:HA	1:B:12:ILE:O	2.19	0.41
1:C:133:GLN:HA	1:C:134:PRO:HD2	1.90	0.41
1:C:241:VAL:HB	1:C:260:ALA:HB3	2.02	0.41
1:C:57:VAL:HB	1:C:91:PHE:HB2	2.01	0.41
1:B:132:LEU:HD12	1:B:245:THR:HG21	2.03	0.41
1:B:211:LYS:H	1:B:211:LYS:HG3	1.73	0.41
1:D:195:GLN:NE2	1:D:204:ARG:HH11	2.18	0.41
1:D:341:GLU:C	1:D:343:THR:H	2.24	0.41
1:A:14:LYS:HA	1:A:24:ILE:O	2.20	0.41
1:A:281:VAL:HG12	1:A:283:LEU:HG	2.02	0.41
1:D:132:LEU:HD12	1:D:245:THR:HG21	2.02	0.41
1:A:104:GLN:HG2	1:A:104:GLN:H	1.62	0.41
1:A:180:ALA:HB2	1:A:215:TYR:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:O	1:A:320:VAL:HG12	2.19	0.41
1:D:79:PHE:CD2	1:D:250:TYR:HB2	2.56	0.41
1:D:230:THR:O	1:D:270:PRO:HB3	2.21	0.41
1:D:320:VAL:HG12	1:D:320:VAL:O	2.19	0.41
1:A:241:VAL:HB	1:A:260:ALA:HB3	2.02	0.41
1:B:318:LYS:NZ	2:B:387:HOH:O	2.53	0.41
1:A:158:ASP:C	1:A:160:GLU:H	2.24	0.41
1:A:71:ASP:O	1:A:72:ILE:HG13	2.21	0.41
1:C:177:VAL:HG23	1:C:179:HIS:CD2	2.55	0.41
1:C:249:LEU:HA	1:C:249:LEU:HD12	1.82	0.41
1:D:191:GLU:O	1:D:192:ALA:CB	2.68	0.41
1:B:177:VAL:HG23	1:B:179:HIS:CD2	2.55	0.41
1:C:281:VAL:HG12	1:C:283:LEU:HG	2.01	0.41
1:C:232:LYS:HG2	1:C:337:GLY:CA	2.51	0.41
1:C:71:ASP:O	1:C:72:ILE:HG13	2.20	0.41
1:C:72:ILE:HG23	1:C:173:LEU:HD11	2.03	0.41
1:A:215:TYR:HA	1:A:356:MET:O	2.21	0.41
1:B:180:ALA:HB2	1:B:215:TYR:HE1	1.86	0.41
1:B:248:VAL:HG23	1:B:319:THR:HA	2.03	0.41
1:A:248:VAL:HG23	1:A:319:THR:HA	2.03	0.41
1:C:215:TYR:HA	1:C:356:MET:O	2.21	0.41
1:D:215:TYR:HA	1:D:356:MET:O	2.21	0.41
1:D:227:THR:HG22	1:D:227:THR:O	2.20	0.41
1:A:264:ALA:HB1	1:A:276:LYS:HE3	2.03	0.41
1:A:91:PHE:O	1:A:93:PRO:N	2.54	0.41
1:B:79:PHE:CD2	1:B:250:TYR:HB2	2.56	0.41
1:C:3:ALA:O	1:C:4:ASN:CB	2.69	0.41
1:B:13:PHE:O	1:B:25:TYR:HA	2.21	0.40
1:B:2:LYS:HE3	1:B:29:ARG:HD2	2.03	0.40
1:B:335:VAL:HG12	1:B:336:SER:N	2.37	0.40
1:D:248:VAL:HG23	1:D:319:THR:HA	2.03	0.40
1:A:266:GLU:OE2	1:A:276:LYS:HE2	2.22	0.40
1:A:341:GLU:C	1:A:343:THR:H	2.25	0.40
1:B:215:TYR:HA	1:B:356:MET:O	2.21	0.40
1:C:91:PHE:O	1:C:93:PRO:CD	2.69	0.40
1:C:19:ASP:O	1:C:20:LYS:HB2	2.21	0.40
1:A:201:LYS:CB	1:A:229:SER:O	2.68	0.40
1:C:62:THR:HG23	1:C:85:PHE:HD1	1.85	0.40
1:B:231:GLU:CA	1:B:270:PRO:HG3	2.51	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	366/368 (100%)	314 (86%)	40 (11%)	12 (3%)	4	28
1	B	361/368 (98%)	310 (86%)	40 (11%)	11 (3%)	5	30
1	C	366/368 (100%)	313 (86%)	41 (11%)	12 (3%)	4	28
1	D	361/368 (98%)	309 (86%)	41 (11%)	11 (3%)	5	30
All	All	1454/1472 (99%)	1246 (86%)	162 (11%)	46 (3%)	5	29

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	11	VAL
1	A	35	VAL
1	A	341	GLU
1	B	4	ASN
1	B	11	VAL
1	B	35	VAL
1	B	76	GLY
1	B	341	GLU
1	C	4	ASN
1	C	11	VAL
1	C	35	VAL
1	C	341	GLU
1	D	4	ASN
1	D	11	VAL
1	D	35	VAL
1	D	76	GLY
1	D	341	GLU
1	A	99	ALA
1	A	181	PRO
1	A	339	LEU
1	B	99	ALA

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Mol	Chain	Res	Type
1	B	192	ALA
1	B	339	LEU
1	C	99	ALA
1	C	181	PRO
1	C	339	LEU
1	D	99	ALA
1	D	192	ALA
1	D	339	LEU
1	A	73	ASP
1	A	91	PHE
1	A	159	VAL
1	B	91	PHE
1	B	159	VAL
1	C	73	ASP
1	C	91	PHE
1	C	159	VAL
1	D	91	PHE
1	D	159	VAL
1	C	185	GLY
1	A	49	PRO
1	A	185	GLY
1	B	49	PRO
1	C	49	PRO
1	D	49	PRO

### 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	327/327 (100%)	247 (76%)	80 (24%)	1	3
1	B	324/327 (99%)	244 (75%)	80 (25%)	1	2
1	C	327/327 (100%)	245 (75%)	82 (25%)	0	2
1	D	324/327 (99%)	246 (76%)	78 (24%)	1	3
All	All	1302/1308 (100%)	982 (75%)	320 (25%)	1	3

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	5	LYS
1	A	18	ARG
1	A	26	LEU
1	A	28	LYS
1	A	35	VAL
1	A	36	GLU
1	A	37	ARG
1	A	38	VAL
1	A	46	LEU
1	A	50	GLU
1	A	53	LYS
1	A	55	LYS
1	A	56	ARG
1	A	62	THR
1	A	69	GLN
1	A	73	ASP
1	A	75	MET
1	A	78	SER
1	A	81	ARG
1	A	94	VAL
1	A	97	SER
1	A	100	THR
1	A	101	THR
1	A	103	LEU
1	A	104	GLN
1	A	105	GLU
1	A	106	SER
1	A	109	LYS
1	A	110	LYS
1	A	130	VAL
1	A	131	MET
1	A	137	GLN
1	A	139	VAL
1	A	141	LYS
1	A	148	GLU
1	A	149	ILE
1	A	156	SER
1	A	159	VAL
1	A	161	GLU
1	A	163	LYS
1	A	167	LYS

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Mol	Chain	Res	Type
1	A	170	VAL
1	A	172	LEU
1	A	184	MET
1	A	193	SER
1	A	199	SER
1	A	200	ASP
1	A	201	LYS
1	A	208	SER
1	A	210	SER
1	A	211	LYS
1	A	212	GLU
1	A	222	VAL
1	A	236	LYS
1	A	240	LEU
1	A	246	ASN
1	A	262	GLU
1	A	265	GLN
1	A	266	GLU
1	A	272	SER
1	A	273	SER
1	A	276	LYS
1	A	279	THR
1	A	280	LEU
1	A	288	ARG
1	A	300	LYS
1	A	305	ASN
1	A	313	LYS
1	A	314	GLU
1	A	318	LYS
1	A	319	THR
1	A	330	LYS
1	A	332	LYS
1	A	334	THR
1	A	341	GLU
1	A	344	SER
1	A	354	ARG
1	A	359	GLN
1	A	367	LYS
1	B	2	LYS
1	B	5	LYS
1	B	18	ARG
1	B	26	LEU

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Mol	Chain	Res	Type
1	B	28	LYS
1	B	35	VAL
1	B	36	GLU
1	B	37	ARG
1	B	38	VAL
1	B	46	LEU
1	B	50	GLU
1	B	53	LYS
1	B	55	LYS
1	B	56	ARG
1	B	62	THR
1	B	69	GLN
1	B	71	ASP
1	B	75	MET
1	B	78	SER
1	B	81	ARG
1	B	94	VAL
1	B	97	SER
1	B	100	THR
1	B	101	THR
1	B	103	LEU
1	B	104	GLN
1	B	105	GLU
1	B	106	SER
1	B	109	LYS
1	B	110	LYS
1	B	130	VAL
1	B	131	MET
1	B	137	GLN
1	B	139	VAL
1	B	141	LYS
1	B	148	GLU
1	B	149	ILE
1	B	156	SER
1	B	159	VAL
1	B	161	GLU
1	B	163	LYS
1	B	167	LYS
1	B	170	VAL
1	B	171	ARG
1	B	172	LEU
1	B	182	ARG

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Mol	Chain	Res	Type
1	B	187	GLN
1	B	189	ARG
1	B	191	GLU
1	B	193	SER
1	B	198	MET
1	B	199	SER
1	B	208	SER
1	B	210	SER
1	B	211	LYS
1	B	212	GLU
1	B	222	VAL
1	B	236	LYS
1	B	240	LEU
1	B	246	ASN
1	B	262	GLU
1	B	265	GLN
1	B	273	SER
1	B	276	LYS
1	B	279	THR
1	B	280	LEU
1	B	288	ARG
1	B	300	LYS
1	B	305	ASN
1	B	313	LYS
1	B	314	GLU
1	B	318	LYS
1	B	319	THR
1	B	330	LYS
1	B	332	LYS
1	B	334	THR
1	B	338	LEU
1	B	341	GLU
1	B	344	SER
1	B	354	ARG
1	C	2	LYS
1	C	5	LYS
1	C	18	ARG
1	C	26	LEU
1	C	28	LYS
1	C	35	VAL
1	C	36	GLU
1	C	37	ARG

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Mol	Chain	Res	Type
1	C	38	VAL
1	C	46	LEU
1	C	50	GLU
1	C	53	LYS
1	C	55	LYS
1	C	56	ARG
1	C	62	THR
1	C	69	GLN
1	C	73	ASP
1	C	75	MET
1	C	78	SER
1	C	81	ARG
1	C	94	VAL
1	C	97	SER
1	C	100	THR
1	C	101	THR
1	C	103	LEU
1	C	104	GLN
1	C	105	GLU
1	C	106	SER
1	C	109	LYS
1	C	110	LYS
1	C	130	VAL
1	C	131	MET
1	C	137	GLN
1	C	139	VAL
1	C	141	LYS
1	C	148	GLU
1	C	149	ILE
1	C	156	SER
1	C	159	VAL
1	C	161	GLU
1	C	163	LYS
1	C	167	LYS
1	C	170	VAL
1	C	171	ARG
1	C	172	LEU
1	C	184	MET
1	C	193	SER
1	C	199	SER
1	C	200	ASP
1	C	201	LYS

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Mol	Chain	Res	Type
1	C	208	SER
1	C	210	SER
1	C	211	LYS
1	C	212	GLU
1	C	222	VAL
1	C	236	LYS
1	C	240	LEU
1	C	246	ASN
1	C	262	GLU
1	C	265	GLN
1	C	266	GLU
1	C	272	SER
1	C	273	SER
1	C	276	LYS
1	C	279	THR
1	C	280	LEU
1	C	288	ARG
1	C	300	LYS
1	C	305	ASN
1	C	313	LYS
1	C	314	GLU
1	C	318	LYS
1	C	319	THR
1	C	330	LYS
1	C	332	LYS
1	C	334	THR
1	C	338	LEU
1	C	341	GLU
1	C	344	SER
1	C	354	ARG
1	C	359	GLN
1	C	367	LYS
1	D	2	LYS
1	D	5	LYS
1	D	18	ARG
1	D	26	LEU
1	D	28	LYS
1	D	35	VAL
1	D	36	GLU
1	D	37	ARG
1	D	38	VAL
1	D	46	LEU

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Mol	Chain	Res	Type
1	D	50	GLU
1	D	53	LYS
1	D	55	LYS
1	D	56	ARG
1	D	62	THR
1	D	69	GLN
1	D	71	ASP
1	D	75	MET
1	D	78	SER
1	D	81	ARG
1	D	94	VAL
1	D	97	SER
1	D	100	THR
1	D	101	THR
1	D	103	LEU
1	D	104	GLN
1	D	105	GLU
1	D	106	SER
1	D	109	LYS
1	D	110	LYS
1	D	130	VAL
1	D	131	MET
1	D	137	GLN
1	D	139	VAL
1	D	141	LYS
1	D	148	GLU
1	D	149	ILE
1	D	156	SER
1	D	159	VAL
1	D	161	GLU
1	D	163	LYS
1	D	167	LYS
1	D	170	VAL
1	D	172	LEU
1	D	182	ARG
1	D	187	GLN
1	D	189	ARG
1	D	191	GLU
1	D	193	SER
1	D	198	MET
1	D	199	SER
1	D	208	SER

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Mol	Chain	Res	Type
1	D	210	SER
1	D	211	LYS
1	D	212	GLU
1	D	222	VAL
1	D	236	LYS
1	D	240	LEU
1	D	246	ASN
1	D	262	GLU
1	D	265	GLN
1	D	273	SER
1	D	276	LYS
1	D	279	THR
1	D	280	LEU
1	D	288	ARG
1	D	300	LYS
1	D	305	ASN
1	D	313	LYS
1	D	314	GLU
1	D	318	LYS
1	D	319	THR
1	D	330	LYS
1	D	332	LYS
1	D	334	THR
1	D	341	GLU
1	D	344	SER
1	D	354	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	34	HIS
1	A	89	GLN
1	A	187	GLN
1	A	265	GLN
1	A	305	ASN
1	A	357	HIS
1	B	34	HIS
1	B	89	GLN
1	B	155	HIS
1	B	195	GLN
1	B	301	HIS

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Mol	Chain	Res	Type
1	C	34	HIS
1	C	89	GLN
1	C	155	HIS
1	C	265	GLN
1	C	301	HIS
1	D	34	HIS
1	D	89	GLN
1	D	155	HIS
1	D	195	GLN
1	D	305	ASN
1	D	357	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	368/368 (100%)	-0.12	17 (4%) 33 31	2, 10, 70, 99	0
1	B	363/368 (98%)	0.08	20 (5%) 26 24	2, 29, 83, 97	0
1	C	368/368 (100%)	-0.09	18 (4%) 30 28	2, 13, 75, 99	0
1	D	363/368 (98%)	0.12	25 (6%) 18 17	2, 25, 83, 99	0
All	All	1462/1472 (99%)	-0.00	80 (5%) 26 24	2, 17, 81, 99	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	ASP	8.7
1	C	76	GLY	6.9
1	A	75	MET	6.6
1	A	76	GLY	6.3
1	C	75	MET	6.2
1	D	98	GLY	6.2
1	D	159	VAL	6.0
1	D	157	THR	5.8
1	C	339	LEU	5.3
1	B	98	GLY	5.1
1	A	74	VAL	5.0
1	C	73	ASP	4.9
1	A	365	THR	4.7
1	D	97	SER	4.7
1	A	337	GLY	4.6
1	A	344	SER	4.4
1	C	74	VAL	4.4
1	D	160	GLU	4.4
1	B	159	VAL	4.3
1	B	158	ASP	4.0
1	A	366	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	157	THR	3.9
1	D	96	ALA	3.9
1	C	340	GLY	3.9
1	C	137	GLN	3.8
1	B	10	HIS	3.8
1	B	96	ALA	3.7
1	A	368	ALA	3.7
1	A	364	ASP	3.7
1	B	340	GLY	3.6
1	C	368	ALA	3.6
1	A	363	PRO	3.5
1	B	339	LEU	3.4
1	A	345	SER	3.3
1	C	77	LEU	3.3
1	B	97	SER	3.2
1	B	56	ARG	3.1
1	B	160	GLU	3.1
1	A	9	ASN	3.0
1	D	155	HIS	3.0
1	D	186	PRO	3.0
1	B	95	GLY	3.0
1	B	137	GLN	3.0
1	C	338	LEU	3.0
1	B	363	PRO	2.9
1	C	363	PRO	2.9
1	C	365	THR	2.8
1	A	343	THR	2.8
1	C	362	ASP	2.8
1	D	95	GLY	2.8
1	A	8	PRO	2.8
1	B	155	HIS	2.8
1	D	103	LEU	2.7
1	A	338	LEU	2.7
1	D	9	ASN	2.7
1	D	362	ASP	2.6
1	B	11	VAL	2.6
1	B	55	LYS	2.6
1	C	367	LYS	2.6
1	D	10	HIS	2.5
1	D	363	PRO	2.5
1	C	10	HIS	2.5
1	D	154	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	2.4
1	C	366	ALA	2.4
1	D	99	ALA	2.4
1	D	56	ARG	2.3
1	C	364	ASP	2.3
1	A	367	LYS	2.3
1	D	73	ASP	2.2
1	B	360	PRO	2.2
1	D	188	PRO	2.2
1	B	9	ASN	2.2
1	D	136	PRO	2.2
1	D	1	MET	2.1
1	B	316	ILE	2.1
1	D	361	GLU	2.1
1	D	187	GLN	2.1
1	D	137	GLN	2.0
1	C	158	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.