



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:40 PM GMT

PDB ID : 1UMY  
Title : BHMT FROM RAT LIVER  
Authors : Gonzalez, B.; Pajares, M.A.; Sanz-Aparicio, J.  
Deposited on : 2003-09-02  
Resolution : 2.50 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  
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

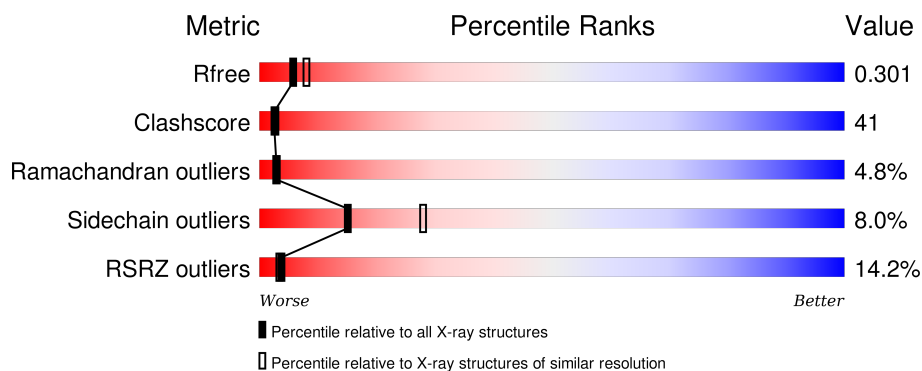
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	407	<div> <div>11%</div> <div>50% 35% 6% 8%</div> </div>
1	B	407	<div> <div>12%</div> <div>47% 40% 6% • 6%</div> </div>
1	C	407	<div> <div>14%</div> <div>45% 40% 8% • 6%</div> </div>
1	D	407	<div> <div>17%</div> <div>40% 46% 7% • 6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12353 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 BETAIN--HOMOCYSTEINE S-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	1
			2908	1847	512	533	16			
1	B	381	Total	C	N	O	S	0	0	1
			2956	1876	519	545	16			
1	C	381	Total	C	N	O	S	0	0	1
			2964	1884	522	542	16			
1	D	382	Total	C	N	O	S	0	0	1
			2975	1893	524	542	16			

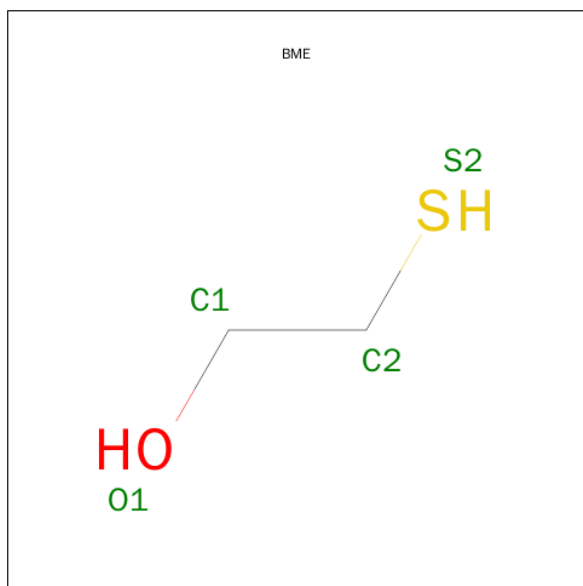
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	GLN	HIS	CONFLICT	UNP O09171
A	248	PRO	ALA	CONFLICT	UNP O09171
B	247	GLN	HIS	CONFLICT	UNP O09171
B	248	PRO	ALA	CONFLICT	UNP O09171
C	247	GLN	HIS	CONFLICT	UNP O09171
C	248	PRO	ALA	CONFLICT	UNP O09171
D	247	GLN	HIS	CONFLICT	UNP O09171
D	248	PRO	ALA	CONFLICT	UNP O09171

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

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

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

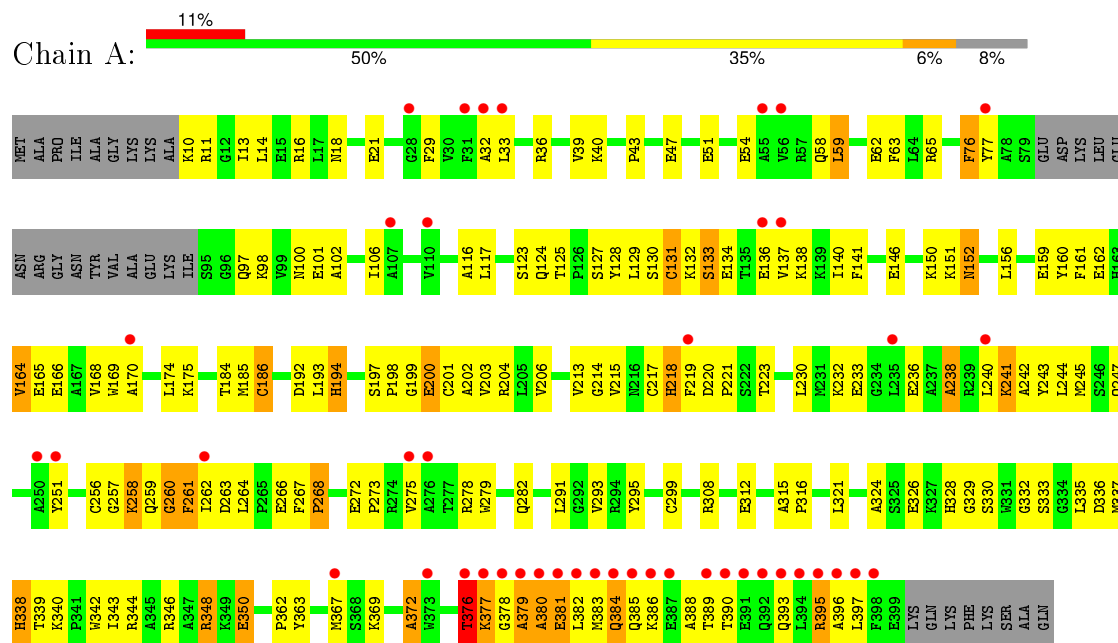
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	149	Total	O	0	0
			149	149		
4	C	107	Total	O	0	0
			107	107		
4	D	142	Total	O	0	0
			142	142		

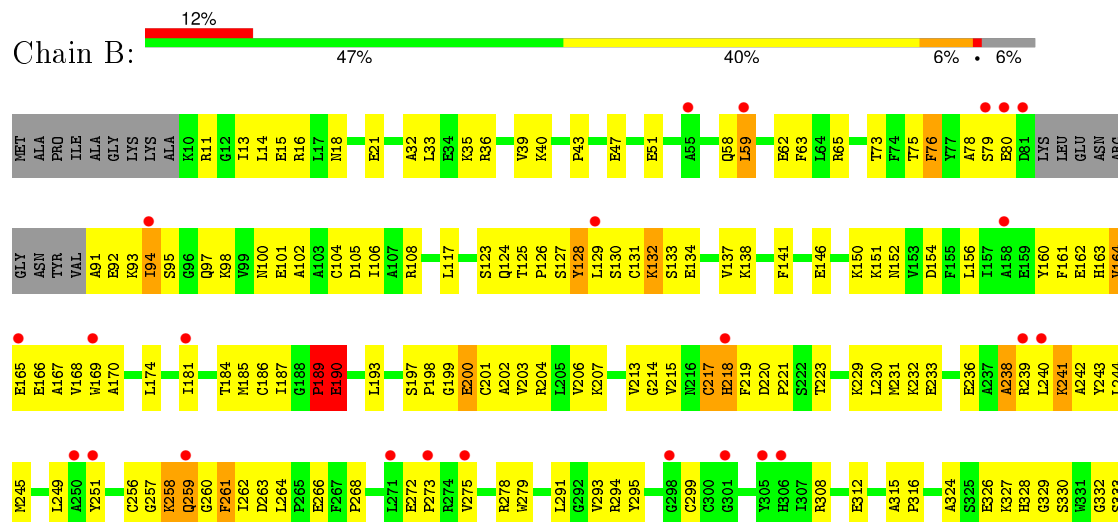
### 3 Residue-property plots

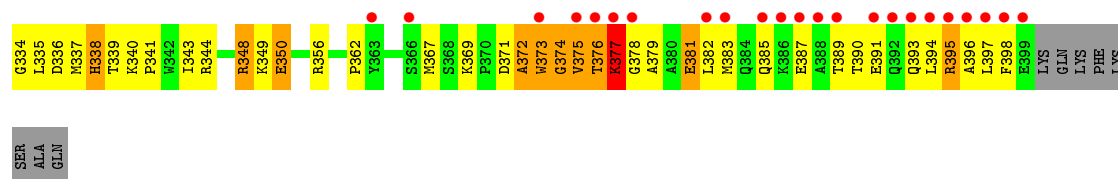
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BETAINE--HOMOCYSTEINE S-METHYLTRANSFERASE

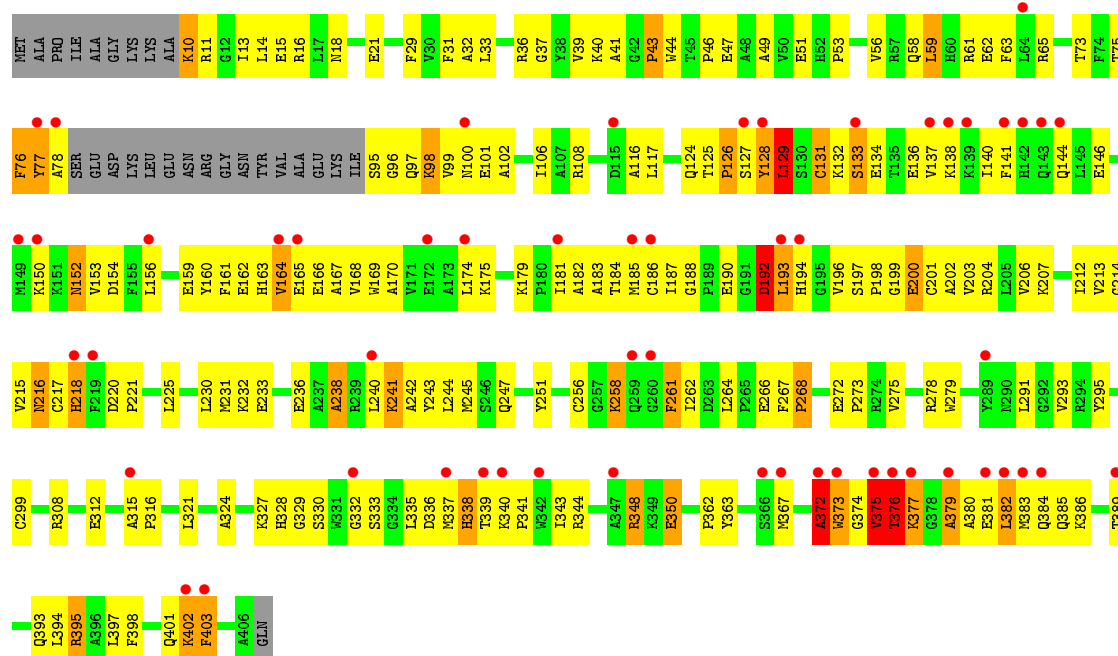
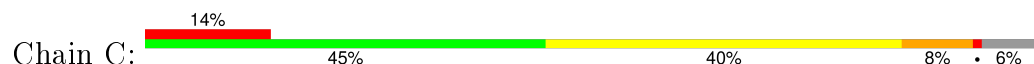


#### • Molecule 1: BETAINE--HOMOCYSTEINE S-METHYLTRANSFERASE

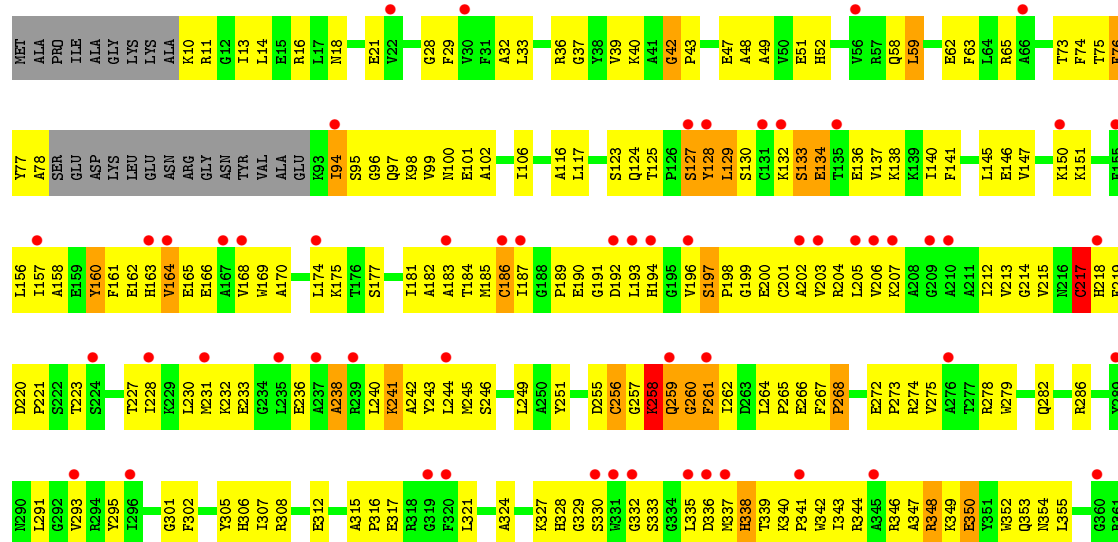


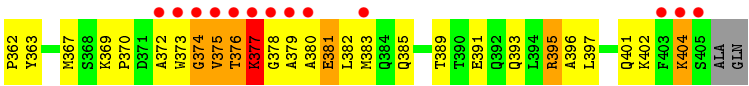


• Molecule 1: BETAIN--HOMOCYSTEINE S-METHYLTRANSFERASE



• Molecule 1: BETAIN--HOMOCYSTEINE S-METHYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.83Å 149.27Å 96.25Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	48.40 – 2.50 48.43 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.40-2.50) 92.1 (48.43-2.44)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.253 , 0.291 0.269 , 0.301	Depositor DCC
$R_{free}$ test set	5549 reflections (11.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.3	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55656 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

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

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	0.44	0/2979	0.64	0/4029
1	B	0.48	0/3027	0.65	1/4093 (0.0%)
1	C	0.52	2/3036 (0.1%)	0.67	3/4102 (0.1%)
1	D	0.50	0/3047	0.68	0/4116
All	All	0.49	2/12089 (0.0%)	0.66	4/16340 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	379	ALA	N-CA	6.12	1.58	1.46
1	C	375	VAL	C-N	-5.34	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	VAL	CB-CA-C	-6.38	99.28	111.40
1	C	372	ALA	CB-CA-C	-5.78	101.44	110.10
1	B	374	GLY	N-CA-C	-5.77	98.67	113.10
1	C	376	THR	O-C-N	5.31	131.20	122.70

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	2908	0	2862	208	0
1	B	2956	0	2906	232	0
1	C	2964	0	2925	276	0
1	D	2975	0	2942	314	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	4	0	5	0	0
3	B	4	0	5	0	0
4	A	140	0	0	19	0
4	B	149	0	0	25	0
4	C	107	0	0	32	0
4	D	142	0	0	67	0
All	All	12353	0	11645	973	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 41.

All (973) 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:D:258:LYS:HG2	1:D:259:GLN:H	0.93	1.09
1:C:126:PRO:HA	1:C:129:LEU:HB2	1.39	1.03
1:D:258:LYS:HG2	1:D:259:GLN:N	1.74	1.02
1:A:377:LYS:HG3	1:A:378:GLY:H	1.23	1.02
1:B:11:ARG:HB2	1:B:11:ARG:HH11	1.26	1.00
1:A:258:LYS:HE3	1:A:259:GLN:H	1.22	1.00
1:C:11:ARG:HH11	1:C:11:ARG:HB2	1.25	1.00
1:A:11:ARG:HB2	1:A:11:ARG:HH11	1.27	0.97
1:A:258:LYS:CE	1:A:259:GLN:H	1.78	0.96
1:C:373:TRP:CH2	1:C:380:ALA:HB2	2.01	0.95
1:D:317:GLU:HB3	4:D:2099:HOH:O	1.67	0.94
1:D:258:LYS:CG	1:D:259:GLN:H	1.81	0.93
1:A:376:THR:HA	1:A:380:ALA:CB	2.00	0.92
1:C:124:GLN:HG3	1:C:161:PHE:HA	1.50	0.90
1:D:11:ARG:HB2	1:D:11:ARG:HH11	1.34	0.90
1:D:375:VAL:HG22	1:D:376:THR:H	1.36	0.90
1:B:381:GLU:O	1:B:385:GLN:HG2	1.72	0.89
1:A:156:LEU:HD13	1:A:174:LEU:HD12	1.55	0.89
1:D:187:ILE:HG21	1:D:192:ASP:HA	1.55	0.89
1:D:374:GLY:O	1:D:375:VAL:O	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LYS:NZ	1:D:404:LYS:HA	1.86	0.88
1:C:156:LEU:HD13	1:C:174:LEU:HD12	1.55	0.88
1:D:124:GLN:HG3	1:D:160:TYR:O	1.74	0.88
1:C:133:SER:HB3	4:C:2037:HOH:O	1.73	0.88
1:A:350:GLU:HB2	4:A:2107:HOH:O	1.74	0.87
1:D:353:GLN:HA	4:D:2122:HOH:O	1.73	0.87
1:B:11:ARG:HB2	1:B:11:ARG:NH1	1.89	0.87
1:A:11:ARG:NH1	1:A:11:ARG:HB2	1.89	0.87
1:C:162:GLU:HB3	1:C:193:LEU:HD23	1.56	0.87
1:C:380:ALA:HA	1:C:383:MET:CE	2.04	0.86
1:C:185:MET:O	1:C:215:VAL:HG23	1.73	0.86
1:C:373:TRP:HH2	1:C:380:ALA:HB2	1.39	0.86
1:C:11:ARG:HB2	1:C:11:ARG:NH1	1.89	0.85
1:C:76:PHE:H	1:C:100:ASN:HD21	1.18	0.85
1:A:185:MET:O	1:A:215:VAL:HG23	1.77	0.84
1:A:258:LYS:HE3	1:A:259:GLN:N	1.92	0.84
1:C:186:CYS:HB2	1:C:218:HIS:HB2	1.58	0.84
1:D:379:ALA:O	1:D:383:MET:HB2	1.76	0.84
1:D:156:LEU:HD13	1:D:174:LEU:HD12	1.57	0.84
1:B:156:LEU:HD13	1:B:174:LEU:HD12	1.57	0.84
1:C:11:ARG:CB	1:C:11:ARG:HH11	1.90	0.83
1:D:382:LEU:HA	1:D:385:GLN:HG2	1.61	0.83
1:D:129:LEU:HD22	1:D:129:LEU:N	1.94	0.82
1:A:11:ARG:CB	1:A:11:ARG:HH11	1.90	0.82
1:C:126:PRO:HA	1:C:129:LEU:CB	2.09	0.82
1:A:377:LYS:HG3	1:A:378:GLY:N	1.94	0.82
1:D:11:ARG:HB2	1:D:11:ARG:NH1	1.92	0.82
1:D:228:ILE:HD11	4:D:2090:HOH:O	1.77	0.82
1:D:11:ARG:CB	1:D:11:ARG:HH11	1.92	0.82
1:B:124:GLN:HG3	1:B:160:TYR:O	1.81	0.81
1:D:99:VAL:HB	4:D:2042:HOH:O	1.79	0.81
1:B:11:ARG:HH11	1:B:11:ARG:CB	1.93	0.81
1:D:36:ARG:NH2	4:D:2018:HOH:O	2.14	0.81
1:B:76:PHE:H	1:B:100:ASN:HD21	1.29	0.81
1:B:217:CYS:HB2	1:B:299:CYS:SG	2.21	0.81
1:C:128:TYR:CE1	1:C:166:GLU:HB2	2.16	0.81
1:B:376:THR:O	1:B:377:LYS:HG2	1.81	0.81
1:B:79:SER:N	1:B:94:ILE:HG21	1.95	0.81
1:B:79:SER:CA	1:B:94:ILE:HG21	2.11	0.81
1:B:185:MET:O	1:B:215:VAL:HG23	1.82	0.80
1:C:153:VAL:HA	4:C:2030:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:H	1:C:401:GLN:HE22	1.28	0.80
1:D:133:SER:OG	1:D:136:GLU:HG3	1.81	0.79
1:B:326:GLU:HA	1:D:402:LYS:HE3	1.63	0.79
1:C:258:LYS:HE2	1:C:258:LYS:N	1.96	0.79
1:D:376:THR:HG21	1:D:380:ALA:HB3	1.65	0.79
1:C:258:LYS:HE2	1:C:258:LYS:H	1.48	0.79
1:D:158:ALA:HB1	1:D:161:PHE:HE1	1.46	0.79
1:C:381:GLU:HA	1:C:384:GLN:HG2	1.65	0.79
1:C:373:TRP:CZ3	1:C:376:THR:OG1	2.36	0.78
1:A:380:ALA:O	1:A:383:MET:HB3	1.84	0.78
1:C:128:TYR:CD1	1:C:166:GLU:HB2	2.20	0.77
1:D:327:LYS:HB2	4:D:2111:HOH:O	1.84	0.77
1:A:382:LEU:HD11	1:A:386:LYS:HB2	1.66	0.76
1:B:11:ARG:HH12	1:B:16:ARG:CZ	1.99	0.76
1:D:77:TYR:CE1	1:D:140:ILE:HG23	2.20	0.76
1:C:37:GLY:HA3	4:C:2009:HOH:O	1.85	0.75
1:B:133:SER:O	1:B:137:VAL:HG12	1.85	0.75
1:A:308:ARG:HD2	4:A:2093:HOH:O	1.86	0.75
1:A:162:GLU:O	1:A:192:ASP:HB2	1.86	0.75
1:C:11:ARG:HH12	1:C:16:ARG:CZ	2.00	0.75
1:B:394:LEU:HD13	1:D:315:ALA:HB3	1.68	0.75
1:B:308:ARG:HD2	4:B:2111:HOH:O	1.86	0.75
1:A:343:ILE:HD11	1:B:262:ILE:HG23	1.69	0.75
1:D:218:HIS:H	1:D:249:LEU:HD21	1.52	0.74
1:A:11:ARG:HH12	1:A:16:ARG:CZ	1.99	0.74
1:D:124:GLN:CG	1:D:161:PHE:HA	2.17	0.74
1:C:327:LYS:O	1:D:40:LYS:HA	1.86	0.74
1:B:348:ARG:HH11	1:B:348:ARG:HG2	1.52	0.74
1:C:380:ALA:HA	1:C:383:MET:HE1	1.68	0.74
1:C:232:LYS:O	1:C:236:GLU:HG3	1.87	0.74
1:A:262:ILE:HG23	1:B:343:ILE:HD11	1.70	0.73
1:C:128:TYR:HB2	1:C:166:GLU:OE2	1.88	0.73
1:D:374:GLY:C	1:D:375:VAL:O	2.25	0.73
1:D:11:ARG:HH12	1:D:16:ARG:CZ	2.02	0.73
1:A:263:ASP:OD2	1:A:372:ALA:HB2	1.88	0.73
1:A:346:ARG:NH2	1:B:371:ASP:OD1	2.20	0.72
1:D:59:LEU:HA	4:D:2018:HOH:O	1.89	0.72
1:B:372:ALA:O	1:B:374:GLY:N	2.23	0.72
1:D:215:VAL:HG12	4:D:2090:HOH:O	1.88	0.72
1:B:185:MET:HE1	4:B:2063:HOH:O	1.88	0.72
1:B:80:GLU:O	1:B:94:ILE:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HD2	1:A:223:THR:HG21	1.53	0.72
1:A:348:ARG:HH11	1:A:348:ARG:HG2	1.54	0.72
1:C:328:HIS:O	1:D:40:LYS:HE2	1.89	0.72
1:C:29:PHE:HA	4:C:2006:HOH:O	1.89	0.72
1:C:95:SER:O	1:C:99:VAL:HG23	1.90	0.72
1:D:232:LYS:O	1:D:236:GLU:HG3	1.89	0.72
1:C:373:TRP:CZ2	1:C:377:LYS:N	2.56	0.71
1:D:184:THR:HA	1:D:214:GLY:O	1.88	0.71
1:A:232:LYS:O	1:A:236:GLU:HG3	1.90	0.71
1:C:376:THR:O	1:C:377:LYS:O	2.07	0.71
1:B:350:GLU:CD	1:B:350:GLU:H	1.93	0.71
1:C:163:HIS:HB3	1:C:194:HIS:CD2	2.24	0.71
1:D:185:MET:O	1:D:215:VAL:HG23	1.90	0.71
1:C:125:THR:O	1:C:127:SER:N	2.23	0.71
1:D:348:ARG:HG2	1:D:348:ARG:HH11	1.56	0.71
1:D:218:HIS:HB3	1:D:260:GLY:HA3	1.72	0.71
1:A:258:LYS:CD	1:A:259:GLN:H	2.04	0.71
1:B:165:GLU:HB3	4:B:2049:HOH:O	1.89	0.71
1:C:198:PRO:HG3	1:C:230:LEU:HD13	1.73	0.71
1:D:214:GLY:HA3	1:D:245:MET:O	1.90	0.71
1:B:202:ALA:O	1:B:206:VAL:HG13	1.90	0.71
1:A:382:LEU:HD12	1:A:386:LYS:H	1.56	0.71
1:D:189:PRO:HD3	1:D:227:THR:OG1	1.91	0.70
1:B:238:ALA:O	1:B:240:LEU:HD22	1.91	0.70
1:B:124:GLN:HG3	1:B:161:PHE:HA	1.73	0.70
1:C:199:GLY:N	4:C:2048:HOH:O	2.25	0.70
1:C:380:ALA:HA	1:C:383:MET:HE2	1.73	0.70
1:D:158:ALA:HB1	1:D:161:PHE:CE1	2.25	0.70
1:A:350:GLU:CD	1:A:350:GLU:H	1.95	0.70
1:A:337:MET:O	1:A:338:HIS:HB2	1.92	0.70
1:C:238:ALA:O	1:C:240:LEU:HD22	1.92	0.70
1:D:48:ALA:HB3	4:D:2024:HOH:O	1.91	0.69
1:C:337:MET:O	1:C:338:HIS:HB2	1.92	0.69
1:D:161:PHE:HB2	1:D:185:MET:HG2	1.73	0.69
1:B:337:MET:O	1:B:338:HIS:HB2	1.93	0.69
1:D:128:TYR:CE2	1:D:166:GLU:HB2	2.27	0.69
1:C:77:TYR:CE2	1:C:140:ILE:HG23	2.28	0.69
1:D:32:ALA:O	1:D:36:ARG:HG3	1.93	0.69
1:D:202:ALA:O	1:D:206:VAL:HG13	1.92	0.69
1:A:198:PRO:HG3	1:A:230:LEU:HD13	1.74	0.69
1:D:257:GLY:HA3	1:D:370:PRO:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HD3	4:C:2024:HOH:O	1.92	0.69
1:B:232:LYS:O	1:B:236:GLU:HG3	1.93	0.69
1:D:382:LEU:O	1:D:385:GLN:N	2.25	0.69
1:D:404:LYS:HZ2	1:D:404:LYS:HA	1.57	0.69
1:C:262:ILE:HG23	1:D:343:ILE:HD11	1.75	0.69
1:A:397:LEU:CD2	1:C:315:ALA:HB1	2.23	0.68
1:D:379:ALA:HA	1:D:382:LEU:HB2	1.75	0.68
1:A:214:GLY:HA3	1:A:245:MET:O	1.93	0.68
1:D:336:ASP:HB2	4:D:2117:HOH:O	1.93	0.68
1:A:238:ALA:O	1:A:240:LEU:HD22	1.93	0.68
1:C:182:ALA:HA	1:C:212:ILE:HB	1.75	0.68
1:A:128:TYR:HB2	1:A:166:GLU:OE2	1.94	0.68
1:A:376:THR:HA	1:A:380:ALA:HB2	1.76	0.68
1:C:348:ARG:HH11	1:C:348:ARG:HG2	1.57	0.68
1:C:202:ALA:O	1:C:206:VAL:HG13	1.93	0.68
1:D:308:ARG:O	1:D:312:GLU:HG3	1.94	0.68
1:D:389:THR:HG21	4:D:2137:HOH:O	1.94	0.68
1:A:381:GLU:O	1:A:384:GLN:HB3	1.94	0.68
1:A:397:LEU:HD22	1:C:315:ALA:HB1	1.75	0.68
1:D:165:GLU:HB3	4:D:2057:HOH:O	1.94	0.68
1:A:326:GLU:HG2	4:C:2106:HOH:O	1.94	0.68
1:C:214:GLY:HA3	1:C:245:MET:O	1.94	0.68
1:A:202:ALA:O	1:A:206:VAL:HG13	1.92	0.67
1:B:97:GLN:O	1:B:101:GLU:HG3	1.94	0.67
1:B:214:GLY:HA3	1:B:245:MET:O	1.94	0.67
1:D:198:PRO:HG3	1:D:230:LEU:HD13	1.75	0.67
1:B:184:THR:HA	1:B:214:GLY:O	1.94	0.67
1:A:124:GLN:HE22	1:A:162:GLU:HG3	1.58	0.67
1:B:379:ALA:HB1	1:B:383:MET:CE	2.24	0.67
1:B:181:ILE:HD12	4:B:2075:HOH:O	1.95	0.67
1:D:337:MET:O	1:D:338:HIS:HB2	1.94	0.66
1:A:97:GLN:O	1:A:101:GLU:HG3	1.95	0.66
1:B:391:GLU:OE1	1:D:349:LYS:HD3	1.94	0.66
1:B:185:MET:H	1:B:215:VAL:HA	1.60	0.66
1:D:238:ALA:O	1:D:240:LEU:HD22	1.94	0.66
1:D:375:VAL:HG22	1:D:376:THR:N	2.09	0.66
1:A:379:ALA:O	1:A:381:GLU:N	2.27	0.66
1:D:347:ALA:N	4:D:2119:HOH:O	2.28	0.66
1:C:216:ASN:HB2	1:C:247:GLN:HB2	1.78	0.66
1:C:335:LEU:HD22	4:C:2090:HOH:O	1.94	0.66
1:A:273:PRO:HA	1:B:273:PRO:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:HG3	1:B:230:LEU:HD13	1.76	0.66
1:A:377:LYS:CG	1:A:378:GLY:H	2.00	0.66
1:A:259:GLN:O	1:A:260:GLY:O	2.14	0.66
1:B:371:ASP:O	1:B:373:TRP:N	2.29	0.66
1:A:13:ILE:HG23	1:A:14:LEU:N	2.11	0.66
1:D:257:GLY:HA2	4:D:2092:HOH:O	1.95	0.66
1:B:337:MET:O	1:B:338:HIS:CB	2.43	0.66
1:D:218:HIS:HE2	1:D:262:ILE:HD12	1.61	0.66
1:C:385:GLN:HA	1:C:385:GLN:NE2	2.10	0.66
1:B:189:PRO:HD3	1:B:223:THR:HG22	1.76	0.66
1:D:385:GLN:NE2	1:D:385:GLN:HA	2.11	0.65
1:D:94:ILE:O	1:D:96:GLY:N	2.29	0.65
1:A:382:LEU:CD1	1:A:386:LYS:H	2.08	0.65
1:C:16:ARG:HE	1:C:117:LEU:HD11	1.62	0.65
1:A:337:MET:O	1:A:338:HIS:CB	2.43	0.65
1:C:132:LYS:O	1:C:136:GLU:HB2	1.97	0.65
1:D:99:VAL:HG23	4:D:2043:HOH:O	1.95	0.65
1:C:350:GLU:CD	1:C:350:GLU:H	1.97	0.65
1:C:379:ALA:C	1:C:381:GLU:H	1.97	0.65
1:C:144:GLN:HG2	4:C:2043:HOH:O	1.96	0.65
1:B:356:ARG:HB2	4:B:2133:HOH:O	1.97	0.65
1:B:394:LEU:HD13	1:D:316:PRO:HD3	1.77	0.65
1:D:376:THR:HG22	4:D:2135:HOH:O	1.95	0.65
1:B:186:CYS:HB2	1:B:218:HIS:CG	2.32	0.65
1:D:350:GLU:H	1:D:350:GLU:CD	2.00	0.65
1:C:192:ASP:OD2	1:C:196:VAL:HB	1.97	0.65
1:D:128:TYR:CD2	1:D:166:GLU:HB2	2.32	0.65
1:D:215:VAL:HG23	4:D:2077:HOH:O	1.96	0.65
1:D:337:MET:O	1:D:338:HIS:CB	2.45	0.65
1:D:127:SER:HB2	4:D:2055:HOH:O	1.97	0.65
1:C:337:MET:O	1:C:338:HIS:CB	2.45	0.64
1:B:16:ARG:HE	1:B:117:LEU:HD11	1.62	0.64
1:B:79:SER:CA	1:B:94:ILE:CG2	2.75	0.64
1:C:343:ILE:HD11	1:D:262:ILE:HG23	1.78	0.64
1:D:124:GLN:HG3	1:D:161:PHE:HA	1.79	0.64
1:D:376:THR:HG21	1:D:380:ALA:CB	2.27	0.64
1:D:129:LEU:CD2	1:D:129:LEU:N	2.60	0.64
1:C:76:PHE:H	1:C:100:ASN:ND2	1.94	0.64
1:D:76:PHE:H	1:D:100:ASN:HD21	1.46	0.64
1:B:394:LEU:HD23	4:D:2113:HOH:O	1.96	0.64
1:C:336:ASP:O	1:C:344:ARG:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ALA:O	1:C:36:ARG:HG3	1.96	0.64
1:C:327:LYS:HA	1:D:40:LYS:HB2	1.78	0.64
1:B:394:LEU:CD1	1:D:315:ALA:HB3	2.28	0.64
1:C:53:PRO:HB3	4:C:2013:HOH:O	1.98	0.64
1:C:97:GLN:O	1:C:101:GLU:HG3	1.99	0.63
1:B:32:ALA:O	1:B:36:ARG:HG3	1.98	0.63
1:C:373:TRP:HZ2	1:C:377:LYS:HA	1.63	0.63
1:D:141:PHE:CE2	4:D:2053:HOH:O	2.49	0.63
1:D:49:ALA:N	4:D:2024:HOH:O	2.30	0.63
1:A:217:CYS:HB2	1:A:299:CYS:SG	2.37	0.63
1:B:133:SER:HA	4:B:2052:HOH:O	1.97	0.63
1:A:385:GLN:NE2	1:A:385:GLN:HA	2.14	0.63
1:C:373:TRP:HZ2	1:C:377:LYS:CA	2.10	0.63
1:D:336:ASP:O	1:D:344:ARG:HD2	1.99	0.63
1:A:54:GLU:HB2	4:A:2012:HOH:O	1.99	0.63
1:C:192:ASP:OD1	1:C:194:HIS:N	2.30	0.63
1:D:128:TYR:OH	1:D:165:GLU:HB3	1.97	0.63
1:C:29:PHE:CD1	1:C:59:LEU:HD13	2.34	0.63
1:D:343:ILE:O	4:D:2119:HOH:O	2.16	0.63
1:B:336:ASP:O	1:B:344:ARG:HD2	1.99	0.63
1:B:14:LEU:HD12	4:B:2003:HOH:O	1.97	0.63
1:D:146:GLU:O	1:D:150:LYS:HG2	1.98	0.63
1:A:146:GLU:O	1:A:150:LYS:HG2	1.98	0.63
1:D:378:GLY:O	1:D:382:LEU:HD13	1.99	0.63
1:D:97:GLN:O	1:D:101:GLU:HG3	1.98	0.63
1:D:13:ILE:HG23	1:D:14:LEU:N	2.14	0.62
1:D:161:PHE:O	1:D:185:MET:HB3	1.99	0.62
1:A:32:ALA:O	1:A:36:ARG:HG3	2.00	0.62
1:C:10:LYS:HE3	1:C:11:ARG:HG3	1.81	0.62
1:A:219:PHE:CD2	1:A:223:THR:HG21	2.34	0.62
1:C:102:ALA:O	1:C:106:ILE:HG13	2.00	0.62
1:A:133:SER:O	1:A:137:VAL:HG12	1.98	0.62
1:B:130:SER:OG	1:B:132:LYS:HG3	2.00	0.62
1:B:385:GLN:HA	1:B:385:GLN:NE2	2.15	0.62
1:A:336:ASP:HA	4:A:2102:HOH:O	2.00	0.62
1:C:308:ARG:O	1:C:312:GLU:HG3	2.00	0.62
1:B:376:THR:O	1:B:377:LYS:CG	2.47	0.62
1:D:404:LYS:HA	1:D:404:LYS:HZ3	1.64	0.62
1:B:198:PRO:HG2	4:B:2071:HOH:O	1.99	0.62
1:A:336:ASP:O	1:A:344:ARG:HD2	2.00	0.61
1:D:77:TYR:CD1	1:D:140:ILE:HG23	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:HE	1:D:117:LEU:HD11	1.65	0.61
1:A:376:THR:HA	1:A:380:ALA:HB3	1.79	0.61
1:C:395:ARG:NH1	1:C:395:ARG:HG2	2.15	0.61
1:B:91:ALA:HB1	4:B:2030:HOH:O	2.00	0.61
1:B:395:ARG:O	1:B:398:PHE:HB2	2.01	0.61
1:C:13:ILE:HG23	1:C:14:LEU:N	2.16	0.61
1:D:186:CYS:O	1:D:187:ILE:HG12	2.01	0.61
1:D:77:TYR:O	1:D:78:ALA:O	2.19	0.61
1:B:308:ARG:O	1:B:312:GLU:HG3	2.00	0.61
1:A:241:LYS:HD3	1:A:242:ALA:N	2.16	0.61
1:C:231:MET:N	4:C:2048:HOH:O	2.33	0.60
1:B:146:GLU:O	1:B:150:LYS:HG2	2.01	0.60
1:A:382:LEU:C	1:A:384:GLN:H	2.04	0.60
1:D:124:GLN:OE1	1:D:162:GLU:HB2	2.01	0.60
1:D:134:GLU:HB2	1:D:169:TRP:CZ2	2.36	0.60
1:D:164:VAL:HG11	1:D:201:CYS:HA	1.84	0.60
1:A:198:PRO:HG2	4:A:2049:HOH:O	2.01	0.60
1:A:165:GLU:HB3	4:A:2033:HOH:O	2.01	0.60
1:A:328:HIS:O	1:B:40:LYS:HE2	2.00	0.60
1:A:197:SER:HB2	1:A:198:PRO:HD2	1.84	0.60
1:D:28:GLY:HA2	4:D:2014:HOH:O	2.01	0.60
1:D:375:VAL:CG2	1:D:376:THR:H	2.13	0.60
1:A:219:PHE:HB3	4:A:2056:HOH:O	2.01	0.60
1:C:162:GLU:O	1:C:192:ASP:HB2	2.00	0.60
1:A:159:GLU:HG3	1:A:160:TYR:HD2	1.66	0.60
1:C:372:ALA:O	1:C:374:GLY:N	2.35	0.60
1:C:241:LYS:HD3	4:C:2060:HOH:O	2.00	0.60
1:A:343:ILE:HD11	1:B:262:ILE:CG2	2.32	0.59
1:D:375:VAL:O	1:D:376:THR:HB	2.01	0.59
1:D:124:GLN:HE21	1:D:160:TYR:C	2.05	0.59
1:A:308:ARG:O	1:A:312:GLU:HG3	2.01	0.59
1:A:258:LYS:HD3	4:A:2072:HOH:O	2.01	0.59
1:C:273:PRO:HA	1:D:273:PRO:HA	1.84	0.59
1:B:59:LEU:HD22	1:B:63:PHE:CE1	2.38	0.59
1:B:394:LEU:HB2	1:D:316:PRO:CG	2.32	0.59
1:A:395:ARG:HG2	1:A:395:ARG:NH1	2.17	0.59
1:A:16:ARG:HE	1:A:117:LEU:HD11	1.67	0.59
1:C:373:TRP:HE1	1:C:377:LYS:HE2	1.66	0.59
1:C:379:ALA:C	1:C:381:GLU:N	2.56	0.59
1:D:124:GLN:CD	1:D:162:GLU:H	2.06	0.59
1:D:59:LEU:HD22	1:D:63:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:CE2	1:C:166:GLU:HG2	2.37	0.59
1:D:197:SER:HB2	1:D:198:PRO:HD2	1.85	0.59
1:D:255:ASP:O	1:D:257:GLY:N	2.35	0.59
1:C:373:TRP:CZ3	1:C:380:ALA:HB2	2.38	0.59
1:A:383:MET:HG3	1:A:383:MET:O	2.01	0.59
1:B:379:ALA:C	1:B:381:GLU:H	2.05	0.59
1:C:197:SER:HB2	1:C:198:PRO:HD2	1.83	0.59
1:B:124:GLN:OE1	1:B:162:GLU:N	2.36	0.58
1:B:79:SER:HA	1:B:94:ILE:CG2	2.31	0.58
1:C:59:LEU:HD22	1:C:63:PHE:CE1	2.37	0.58
1:B:189:PRO:HD3	1:B:223:THR:CG2	2.33	0.58
1:A:257:GLY:HA2	4:A:2070:HOH:O	2.03	0.58
1:C:16:ARG:O	1:C:21:GLU:HB2	2.02	0.58
1:C:29:PHE:CE1	1:C:59:LEU:HB3	2.38	0.58
1:A:175:LYS:HB3	4:A:2046:HOH:O	2.02	0.58
1:D:74:PHE:HE2	4:D:2024:HOH:O	1.85	0.58
1:B:378:GLY:O	1:B:382:LEU:N	2.33	0.58
1:C:381:GLU:HA	1:C:384:GLN:CG	2.32	0.58
1:A:382:LEU:C	1:A:384:GLN:N	2.55	0.58
1:C:373:TRP:CH2	1:C:380:ALA:CB	2.82	0.58
1:A:102:ALA:O	1:A:106:ILE:HG13	2.03	0.58
1:D:129:LEU:CD2	1:D:129:LEU:H	2.17	0.58
1:C:196:VAL:CG1	1:C:200:GLU:HB3	2.34	0.58
1:A:124:GLN:HE21	1:A:161:PHE:HA	1.68	0.58
1:D:124:GLN:HE22	1:D:162:GLU:HG3	1.68	0.58
1:B:394:LEU:CA	1:D:316:PRO:HG3	2.34	0.58
1:A:397:LEU:HB3	1:C:321:LEU:CD1	2.34	0.58
1:D:355:LEU:N	4:D:2124:HOH:O	2.36	0.58
1:C:129:LEU:C	1:C:131:CYS:H	2.06	0.58
1:B:395:ARG:NH1	1:B:395:ARG:HG2	2.19	0.58
1:C:124:GLN:NE2	1:C:166:GLU:OE1	2.36	0.58
1:D:16:ARG:O	1:D:21:GLU:HB2	2.04	0.58
1:C:230:LEU:C	4:C:2048:HOH:O	2.42	0.58
1:B:163:HIS:NE2	1:B:193:LEU:HD12	2.19	0.58
1:B:338:HIS:CE1	1:B:343:ILE:HD12	2.39	0.57
1:C:241:LYS:HD3	1:C:242:ALA:N	2.19	0.57
1:B:13:ILE:HG23	1:B:14:LEU:N	2.18	0.57
1:D:102:ALA:O	1:D:106:ILE:HG13	2.02	0.57
1:C:395:ARG:CG	1:C:395:ARG:HH11	2.17	0.57
1:A:395:ARG:HH11	1:A:395:ARG:HG2	1.69	0.57
1:D:37:GLY:HA2	4:D:2020:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLU:OE1	1:C:204:ARG:HD2	2.04	0.57
1:C:258:LYS:HE2	4:C:2067:HOH:O	2.05	0.57
1:A:200:GLU:OE1	1:A:204:ARG:HD2	2.04	0.57
1:D:385:GLN:HE21	1:D:385:GLN:HA	1.70	0.57
1:C:395:ARG:HH11	1:C:395:ARG:HG2	1.68	0.57
1:A:59:LEU:HD22	1:A:63:PHE:CE1	2.40	0.57
1:D:129:LEU:HD21	4:D:2054:HOH:O	2.05	0.57
1:B:197:SER:HB2	1:B:198:PRO:HD2	1.85	0.57
1:A:13:ILE:HG23	1:A:14:LEU:H	1.69	0.57
1:D:328:HIS:CG	1:D:329:GLY:H	2.23	0.57
1:C:31:PHE:CE2	1:C:44:TRP:CH2	2.93	0.57
1:C:46:PRO:HD2	1:C:76:PHE:CD1	2.40	0.56
1:A:164:VAL:HG11	1:A:201:CYS:HA	1.87	0.56
1:C:247:GLN:NE2	4:C:2062:HOH:O	2.27	0.56
1:D:146:GLU:HB3	4:D:2064:HOH:O	2.05	0.56
1:D:302:PHE:HE2	4:D:2106:HOH:O	1.88	0.56
1:C:146:GLU:O	1:C:150:LYS:HG2	2.04	0.56
1:A:10:LYS:NZ	1:A:10:LYS:CB	2.68	0.56
1:A:382:LEU:HD12	1:A:385:GLN:HB2	1.87	0.56
1:B:373:TRP:O	1:B:375:VAL:N	2.36	0.56
1:C:144:GLN:HA	4:C:2042:HOH:O	2.04	0.56
1:D:338:HIS:CE1	1:D:343:ILE:HD12	2.40	0.56
1:B:124:GLN:CG	1:B:161:PHE:HA	2.35	0.56
1:D:261:PHE:HB2	1:D:264:LEU:HD12	1.87	0.56
1:D:128:TYR:HB3	1:D:129:LEU:HD22	1.88	0.56
1:D:164:VAL:HG21	1:D:196:VAL:HG11	1.86	0.56
1:B:241:LYS:HD3	1:B:242:ALA:N	2.21	0.56
1:B:258:LYS:O	1:B:260:GLY:N	2.36	0.56
1:C:375:VAL:O	1:C:375:VAL:HG12	2.06	0.56
1:D:162:GLU:N	4:D:2074:HOH:O	2.37	0.56
1:B:395:ARG:HH11	1:B:395:ARG:HG2	1.70	0.56
1:D:128:TYR:OH	1:D:165:GLU:CB	2.54	0.56
1:B:123:SER:HB2	1:B:160:TYR:HB2	1.88	0.56
1:A:382:LEU:O	1:A:384:GLN:N	2.29	0.56
1:C:372:ALA:O	1:C:373:TRP:C	2.42	0.56
1:C:379:ALA:O	1:C:383:MET:HG2	2.06	0.56
1:D:192:ASP:OD2	1:D:192:ASP:C	2.44	0.56
1:C:262:ILE:CG2	1:D:343:ILE:HD11	2.36	0.56
1:B:261:PHE:HB2	1:B:264:LEU:HD12	1.88	0.56
1:D:200:GLU:OE1	1:D:204:ARG:HD2	2.05	0.56
1:B:131:CYS:O	1:B:132:LYS:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HH11	1:A:395:ARG:CG	2.19	0.55
1:C:343:ILE:HD11	1:D:262:ILE:CG2	2.36	0.55
1:D:125:THR:O	1:D:129:LEU:HD23	2.05	0.55
1:A:40:LYS:HA	1:B:327:LYS:O	2.06	0.55
1:C:164:VAL:HG11	1:C:201:CYS:HA	1.87	0.55
1:C:383:MET:C	1:C:385:GLN:H	2.10	0.55
1:B:263:ASP:O	1:B:371:ASP:HB2	2.05	0.55
1:D:13:ILE:HG23	1:D:14:LEU:H	1.72	0.55
1:A:378:GLY:O	1:A:379:ALA:O	2.23	0.55
1:B:379:ALA:HB1	1:B:383:MET:HE1	1.88	0.55
1:C:328:HIS:CG	1:C:329:GLY:H	2.25	0.55
1:B:164:VAL:HG11	1:B:201:CYS:HA	1.88	0.55
1:D:132:LYS:O	1:D:133:SER:O	2.25	0.55
1:D:185:MET:H	1:D:215:VAL:HA	1.72	0.55
1:A:10:LYS:NZ	1:A:10:LYS:HB2	2.22	0.55
1:B:376:THR:OG1	1:B:379:ALA:HB3	2.06	0.55
1:D:129:LEU:HD22	1:D:129:LEU:H	1.69	0.55
1:D:136:GLU:HA	4:D:2063:HOH:O	2.07	0.55
1:A:261:PHE:HB2	1:A:264:LEU:HD12	1.88	0.55
1:D:241:LYS:HD3	1:D:242:ALA:N	2.21	0.55
1:D:395:ARG:HG2	1:D:395:ARG:NH1	2.22	0.55
1:C:134:GLU:HB2	1:C:169:TRP:CZ2	2.42	0.55
1:D:123:SER:CB	1:D:160:TYR:HB2	2.36	0.55
1:C:198:PRO:HB2	4:C:2048:HOH:O	2.07	0.54
1:A:40:LYS:HE2	1:B:328:HIS:O	2.07	0.54
1:C:382:LEU:O	1:C:385:GLN:HB2	2.07	0.54
1:C:128:TYR:OH	1:C:165:GLU:HB3	2.08	0.54
1:C:13:ILE:HG23	1:C:14:LEU:H	1.71	0.54
1:B:315:ALA:HB3	1:B:316:PRO:HD3	1.88	0.54
1:D:315:ALA:HB3	1:D:316:PRO:HD3	1.90	0.54
1:B:134:GLU:HB2	1:B:169:TRP:CZ2	2.41	0.54
1:B:128:TYR:C	1:B:130:SER:H	2.10	0.54
4:A:2122:HOH:O	1:D:369:LYS:HE2	2.07	0.54
1:B:375:VAL:O	1:B:377:LYS:HE3	2.06	0.54
1:C:315:ALA:HB3	1:C:316:PRO:HD3	1.88	0.54
1:C:40:LYS:HB2	1:D:327:LYS:HA	1.90	0.54
1:B:333:SER:C	1:B:335:LEU:H	2.12	0.54
1:C:162:GLU:HB3	1:C:193:LEU:CD2	2.33	0.54
1:D:164:VAL:HG22	1:D:192:ASP:OD1	2.08	0.54
1:C:76:PHE:C	1:C:76:PHE:CD2	2.77	0.54
1:B:79:SER:H	1:B:94:ILE:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:HA	1:A:214:GLY:O	2.07	0.54
1:B:328:HIS:CG	1:B:329:GLY:H	2.26	0.53
1:D:187:ILE:CG2	1:D:191:GLY:O	2.57	0.53
1:B:398:PHE:CD1	1:D:321:LEU:HD11	2.43	0.53
1:A:43:PRO:HD3	1:B:337:MET:CE	2.38	0.53
1:C:161:PHE:HE2	1:C:166:GLU:CG	2.21	0.53
1:B:170:ALA:O	1:B:174:LEU:HD23	2.09	0.53
1:D:28:GLY:HA3	4:D:2103:HOH:O	2.08	0.53
1:A:369:LYS:HE3	1:D:363:TYR:CZ	2.43	0.53
1:A:124:GLN:HE21	1:A:161:PHE:CA	2.21	0.53
1:A:262:ILE:CG2	1:B:343:ILE:HD11	2.37	0.53
1:C:261:PHE:HB2	1:C:264:LEU:HD12	1.90	0.53
1:D:123:SER:HB2	1:D:160:TYR:HB2	1.90	0.53
1:A:130:SER:O	1:A:131:CYS:C	2.46	0.53
1:B:104:CYS:CB	1:B:151:LYS:HG2	2.38	0.53
1:C:77:TYR:HA	4:C:2043:HOH:O	2.08	0.53
1:A:328:HIS:CG	1:A:329:GLY:H	2.26	0.53
1:B:379:ALA:O	1:B:383:MET:HE2	2.09	0.53
1:C:232:LYS:NZ	4:C:2055:HOH:O	2.41	0.53
1:A:385:GLN:HE21	1:A:385:GLN:HA	1.73	0.53
1:B:373:TRP:C	1:B:375:VAL:N	2.61	0.53
1:C:127:SER:HB3	1:C:140:ILE:HD12	1.89	0.53
1:C:77:TYR:HE2	1:C:140:ILE:CG2	2.21	0.53
1:B:79:SER:HA	1:B:94:ILE:HG21	1.88	0.53
1:A:16:ARG:O	1:A:21:GLU:HB2	2.10	0.52
1:C:127:SER:HB3	1:C:140:ILE:CD1	2.39	0.52
1:D:336:ASP:N	4:D:2117:HOH:O	2.41	0.52
1:D:302:PHE:CE2	4:D:2106:HOH:O	2.54	0.52
1:C:41:ALA:C	1:C:43:PRO:HD2	2.30	0.52
1:A:388:ALA:HB2	4:A:2132:HOH:O	2.07	0.52
1:C:161:PHE:HE2	1:C:166:GLU:HG2	1.72	0.52
1:C:161:PHE:CD2	1:C:167:ALA:HB2	2.44	0.52
1:A:185:MET:H	1:A:215:VAL:HA	1.74	0.52
1:A:338:HIS:CE1	1:A:343:ILE:HD12	2.44	0.52
1:D:340:LYS:O	1:D:344:ARG:HG3	2.09	0.52
1:D:395:ARG:HH11	1:D:395:ARG:CG	2.23	0.52
1:C:373:TRP:CH2	1:C:376:THR:OG1	2.51	0.52
1:C:124:GLN:HG2	1:C:161:PHE:CE2	2.44	0.52
1:C:77:TYR:C	1:C:77:TYR:CD1	2.82	0.52
1:D:324:ALA:O	4:D:2111:HOH:O	2.19	0.52
1:C:327:LYS:C	1:D:40:LYS:HG3	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLY:O	1:C:203:VAL:HG23	2.10	0.52
1:B:395:ARG:CG	1:B:395:ARG:HH11	2.22	0.52
1:B:232:LYS:HD3	4:B:2083:HOH:O	2.10	0.52
1:C:213:VAL:HG12	1:C:214:GLY:N	2.25	0.52
1:B:257:GLY:N	4:B:2090:HOH:O	2.42	0.52
1:B:123:SER:CB	1:B:160:TYR:HB2	2.39	0.52
1:D:203:VAL:O	1:D:206:VAL:HG22	2.09	0.52
1:B:16:ARG:O	1:B:21:GLU:HB2	2.09	0.52
1:C:373:TRP:NE1	1:C:377:LYS:HE2	2.24	0.52
1:C:262:ILE:HG23	1:D:343:ILE:CD1	2.39	0.52
1:A:382:LEU:CD1	1:A:385:GLN:HB2	2.39	0.52
1:C:132:LYS:O	1:C:133:SER:HB2	2.10	0.52
1:C:95:SER:HB3	1:C:98:LYS:HE2	1.92	0.52
1:C:340:LYS:O	1:C:344:ARG:HG3	2.10	0.52
1:D:258:LYS:CG	1:D:259:GLN:N	2.52	0.52
1:D:246:SER:CB	4:D:2090:HOH:O	2.57	0.52
1:B:134:GLU:O	1:B:138:LYS:HB2	2.10	0.52
1:D:348:ARG:CG	1:D:348:ARG:HH11	2.23	0.52
1:A:134:GLU:HB2	1:A:169:TRP:CZ2	2.45	0.52
1:C:333:SER:C	1:C:335:LEU:H	2.13	0.52
1:D:376:THR:O	1:D:377:LYS:HB3	2.09	0.52
1:C:203:VAL:O	1:C:206:VAL:HG22	2.09	0.52
1:C:332:GLY:O	1:C:335:LEU:HB2	2.10	0.52
4:A:2085:HOH:O	1:C:386:LYS:HG3	2.10	0.52
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.91	0.52
1:B:239:ARG:HA	4:B:2084:HOH:O	2.10	0.52
1:C:373:TRP:CZ2	1:C:377:LYS:CA	2.92	0.51
1:C:18:ASN:ND2	1:C:243:TYR:OH	2.41	0.51
1:A:385:GLN:NE2	4:A:2133:HOH:O	2.43	0.51
1:A:170:ALA:O	1:A:174:LEU:HD23	2.10	0.51
1:A:124:GLN:HG3	1:A:161:PHE:HA	1.92	0.51
1:A:367:MET:HE3	1:D:362:PRO:HB2	1.92	0.51
1:C:338:HIS:CE1	1:C:343:ILE:HD12	2.45	0.51
1:B:217:CYS:O	1:B:218:HIS:HB2	2.09	0.51
1:B:102:ALA:O	1:B:106:ILE:HG13	2.10	0.51
1:B:58:GLN:O	1:B:62:GLU:HG3	2.10	0.51
1:A:382:LEU:HD11	1:A:386:LYS:CB	2.38	0.51
1:B:93:LYS:HB2	4:B:2033:HOH:O	2.09	0.51
1:D:58:GLN:O	1:D:62:GLU:HG3	2.10	0.51
1:C:134:GLU:O	1:C:138:LYS:HB2	2.10	0.51
1:B:373:TRP:C	1:B:375:VAL:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:HIS:N	4:D:2074:HOH:O	2.44	0.51
1:B:78:ALA:C	1:B:80:GLU:H	2.14	0.51
1:A:343:ILE:CD1	1:B:262:ILE:HG23	2.39	0.51
1:D:199:GLY:O	1:D:203:VAL:HG23	2.11	0.51
1:A:333:SER:C	1:A:335:LEU:H	2.14	0.51
1:A:76:PHE:H	1:A:100:ASN:HD21	1.57	0.51
1:D:382:LEU:O	1:D:383:MET:C	2.49	0.51
1:C:127:SER:O	1:C:132:LYS:HB2	2.11	0.51
1:C:402:LYS:O	1:C:403:PHE:HB2	2.09	0.51
1:A:123:SER:CB	1:A:160:TYR:HB2	2.40	0.51
1:A:123:SER:HB2	1:A:160:TYR:HB2	1.93	0.51
1:A:348:ARG:CG	1:A:348:ARG:HH11	2.22	0.51
1:C:183:ALA:N	1:C:212:ILE:O	2.39	0.51
1:B:126:PRO:O	1:B:128:TYR:N	2.42	0.51
1:B:203:VAL:O	1:B:206:VAL:HG22	2.10	0.51
1:C:343:ILE:CD1	1:D:262:ILE:HG23	2.41	0.51
1:C:124:GLN:HG2	1:C:161:PHE:CD2	2.45	0.51
1:B:76:PHE:H	1:B:100:ASN:ND2	2.05	0.51
1:D:18:ASN:ND2	1:D:243:TYR:OH	2.43	0.51
1:D:190:GLU:HB2	4:D:2078:HOH:O	2.09	0.51
1:D:274:ARG:NE	4:D:2095:HOH:O	2.36	0.50
1:C:165:GLU:OE1	1:C:194:HIS:CD2	2.64	0.50
1:C:170:ALA:O	1:C:174:LEU:HD23	2.11	0.50
1:A:272:GLU:O	1:A:275:VAL:HG23	2.11	0.50
1:D:306:HIS:C	4:D:2106:HOH:O	2.50	0.50
1:D:333:SER:C	1:D:335:LEU:H	2.15	0.50
1:A:266:GLU:N	1:A:266:GLU:OE1	2.43	0.50
1:B:187:ILE:HG13	1:B:187:ILE:O	2.12	0.50
1:C:394:LEU:HD11	1:C:398:PHE:HE1	1.75	0.50
1:D:190:GLU:HA	1:D:190:GLU:OE2	2.11	0.50
1:C:385:GLN:HA	1:C:385:GLN:HE21	1.76	0.50
1:D:137:VAL:HB	4:D:2061:HOH:O	2.12	0.50
1:A:159:GLU:O	1:A:160:TYR:HB2	2.11	0.50
1:A:10:LYS:HB2	1:A:10:LYS:HZ2	1.77	0.50
1:C:108:ARG:NH1	4:C:2031:HOH:O	2.44	0.50
1:C:125:THR:C	1:C:127:SER:H	2.14	0.50
1:A:203:VAL:O	1:A:206:VAL:HG22	2.11	0.50
1:D:374:GLY:O	1:D:375:VAL:C	2.50	0.50
1:D:134:GLU:O	1:D:138:LYS:HB2	2.12	0.50
1:B:394:LEU:HB2	1:D:316:PRO:HG3	1.93	0.50
1:A:164:VAL:HG13	1:A:201:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:OE1	1:B:204:ARG:HD2	2.10	0.50
1:D:47:GLU:O	1:D:51:GLU:HG3	2.11	0.50
1:B:108:ARG:NH2	1:B:154:ASP:OD2	2.43	0.50
1:B:105:ASP:OD2	1:B:151:LYS:HE3	2.12	0.50
1:B:33:LEU:HB3	1:B:39:VAL:HG23	1.94	0.50
1:D:33:LEU:HB3	1:D:39:VAL:HG23	1.94	0.50
1:C:373:TRP:CZ2	1:C:377:LYS:HA	2.45	0.49
1:D:380:ALA:C	1:D:382:LEU:H	2.14	0.49
1:D:129:LEU:HB2	4:D:2056:HOH:O	2.12	0.49
1:D:395:ARG:HG2	1:D:395:ARG:HH11	1.77	0.49
1:A:47:GLU:O	1:A:51:GLU:HG3	2.12	0.49
1:C:58:GLN:O	1:C:62:GLU:HG3	2.12	0.49
1:C:117:LEU:HB3	1:C:154:ASP:HB2	1.93	0.49
1:C:164:VAL:O	1:C:168:VAL:HG23	2.12	0.49
1:D:186:CYS:SG	1:D:186:CYS:O	2.70	0.49
1:D:346:ARG:N	4:D:2119:HOH:O	2.45	0.49
1:A:133:SER:OG	1:A:136:GLU:HG3	2.12	0.49
1:B:258:LYS:C	1:B:260:GLY:H	2.14	0.49
1:B:244:LEU:HB2	1:B:293:VAL:HA	1.94	0.49
1:C:382:LEU:HD23	1:C:382:LEU:O	2.12	0.49
1:A:213:VAL:HG12	1:A:214:GLY:N	2.27	0.49
1:A:134:GLU:O	1:A:138:LYS:HB2	2.13	0.49
1:B:204:ARG:NH2	4:B:2072:HOH:O	2.43	0.49
1:D:376:THR:OG1	1:D:377:LYS:N	2.42	0.49
1:D:218:HIS:HA	1:D:249:LEU:HD11	1.94	0.49
1:A:376:THR:O	1:A:377:LYS:O	2.30	0.49
1:D:379:ALA:O	1:D:383:MET:CB	2.57	0.49
1:D:164:VAL:O	1:D:168:VAL:HG23	2.13	0.49
1:C:240:LEU:O	4:C:2059:HOH:O	2.20	0.49
1:B:220:ASP:HB2	1:B:221:PRO:HD2	1.95	0.49
1:C:76:PHE:HD2	1:C:100:ASN:HD21	1.60	0.49
1:C:76:PHE:CE2	1:C:78:ALA:HB2	2.47	0.49
1:B:213:VAL:HG12	1:B:214:GLY:N	2.27	0.49
1:C:33:LEU:HB3	1:C:39:VAL:HG23	1.94	0.49
1:D:259:GLN:O	1:D:260:GLY:O	2.31	0.49
1:D:187:ILE:HG23	1:D:191:GLY:O	2.12	0.49
1:C:401:GLN:C	1:C:402:LYS:HE2	2.33	0.49
1:A:397:LEU:HB3	1:C:321:LEU:HG	1.95	0.49
1:D:308:ARG:HG2	1:D:308:ARG:O	2.13	0.49
1:D:389:THR:O	1:D:393:GLN:HG3	2.13	0.49
1:A:33:LEU:HB3	1:A:39:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:MET:HE3	1:C:362:PRO:HB2	1.94	0.49
1:B:375:VAL:O	1:B:375:VAL:HG13	2.12	0.49
1:D:189:PRO:CD	1:D:227:THR:OG1	2.59	0.49
1:B:167:ALA:CB	1:B:185:MET:HE3	2.43	0.49
1:D:257:GLY:CA	1:D:370:PRO:HG2	2.40	0.49
1:D:241:LYS:NZ	4:D:2087:HOH:O	2.43	0.49
1:C:251:TYR:CE1	1:C:275:VAL:HG22	2.48	0.49
1:B:151:LYS:NZ	4:B:2058:HOH:O	2.44	0.49
1:A:215:VAL:HG22	4:A:2053:HOH:O	2.13	0.48
1:B:199:GLY:O	1:B:203:VAL:HG23	2.12	0.48
1:B:398:PHE:CE1	1:D:321:LEU:HD21	2.48	0.48
1:B:348:ARG:HH11	1:B:348:ARG:CG	2.19	0.48
1:B:163:HIS:CE1	1:B:193:LEU:HD12	2.48	0.48
1:A:385:GLN:HA	4:A:2133:HOH:O	2.12	0.48
1:B:383:MET:O	1:B:387:GLU:HG2	2.13	0.48
1:B:385:GLN:HA	1:B:385:GLN:HE21	1.78	0.48
1:B:164:VAL:CG1	1:B:201:CYS:SG	3.02	0.48
1:B:272:GLU:O	1:B:275:VAL:HG23	2.12	0.48
1:A:390:THR:HG22	4:C:2087:HOH:O	2.12	0.48
1:C:163:HIS:HB3	1:C:194:HIS:HD2	1.76	0.48
1:A:127:SER:O	1:A:128:TYR:C	2.51	0.48
1:B:220:ASP:HB3	1:B:251:TYR:O	2.13	0.48
1:A:340:LYS:O	1:A:344:ARG:HG3	2.13	0.48
1:C:152:ASN:HA	1:C:179:LYS:HZ1	1.78	0.48
1:D:127:SER:O	1:D:130:SER:N	2.35	0.48
1:A:164:VAL:CG1	1:A:201:CYS:SG	3.01	0.48
1:D:218:HIS:NE2	1:D:262:ILE:HD12	2.26	0.48
1:A:159:GLU:HG3	1:A:160:TYR:CD2	2.47	0.48
1:B:184:THR:HG22	1:B:214:GLY:C	2.34	0.48
1:D:157:ILE:HG12	1:D:182:ALA:HB3	1.95	0.48
1:C:188:GLY:C	1:C:190:GLU:H	2.15	0.48
1:D:377:LYS:HA	1:D:381:GLU:OE1	2.13	0.48
1:A:124:GLN:NE2	1:A:162:GLU:HG3	2.27	0.48
1:B:164:VAL:O	1:B:168:VAL:HG23	2.13	0.48
1:B:340:LYS:O	1:B:344:ARG:HG3	2.14	0.48
1:A:244:LEU:HB2	1:A:293:VAL:HA	1.95	0.48
1:B:65:ARG:HG2	1:B:324:ALA:HB2	1.96	0.48
1:D:220:ASP:HB3	1:D:251:TYR:O	2.13	0.48
1:B:94:ILE:HG12	1:B:97:GLN:H	1.79	0.48
1:A:348:ARG:NH1	1:A:348:ARG:HG2	2.24	0.48
1:A:241:LYS:HE3	4:A:2062:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:CYS:HB2	1:C:218:HIS:CB	2.36	0.48
1:B:348:ARG:HG2	1:B:348:ARG:NH1	2.23	0.48
1:B:238:ALA:HB1	1:B:240:LEU:HD23	1.95	0.48
1:B:13:ILE:HG23	1:B:14:LEU:H	1.79	0.48
1:A:363:TYR:CZ	1:D:369:LYS:HE3	2.48	0.48
1:C:401:GLN:CB	1:C:402:LYS:HE2	2.44	0.47
1:C:266:GLU:OE1	1:C:266:GLU:N	2.47	0.47
1:D:376:THR:CG2	1:D:380:ALA:HB3	2.39	0.47
1:B:376:THR:O	1:B:377:LYS:CB	2.63	0.47
1:C:141:PHE:CD1	1:C:170:ALA:HA	2.49	0.47
1:D:40:LYS:HG2	1:D:42:GLY:H	1.77	0.47
1:D:213:VAL:HG12	1:D:214:GLY:N	2.30	0.47
1:A:164:VAL:O	1:A:165:GLU:C	2.53	0.47
1:C:244:LEU:HB2	1:C:293:VAL:HA	1.96	0.47
1:C:393:GLN:O	1:C:397:LEU:HD13	2.14	0.47
1:D:164:VAL:CG1	1:D:201:CYS:SG	3.02	0.47
1:B:238:ALA:CB	1:B:240:LEU:HD23	2.45	0.47
1:B:377:LYS:C	1:B:379:ALA:H	2.17	0.47
1:C:132:LYS:HA	4:C:2035:HOH:O	2.14	0.47
1:C:98:LYS:HD3	4:C:2028:HOH:O	2.15	0.47
1:D:220:ASP:HB2	1:D:221:PRO:HD2	1.96	0.47
1:B:18:ASN:ND2	1:B:243:TYR:OH	2.45	0.47
1:B:294:ARG:HB2	4:B:2103:HOH:O	2.13	0.47
1:C:65:ARG:HB3	4:C:2026:HOH:O	2.14	0.47
1:D:96:GLY:N	4:D:2043:HOH:O	2.47	0.47
1:C:238:ALA:HB1	1:C:240:LEU:HD23	1.96	0.47
1:A:220:ASP:HB3	1:A:251:TYR:O	2.13	0.47
1:A:164:VAL:O	1:A:168:VAL:HG23	2.14	0.47
1:C:337:MET:CE	1:D:43:PRO:HD3	2.44	0.47
1:B:372:ALA:C	1:B:374:GLY:N	2.68	0.47
1:D:128:TYR:HB2	1:D:166:GLU:OE2	2.15	0.47
1:B:78:ALA:O	1:B:80:GLU:HG2	2.14	0.47
1:B:164:VAL:HG13	1:B:201:CYS:SG	2.54	0.47
1:D:238:ALA:HB1	1:D:240:LEU:HD23	1.96	0.47
1:A:13:ILE:CG2	1:A:14:LEU:N	2.78	0.47
1:D:272:GLU:O	1:D:275:VAL:HG23	2.14	0.47
1:D:354:ASN:C	4:D:2124:HOH:O	2.52	0.47
1:B:47:GLU:O	1:B:51:GLU:HG3	2.14	0.47
1:C:47:GLU:O	1:C:51:GLU:HG3	2.15	0.47
1:D:133:SER:O	1:D:137:VAL:HG12	2.15	0.47
1:D:215:VAL:HG22	4:D:2083:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:C	1:C:77:TYR:HD1	2.19	0.47
1:C:389:THR:O	1:C:393:GLN:HG3	2.14	0.47
1:B:373:TRP:O	1:B:373:TRP:CG	2.67	0.47
1:D:186:CYS:O	1:D:187:ILE:CG1	2.63	0.47
1:A:192:ASP:C	1:A:194:HIS:H	2.18	0.47
1:D:73:THR:HB	1:D:75:THR:HG23	1.97	0.47
1:D:244:LEU:HB2	1:D:293:VAL:HA	1.96	0.47
1:A:18:ASN:ND2	1:A:243:TYR:OH	2.45	0.47
1:A:124:GLN:NE2	1:A:160:TYR:O	2.48	0.47
1:A:238:ALA:HB1	1:A:240:LEU:HD23	1.97	0.47
1:B:393:GLN:O	1:B:397:LEU:HD13	2.15	0.47
1:C:77:TYR:CE2	1:C:140:ILE:CG2	2.95	0.46
1:B:348:ARG:CG	1:B:348:ARG:NH1	2.74	0.46
1:D:147:VAL:HG23	4:D:2064:HOH:O	2.15	0.46
1:B:266:GLU:OE1	1:B:266:GLU:N	2.48	0.46
1:C:11:ARG:NH1	1:C:16:ARG:HG2	2.30	0.46
1:D:187:ILE:HG21	1:D:192:ASP:CA	2.37	0.46
1:B:141:PHE:CD1	1:B:170:ALA:HA	2.50	0.46
1:D:40:LYS:C	1:D:42:GLY:H	2.18	0.46
1:B:349:LYS:NZ	4:B:2128:HOH:O	2.48	0.46
1:D:183:ALA:O	1:D:213:VAL:HA	2.15	0.46
1:A:369:LYS:HE3	1:D:363:TYR:CE1	2.50	0.46
1:C:29:PHE:CE1	1:C:59:LEU:HD13	2.51	0.46
1:B:104:CYS:HB3	1:B:151:LYS:HG2	1.96	0.46
1:B:95:SER:HB3	4:B:2036:HOH:O	2.15	0.46
1:D:218:HIS:HE2	1:D:262:ILE:CD1	2.25	0.46
1:D:162:GLU:HG3	1:D:186:CYS:SG	2.56	0.46
1:D:215:VAL:CG1	4:D:2090:HOH:O	2.54	0.46
1:D:151:LYS:HD3	4:D:2068:HOH:O	2.15	0.46
1:C:159:GLU:O	1:C:161:PHE:HD1	1.98	0.46
1:C:220:ASP:HB3	1:C:251:TYR:O	2.16	0.46
1:B:393:GLN:O	1:B:396:ALA:HB3	2.16	0.46
1:C:77:TYR:HE2	1:C:140:ILE:HG23	1.72	0.46
1:A:348:ARG:CG	1:A:348:ARG:NH1	2.76	0.46
1:D:348:ARG:CG	1:D:348:ARG:NH1	2.78	0.46
1:A:220:ASP:HB2	1:A:221:PRO:HD2	1.98	0.46
1:B:332:GLY:O	1:B:335:LEU:HB2	2.16	0.46
1:D:218:HIS:HB3	1:D:260:GLY:CA	2.43	0.46
1:C:164:VAL:O	1:C:165:GLU:C	2.53	0.46
1:D:348:ARG:HG2	1:D:348:ARG:NH1	2.27	0.46
1:A:389:THR:O	1:A:393:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:O	1:A:397:LEU:HD13	2.16	0.46
1:D:393:GLN:O	1:D:397:LEU:HD13	2.15	0.46
1:B:35:LYS:HE2	4:B:2094:HOH:O	2.16	0.46
1:A:377:LYS:CG	1:A:378:GLY:N	2.64	0.46
1:C:241:LYS:HZ2	1:C:242:ALA:H	1.63	0.46
1:D:238:ALA:CB	1:D:240:LEU:HD23	2.46	0.46
1:B:125:THR:O	1:B:128:TYR:HB3	2.16	0.46
1:D:352:TRP:HE3	4:D:2121:HOH:O	1.99	0.46
1:D:379:ALA:C	1:D:383:MET:H	2.19	0.46
1:A:43:PRO:HD3	1:B:337:MET:HE3	1.96	0.46
1:A:238:ALA:CB	1:A:240:LEU:HD23	2.46	0.46
1:A:141:PHE:CD1	1:A:170:ALA:HA	2.51	0.45
1:B:11:ARG:NH1	1:B:16:ARG:HG2	2.31	0.45
1:C:373:TRP:CH2	1:C:377:LYS:N	2.78	0.45
1:D:378:GLY:O	1:D:382:LEU:HB2	2.15	0.45
1:D:164:VAL:HG13	1:D:201:CYS:SG	2.55	0.45
1:D:141:PHE:CD1	1:D:170:ALA:HA	2.51	0.45
1:C:230:LEU:HB3	4:C:2048:HOH:O	2.17	0.45
1:D:166:GLU:O	1:D:169:TRP:HB2	2.16	0.45
1:D:246:SER:HB3	4:D:2090:HOH:O	2.16	0.45
1:C:401:GLN:HB2	1:C:402:LYS:CE	2.47	0.45
1:B:166:GLU:O	1:B:169:TRP:HB2	2.16	0.45
1:D:145:LEU:HD11	1:D:177:SER:HB3	1.98	0.45
1:D:266:GLU:OE1	1:D:266:GLU:N	2.47	0.45
1:B:79:SER:C	1:B:94:ILE:CG2	2.84	0.45
1:A:262:ILE:HG23	1:B:343:ILE:CD1	2.43	0.45
1:D:183:ALA:HB1	1:D:205:LEU:HD13	1.99	0.45
1:B:73:THR:HB	1:B:75:THR:HG23	1.99	0.45
1:B:308:ARG:HG2	1:B:308:ARG:O	2.16	0.45
1:B:389:THR:O	1:B:393:GLN:HG3	2.17	0.45
1:A:258:LYS:HE3	1:A:259:GLN:CA	2.45	0.45
1:A:116:ALA:C	1:A:117:LEU:HD12	2.37	0.45
1:C:163:HIS:CD2	1:C:193:LEU:HB2	2.51	0.45
1:D:124:GLN:CD	1:D:162:GLU:N	2.69	0.45
1:B:251:TYR:CE1	1:B:275:VAL:HG22	2.51	0.45
1:D:124:GLN:HE21	1:D:161:PHE:N	2.15	0.45
1:C:76:PHE:HZ	1:C:96:GLY:CA	2.29	0.45
1:D:170:ALA:O	1:D:174:LEU:HD23	2.15	0.45
1:C:373:TRP:HH2	1:C:380:ALA:CB	2.21	0.45
1:B:164:VAL:O	1:B:165:GLU:C	2.55	0.45
1:C:238:ALA:CB	1:C:240:LEU:HD23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:O	1:A:203:VAL:HG23	2.16	0.45
1:C:220:ASP:HB2	1:C:221:PRO:HD2	1.98	0.45
1:C:217:CYS:HB2	1:C:299:CYS:SG	2.57	0.45
1:A:258:LYS:CD	1:A:259:GLN:N	2.78	0.45
1:A:138:LYS:HD3	4:A:2035:HOH:O	2.17	0.45
1:A:241:LYS:HZ2	1:A:242:ALA:H	1.64	0.45
1:C:164:VAL:CG1	1:C:201:CYS:SG	3.05	0.44
1:B:379:ALA:HB1	1:B:383:MET:HE2	1.97	0.44
1:B:333:SER:C	1:B:335:LEU:N	2.70	0.44
1:A:393:GLN:OE1	1:C:316:PRO:HB3	2.17	0.44
1:B:391:GLU:OE2	1:D:349:LYS:HB2	2.16	0.44
1:A:146:GLU:HG3	1:A:150:LYS:HE2	1.99	0.44
1:A:363:TYR:CE1	1:D:369:LYS:HE3	2.52	0.44
1:C:58:GLN:HE21	1:C:62:GLU:CG	2.31	0.44
1:C:333:SER:C	1:C:335:LEU:N	2.71	0.44
1:C:272:GLU:N	1:C:273:PRO:HD2	2.33	0.44
1:B:258:LYS:HE3	1:B:258:LYS:N	2.31	0.44
1:C:213:VAL:CG1	1:C:214:GLY:N	2.80	0.44
1:D:251:TYR:CE1	1:D:275:VAL:HG22	2.53	0.44
1:D:332:GLY:O	1:D:335:LEU:HB2	2.17	0.44
1:B:117:LEU:HD12	1:B:117:LEU:N	2.33	0.44
1:C:162:GLU:HA	1:C:187:ILE:CG2	2.47	0.44
1:B:375:VAL:HG22	1:B:377:LYS:N	2.32	0.44
1:D:146:GLU:HG3	1:D:150:LYS:HE2	2.00	0.44
1:C:65:ARG:HG2	1:C:324:ALA:HB2	1.99	0.44
1:C:117:LEU:N	1:C:117:LEU:HD12	2.32	0.44
1:D:59:LEU:HD23	4:D:2018:HOH:O	2.17	0.44
1:A:338:HIS:HD2	4:B:2013:HOH:O	2.00	0.44
1:C:184:THR:HA	1:C:214:GLY:O	2.18	0.44
1:D:301:GLY:N	4:D:2103:HOH:O	2.50	0.44
1:B:333:SER:O	1:B:335:LEU:N	2.51	0.44
1:D:278:ARG:HG3	1:D:279:TRP:CE3	2.53	0.44
1:D:117:LEU:HD12	1:D:117:LEU:N	2.33	0.44
1:C:206:VAL:HG23	1:C:207:LYS:N	2.33	0.44
1:D:74:PHE:CB	4:D:2030:HOH:O	2.66	0.44
1:B:220:ASP:HB2	1:B:221:PRO:CD	2.48	0.44
1:C:272:GLU:O	1:C:275:VAL:HG23	2.18	0.44
1:C:383:MET:C	1:C:385:GLN:N	2.71	0.44
1:C:161:PHE:CE2	1:C:167:ALA:N	2.85	0.44
1:C:187:ILE:O	1:C:187:ILE:HD12	2.18	0.44
1:D:164:VAL:O	1:D:165:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ALA:HB2	1:C:96:GLY:HA3	1.99	0.44
1:A:336:ASP:CA	4:A:2102:HOH:O	2.59	0.44
1:D:220:ASP:HB2	1:D:221:PRO:CD	2.48	0.44
1:D:282:GLN:HB3	1:D:282:GLN:HE21	1.58	0.44
1:B:15:GLU:OE2	1:B:15:GLU:N	2.45	0.44
1:D:380:ALA:C	1:D:382:LEU:N	2.67	0.44
1:D:129:LEU:CD2	4:D:2054:HOH:O	2.62	0.44
1:B:186:CYS:HB2	1:B:218:HIS:ND1	2.33	0.44
1:A:134:GLU:O	1:A:134:GLU:HG2	2.18	0.44
1:D:13:ILE:CG2	1:D:14:LEU:N	2.80	0.44
1:C:278:ARG:HG3	1:C:279:TRP:CE3	2.52	0.44
1:D:187:ILE:HD13	1:D:187:ILE:HA	1.88	0.43
1:C:29:PHE:CE2	1:C:56:VAL:HG13	2.53	0.43
1:D:333:SER:C	1:D:335:LEU:N	2.71	0.43
1:B:291:LEU:O	1:B:291:LEU:HG	2.18	0.43
1:A:65:ARG:HG2	1:A:324:ALA:HB2	2.00	0.43
1:A:117:LEU:HD12	1:A:117:LEU:N	2.32	0.43
1:D:11:ARG:NH1	1:D:16:ARG:HG2	2.32	0.43
1:C:77:TYR:O	1:C:77:TYR:HD1	2.01	0.43
1:C:398:PHE:O	1:C:402:LYS:HB2	2.18	0.43
1:B:137:VAL:HG11	1:B:169:TRP:CZ3	2.53	0.43
1:C:182:ALA:CB	1:C:212:ILE:HB	2.48	0.43
1:A:291:LEU:HG	1:A:291:LEU:O	2.19	0.43
1:B:229:LYS:NZ	4:B:2080:HOH:O	2.51	0.43
1:A:382:LEU:CD1	1:A:386:LYS:N	2.80	0.43
1:D:187:ILE:CG2	1:D:192:ASP:HA	2.36	0.43
1:D:272:GLU:N	1:D:273:PRO:HD2	2.33	0.43
1:C:225:LEU:HG	4:C:2050:HOH:O	2.19	0.43
1:A:362:PRO:HB2	1:D:367:MET:HE3	2.00	0.43
1:A:186:CYS:HB2	1:A:218:HIS:HB2	2.00	0.43
1:C:164:VAL:HG13	1:C:201:CYS:SG	2.58	0.43
1:D:401:GLN:O	1:D:404:LYS:HG2	2.18	0.43
1:C:78:ALA:CB	1:C:96:GLY:HA3	2.48	0.43
1:D:206:VAL:HG23	1:D:207:LYS:N	2.33	0.43
1:A:130:SER:O	1:A:132:LYS:HG2	2.18	0.43
1:A:332:GLY:O	1:A:335:LEU:HB2	2.18	0.43
1:B:362:PRO:HB2	1:C:367:MET:HE3	1.99	0.43
1:C:128:TYR:CE2	1:C:169:TRP:CZ3	3.06	0.43
1:C:134:GLU:HG2	1:C:134:GLU:O	2.19	0.43
1:A:308:ARG:HG2	1:A:308:ARG:O	2.19	0.43
1:C:182:ALA:CA	1:C:212:ILE:HB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HB	4:B:2075:HOH:O	2.18	0.43
1:D:267:PHE:HA	1:D:268:PRO:HA	1.71	0.43
1:C:136:GLU:HG3	4:C:2038:HOH:O	2.18	0.43
1:D:116:ALA:C	1:D:117:LEU:HD12	2.38	0.43
1:D:186:CYS:HB2	1:D:217:CYS:O	2.18	0.43
1:B:394:LEU:O	1:B:398:PHE:HD1	2.02	0.43
1:B:340:LYS:HA	1:B:341:PRO:HD3	1.81	0.43
1:A:267:PHE:HA	1:A:268:PRO:HA	1.74	0.43
1:D:175:LYS:N	1:D:181:ILE:HD11	2.33	0.43
1:A:342:TRP:CE3	1:B:373:TRP:HB3	2.54	0.43
1:B:379:ALA:C	1:B:381:GLU:N	2.71	0.43
1:D:166:GLU:O	1:D:169:TRP:N	2.51	0.43
1:B:394:LEU:HA	1:D:316:PRO:HG3	2.00	0.43
1:A:220:ASP:HB2	1:A:221:PRO:CD	2.49	0.43
1:A:278:ARG:HG3	1:A:279:TRP:CE3	2.54	0.43
1:A:11:ARG:NH1	1:A:16:ARG:HG2	2.34	0.43
1:C:161:PHE:CE2	1:C:166:GLU:CG	2.98	0.43
1:C:175:LYS:N	1:C:181:ILE:HD11	2.34	0.43
1:D:52:HIS:CE1	4:D:2026:HOH:O	2.72	0.43
1:C:206:VAL:CG2	1:C:207:LYS:N	2.82	0.42
1:D:393:GLN:O	1:D:396:ALA:HB3	2.20	0.42
1:C:73:THR:HB	1:C:75:THR:HG23	2.00	0.42
1:C:161:PHE:HE2	1:C:166:GLU:CB	2.31	0.42
1:C:166:GLU:O	1:C:169:TRP:N	2.51	0.42
1:D:123:SER:HB3	1:D:160:TYR:HB2	2.00	0.42
1:A:337:MET:CE	1:B:43:PRO:HD3	2.50	0.42
1:A:58:GLN:O	1:A:62:GLU:HG3	2.18	0.42
1:A:282:GLN:HB3	1:A:282:GLN:HE21	1.60	0.42
1:A:151:LYS:O	1:A:152:ASN:C	2.57	0.42
1:D:125:THR:C	4:D:2054:HOH:O	2.57	0.42
1:C:241:LYS:HG2	4:C:2059:HOH:O	2.19	0.42
1:C:348:ARG:CG	1:C:348:ARG:NH1	2.79	0.42
1:C:13:ILE:CG2	1:C:14:LEU:N	2.83	0.42
1:C:166:GLU:O	1:C:169:TRP:HB2	2.19	0.42
1:D:186:CYS:C	1:D:219:PHE:HE1	2.22	0.42
1:B:164:VAL:HG23	1:B:165:GLU:OE1	2.20	0.42
1:A:213:VAL:CG1	1:A:214:GLY:N	2.82	0.42
1:A:76:PHE:CG	1:A:77:TYR:N	2.85	0.42
1:C:188:GLY:C	1:C:190:GLU:N	2.73	0.42
1:D:385:GLN:NE2	1:D:385:GLN:CA	2.77	0.42
1:B:79:SER:HA	1:B:94:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:CG1	1:B:214:GLY:N	2.83	0.42
1:A:251:TYR:CE1	1:A:275:VAL:HG22	2.54	0.42
1:B:134:GLU:O	1:B:134:GLU:HG2	2.19	0.42
1:A:333:SER:C	1:A:335:LEU:N	2.72	0.42
1:C:198:PRO:CB	4:C:2048:HOH:O	2.66	0.42
1:D:150:LYS:HD2	4:D:2066:HOH:O	2.18	0.42
1:B:146:GLU:HG3	1:B:150:LYS:HE2	2.02	0.42
1:C:220:ASP:HB2	1:C:221:PRO:CD	2.50	0.42
1:D:307:ILE:HA	4:D:2106:HOH:O	2.19	0.42
1:D:340:LYS:HD2	1:D:342:TRP:CZ2	2.55	0.42
1:A:10:LYS:CB	1:A:10:LYS:HZ3	2.33	0.42
1:A:77:TYR:OH	1:A:140:ILE:HG12	2.20	0.42
1:C:11:ARG:CB	1:C:11:ARG:NH1	2.66	0.42
1:D:65:ARG:HG2	1:D:324:ALA:HB2	2.02	0.42
1:B:241:LYS:HZ2	1:B:242:ALA:H	1.68	0.42
1:D:259:GLN:OE1	1:D:260:GLY:N	2.48	0.41
1:C:127:SER:CB	1:C:140:ILE:HD12	2.50	0.41
1:C:76:PHE:CZ	1:C:78:ALA:HB2	2.54	0.41
1:D:231:MET:O	1:D:232:LYS:C	2.58	0.41
1:A:369:LYS:HE2	4:D:2130:HOH:O	2.20	0.41
1:B:390:THR:HG21	1:D:286:ARG:NH1	2.35	0.41
1:C:291:LEU:HG	1:C:291:LEU:O	2.19	0.41
1:D:291:LEU:O	1:D:291:LEU:HG	2.18	0.41
1:C:116:ALA:C	1:C:117:LEU:HD12	2.40	0.41
1:D:189:PRO:C	1:D:191:GLY:N	2.73	0.41
1:D:206:VAL:CG2	1:D:207:LYS:N	2.83	0.41
1:C:340:LYS:HA	1:C:341:PRO:HD3	1.83	0.41
1:A:29:PHE:CD1	1:A:59:LEU:HD13	2.55	0.41
1:C:377:LYS:O	1:C:379:ALA:N	2.51	0.41
1:C:98:LYS:HB2	1:C:98:LYS:HE2	1.94	0.41
1:C:348:ARG:NH1	1:C:348:ARG:HG2	2.29	0.41
1:B:294:ARG:HG3	4:B:2004:HOH:O	2.20	0.41
1:D:308:ARG:HB2	4:D:2107:HOH:O	2.20	0.41
1:A:13:ILE:CG2	1:A:14:LEU:H	2.33	0.41
1:D:333:SER:O	1:D:335:LEU:N	2.54	0.41
1:D:291:LEU:HA	4:D:2102:HOH:O	2.20	0.41
1:C:15:GLU:N	1:C:15:GLU:OE2	2.43	0.41
1:C:161:PHE:HE2	1:C:166:GLU:HB3	1.86	0.41
1:A:272:GLU:N	1:A:273:PRO:HD2	2.36	0.41
1:D:267:PHE:CE1	1:D:268:PRO:HB3	2.56	0.41
1:A:258:LYS:HA	1:A:258:LYS:HD2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ALA:O	1:B:373:TRP:C	2.58	0.41
1:B:94:ILE:H	1:B:94:ILE:HD13	1.85	0.41
1:A:166:GLU:O	1:A:169:TRP:N	2.54	0.41
1:A:247:GLN:O	1:A:299:CYS:HB2	2.20	0.41
1:D:354:ASN:HB2	4:D:2124:HOH:O	2.21	0.41
1:D:223:THR:HG22	4:D:2084:HOH:O	2.20	0.41
1:B:190:GLU:HG2	4:B:2069:HOH:O	2.21	0.41
1:B:217:CYS:SG	1:B:249:LEU:HD21	2.60	0.41
1:C:198:PRO:HG3	1:C:230:LEU:CD1	2.47	0.41
1:B:377:LYS:C	1:B:379:ALA:N	2.72	0.41
1:D:134:GLU:HA	1:D:137:VAL:CG1	2.50	0.41
1:C:127:SER:OG	1:C:137:VAL:HG23	2.21	0.41
1:B:134:GLU:HA	1:B:137:VAL:CG1	2.50	0.41
1:D:373:TRP:O	1:D:375:VAL:N	2.53	0.41
1:D:196:VAL:O	1:D:197:SER:O	2.38	0.41
1:D:207:LYS:HB2	4:D:2081:HOH:O	2.21	0.41
1:D:257:GLY:H	1:D:370:PRO:CG	2.34	0.41
1:A:132:LYS:O	1:A:133:SER:OG	2.37	0.41
1:A:134:GLU:HA	1:A:137:VAL:CG1	2.51	0.41
1:A:166:GLU:O	1:A:169:TRP:HB2	2.21	0.41
1:C:333:SER:O	1:C:335:LEU:N	2.53	0.41
1:B:272:GLU:N	1:B:273:PRO:HD2	2.36	0.41
1:D:264:LEU:HA	1:D:265:PRO:HD3	1.96	0.41
1:B:58:GLN:HE21	1:B:62:GLU:CG	2.34	0.41
1:B:278:ARG:HG3	1:B:279:TRP:CE3	2.56	0.41
1:C:126:PRO:CA	1:C:129:LEU:HB2	2.30	0.41
1:D:134:GLU:HG2	1:D:134:GLU:O	2.21	0.41
1:D:182:ALA:HA	1:D:212:ILE:HB	2.03	0.41
1:B:369:LYS:HE3	1:C:363:TYR:CZ	2.56	0.41
1:D:132:LYS:O	1:D:136:GLU:HB2	2.21	0.40
1:D:187:ILE:N	1:D:219:PHE:CE1	2.89	0.40
1:C:49:ALA:HA	1:C:56:VAL:HG21	2.03	0.40
1:B:206:VAL:HG23	1:B:207:LYS:N	2.35	0.40
1:C:308:ARG:HD2	4:C:2071:HOH:O	2.20	0.40
1:C:146:GLU:HG3	1:C:150:LYS:HE2	2.03	0.40
1:C:76:PHE:HZ	1:C:96:GLY:HA3	1.86	0.40
1:A:393:GLN:O	1:A:396:ALA:HB3	2.21	0.40
1:D:305:TYR:HA	4:D:2107:HOH:O	2.20	0.40
1:D:213:VAL:CG1	1:D:214:GLY:N	2.84	0.40
1:C:241:LYS:NZ	1:C:242:ALA:H	2.19	0.40
1:D:340:LYS:HA	1:D:341:PRO:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:PHE:HB3	1:B:223:THR:HB	2.04	0.40
1:D:391:GLU:O	1:D:395:ARG:HG3	2.22	0.40
1:B:374:GLY:O	1:B:375:VAL:C	2.60	0.40
1:B:238:ALA:C	1:B:240:LEU:H	2.25	0.40
1:B:231:MET:O	1:B:232:LYS:C	2.59	0.40
1:C:267:PHE:HA	1:C:268:PRO:HA	1.71	0.40
1:B:124:GLN:OE1	1:B:162:GLU:HG3	2.21	0.40
1:C:40:LYS:HB2	1:D:327:LYS:CA	2.50	0.40
1:B:166:GLU:OE1	4:B:2064:HOH:O	2.22	0.40
1:C:327:LYS:HE2	4:C:2078:HOH:O	2.21	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	371/407 (91%)	320 (86%)	34 (9%)	17 (5%)	3	3
1	B	377/407 (93%)	322 (85%)	38 (10%)	17 (4%)	3	3
1	C	377/407 (93%)	320 (85%)	41 (11%)	16 (4%)	3	4
1	D	378/407 (93%)	322 (85%)	34 (9%)	22 (6%)	2	2
All	All	1503/1628 (92%)	1284 (85%)	147 (10%)	72 (5%)	3	3

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	260	GLY
1	A	338	HIS
1	A	376	THR
1	A	377	LYS

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Mol	Chain	Res	Type
1	A	379	ALA
1	B	132	LYS
1	B	189	PRO
1	B	190	GLU
1	B	259	GLN
1	B	338	HIS
1	B	372	ALA
1	B	373	TRP
1	B	377	LYS
1	C	126	PRO
1	C	129	LEU
1	C	218	HIS
1	C	338	HIS
1	C	372	ALA
1	C	375	VAL
1	C	377	LYS
1	C	403	PHE
1	D	95	SER
1	D	133	SER
1	D	338	HIS
1	D	372	ALA
1	D	375	VAL
1	D	377	LYS
1	A	131	CYS
1	A	330	SER
1	A	380	ALA
1	A	381	GLU
1	A	384	GLN
1	B	330	SER
1	B	375	VAL
1	C	330	SER
1	C	373	TRP
1	D	127	SER
1	D	134	GLU
1	D	260	GLY
1	D	330	SER
1	D	374	GLY
1	D	376	THR
1	A	193	LEU
1	A	218	HIS
1	A	238	ALA
1	A	372	ALA

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Mol	Chain	Res	Type
1	B	92	GLU
1	B	217	CYS
1	B	238	ALA
1	C	133	SER
1	C	238	ALA
1	D	217	CYS
1	D	238	ALA
1	D	256	CYS
1	D	258	LYS
1	B	128	TYR
1	C	131	CYS
1	C	192	ASP
1	D	128	TYR
1	D	339	THR
1	A	133	SER
1	A	339	THR
1	B	127	SER
1	B	339	THR
1	C	43	PRO
1	C	339	THR
1	D	94	ILE
1	D	160	TYR
1	D	197	SER
1	D	42	GLY
1	B	334	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	297/323 (92%)	277 (93%)	20 (7%)	20	37
1	B	302/323 (94%)	277 (92%)	25 (8%)	14	26
1	C	303/323 (94%)	276 (91%)	27 (9%)	12	23
1	D	304/323 (94%)	279 (92%)	25 (8%)	14	27
All	All	1206/1292 (93%)	1109 (92%)	97 (8%)	15	28

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	76	PHE
1	A	98	LYS
1	A	125	THR
1	A	129	LEU
1	A	164	VAL
1	A	186	CYS
1	A	194	HIS
1	A	200	GLU
1	A	233	GLU
1	A	241	LYS
1	A	256	CYS
1	A	258	LYS
1	A	261	PHE
1	A	268	PRO
1	A	295	TYR
1	A	348	ARG
1	A	350	GLU
1	A	376	THR
1	A	395	ARG
1	B	59	LEU
1	B	76	PHE
1	B	94	ILE
1	B	98	LYS
1	B	129	LEU
1	B	152	ASN
1	B	164	VAL
1	B	189	PRO
1	B	190	GLU
1	B	200	GLU
1	B	218	HIS
1	B	233	GLU
1	B	241	LYS
1	B	256	CYS
1	B	258	LYS
1	B	259	GLN
1	B	261	PHE
1	B	268	PRO
1	B	295	TYR
1	B	348	ARG
1	B	350	GLU
1	B	376	THR

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Mol	Chain	Res	Type
1	B	377	LYS
1	B	381	GLU
1	B	395	ARG
1	C	10	LYS
1	C	59	LEU
1	C	76	PHE
1	C	77	TYR
1	C	98	LYS
1	C	128	TYR
1	C	129	LEU
1	C	152	ASN
1	C	160	TYR
1	C	164	VAL
1	C	192	ASP
1	C	193	LEU
1	C	200	GLU
1	C	216	ASN
1	C	233	GLU
1	C	241	LYS
1	C	256	CYS
1	C	258	LYS
1	C	261	PHE
1	C	268	PRO
1	C	295	TYR
1	C	348	ARG
1	C	350	GLU
1	C	376	THR
1	C	382	LEU
1	C	395	ARG
1	C	402	LYS
1	D	10	LYS
1	D	29	PHE
1	D	59	LEU
1	D	76	PHE
1	D	98	LYS
1	D	129	LEU
1	D	164	VAL
1	D	186	CYS
1	D	193	LEU
1	D	194	HIS
1	D	217	CYS
1	D	233	GLU

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Mol	Chain	Res	Type
1	D	241	LYS
1	D	256	CYS
1	D	258	LYS
1	D	259	GLN
1	D	261	PHE
1	D	268	PRO
1	D	295	TYR
1	D	348	ARG
1	D	350	GLU
1	D	377	LYS
1	D	381	GLU
1	D	395	ARG
1	D	404	LYS

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	58	GLN
1	A	72	GLN
1	A	97	GLN
1	A	100	ASN
1	A	124	GLN
1	A	143	GLN
1	A	144	GLN
1	A	152	ASN
1	A	282	GLN
1	A	290	ASN
1	A	385	GLN
1	B	18	ASN
1	B	58	GLN
1	B	72	GLN
1	B	97	GLN
1	B	100	ASN
1	B	143	GLN
1	B	144	GLN
1	B	152	ASN
1	B	194	HIS
1	B	247	GLN
1	B	282	GLN
1	B	290	ASN
1	B	385	GLN

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Mol	Chain	Res	Type
1	C	18	ASN
1	C	58	GLN
1	C	72	GLN
1	C	97	GLN
1	C	100	ASN
1	C	124	GLN
1	C	143	GLN
1	C	144	GLN
1	C	152	ASN
1	C	194	HIS
1	C	216	ASN
1	C	247	GLN
1	C	282	GLN
1	C	290	ASN
1	C	385	GLN
1	C	401	GLN
1	D	18	ASN
1	D	52	HIS
1	D	58	GLN
1	D	72	GLN
1	D	97	GLN
1	D	100	ASN
1	D	124	GLN
1	D	143	GLN
1	D	247	GLN
1	D	282	GLN
1	D	290	ASN
1	D	385	GLN
1	D	401	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	BME	A	1400	-	3,3,3	1.98	1 (33%)	2,2,2	1.61	1 (50%)
3	BME	B	1400	-	3,3,3	1.88	1 (33%)	2,2,2	1.74	1 (50%)

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	BME	A	1400	-	-	0/1/1/1	0/0/0/0
3	BME	B	1400	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	BME	O1-C1	-3.42	1.23	1.42
3	B	1400	BME	O1-C1	-3.22	1.24	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1400	BME	O1-C1-C2	2.26	120.72	110.83
3	B	1400	BME	O1-C1-C2	2.41	121.40	110.83

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<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	375/407 (92%)	0.99	44 (11%) 6 6	31, 49, 65, 74	0
1	B	381/407 (93%)	0.97	47 (12%) 5 5	30, 49, 63, 70	24 (6%)
1	C	381/407 (93%)	0.83	55 (14%) 3 3	32, 52, 68, 73	0
1	D	382/407 (93%)	1.07	70 (18%) 2 2	32, 53, 69, 73	0
All	All	1519/1628 (93%)	0.97	216 (14%) 4 3	30, 51, 67, 74	24 (1%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	ALA	11.7
1	B	388	ALA	9.8
1	B	389	THR	9.0
1	B	376	THR	7.6
1	A	395	ARG	6.9
1	A	394	LEU	6.8
1	B	395	ARG	6.5
1	A	397	LEU	6.3
1	A	380	ALA	6.3
1	D	375	VAL	6.3
1	D	296	ILE	6.0
1	B	383	MET	5.8
1	B	391	GLU	5.7
1	B	378	GLY	5.7
1	A	376	THR	5.7
1	C	240	LEU	5.6
1	D	187	ILE	5.5
1	B	377	LYS	5.4
1	D	127	SER	5.0
1	A	379	ALA	5.0
1	B	398	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	399	GLU	4.9
1	B	393	GLN	4.9
1	D	209	GLY	4.9
1	C	156	LEU	4.9
1	B	94	ILE	4.9
1	A	390	THR	4.8
1	D	168	VAL	4.8
1	B	397	LEU	4.7
1	B	392	GLN	4.7
1	D	135	THR	4.7
1	A	378	GLY	4.6
1	D	203	VAL	4.5
1	D	235	LEU	4.5
1	C	315	ALA	4.4
1	A	373	TRP	4.4
1	D	207	LYS	4.4
1	D	379	ALA	4.4
1	A	398	PHE	4.3
1	A	235	LEU	4.3
1	D	205	LEU	4.3
1	B	129	LEU	4.3
1	D	186	CYS	4.3
1	A	392	GLN	4.2
1	A	137	VAL	4.2
1	A	384	GLN	4.1
1	C	142	HIS	4.0
1	D	22	VAL	4.0
1	D	377	LYS	4.0
1	C	375	VAL	4.0
1	D	261	PHE	3.9
1	C	376	THR	3.9
1	D	167	ALA	3.9
1	C	381	GLU	3.9
1	D	383	MET	3.9
1	D	244	LEU	3.9
1	B	79	SER	3.9
1	B	386	LYS	3.8
1	D	164	VAL	3.8
1	B	394	LEU	3.8
1	D	320	PHE	3.7
1	D	192	ASP	3.7
1	D	405	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	150	LYS	3.7
1	A	385	GLN	3.7
1	C	185	MET	3.6
1	C	143	GLN	3.6
1	D	319	GLY	3.6
1	B	382	LEU	3.6
1	D	403	PHE	3.5
1	D	228	ILE	3.5
1	B	387	GLU	3.5
1	C	382	LEU	3.5
1	A	381	GLU	3.5
1	D	163	HIS	3.5
1	A	377	LYS	3.4
1	A	386	LYS	3.4
1	C	137	VAL	3.4
1	C	403	PHE	3.3
1	A	391	GLU	3.3
1	D	194	HIS	3.3
1	A	383	MET	3.3
1	A	77	TYR	3.3
1	B	385	GLN	3.3
1	C	377	LYS	3.2
1	D	196	VAL	3.2
1	C	219	PHE	3.2
1	C	141	PHE	3.2
1	A	275	VAL	3.2
1	C	138	LYS	3.2
1	A	382	LEU	3.1
1	B	81	ASP	3.1
1	D	341	PRO	3.1
1	B	373	TRP	3.0
1	A	219	PHE	3.0
1	D	239	ARG	3.0
1	D	330	SER	3.0
1	D	293	VAL	3.0
1	D	373	TRP	3.0
1	D	345	ALA	2.9
1	D	128	TYR	2.9
1	C	128	TYR	2.9
1	C	174	LEU	2.9
1	D	335	LEU	2.9
1	A	393	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	275	VAL	2.9
1	D	131	CYS	2.9
1	B	273	PRO	2.9
1	D	337	MET	2.8
1	D	202	ALA	2.8
1	D	237	ALA	2.8
1	C	337	MET	2.8
1	D	150	LYS	2.8
1	A	251	TYR	2.8
1	A	55	ALA	2.8
1	B	240	LEU	2.8
1	A	389	THR	2.8
1	D	183	ALA	2.7
1	B	239	ARG	2.7
1	C	77	TYR	2.7
1	A	387	GLU	2.7
1	C	181	ILE	2.7
1	C	366	SER	2.6
1	D	374	GLY	2.6
1	C	340	LYS	2.6
1	D	224	SER	2.6
1	D	360	GLY	2.6
1	C	139	LYS	2.6
1	D	155	PHE	2.6
1	C	332	GLY	2.6
1	D	331	TRP	2.6
1	B	250	ALA	2.6
1	C	186	CYS	2.6
1	D	206	VAL	2.5
1	C	367	MET	2.5
1	C	149	MET	2.5
1	A	32	ALA	2.5
1	C	78	ALA	2.5
1	D	378	GLY	2.5
1	B	165	GLU	2.5
1	C	289	TYR	2.5
1	D	336	ASP	2.5
1	A	250	ALA	2.5
1	A	110	VAL	2.4
1	C	64	LEU	2.4
1	D	376	THR	2.4
1	A	367	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	169	TRP	2.4
1	C	384	GLN	2.4
1	C	115	ASP	2.4
1	B	259	GLN	2.4
1	D	276	ALA	2.4
1	B	59	LEU	2.4
1	C	144	GLN	2.4
1	C	342	TRP	2.4
1	B	80	GLU	2.4
1	D	174	LEU	2.4
1	D	66	ALA	2.4
1	D	380	ALA	2.4
1	A	33	LEU	2.3
1	B	375	VAL	2.3
1	C	127	SER	2.3
1	C	218	HIS	2.3
1	A	276	ALA	2.3
1	C	193	LEU	2.3
1	A	31	PHE	2.3
1	B	363	TYR	2.3
1	A	136	GLU	2.3
1	A	170	ALA	2.3
1	B	55	ALA	2.3
1	C	172	GLU	2.3
1	B	305	TYR	2.3
1	C	194	HIS	2.3
1	C	339	THR	2.3
1	D	30	VAL	2.3
1	D	210	ALA	2.3
1	D	94	ILE	2.3
1	A	107	ALA	2.2
1	A	396	ALA	2.2
1	B	306	HIS	2.2
1	D	372	ALA	2.2
1	D	218	HIS	2.2
1	A	56	VAL	2.2
1	D	231	MET	2.2
1	B	366	SER	2.2
1	B	301	GLY	2.2
1	C	165	GLU	2.2
1	A	28	GLY	2.2
1	C	402	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	373	TRP	2.2
1	C	164	VAL	2.2
1	B	298	GLY	2.2
1	B	181	ILE	2.2
1	C	259	GLN	2.2
1	B	158	ALA	2.1
1	B	251	TYR	2.1
1	C	383	MET	2.1
1	A	240	LEU	2.1
1	C	379	ALA	2.1
1	B	271	LEU	2.1
1	C	372	ALA	2.1
1	D	289	TYR	2.1
1	D	259	GLN	2.1
1	B	218	HIS	2.1
1	D	56	VAL	2.1
1	D	157	ILE	2.1
1	C	347	ALA	2.1
1	C	100	ASN	2.1
1	D	404	LYS	2.1
1	C	260	GLY	2.1
1	D	193	LEU	2.0
1	C	133	SER	2.0
1	C	389	THR	2.0
1	D	332	GLY	2.0
1	A	262	ILE	2.0
1	D	132	LYS	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<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BME	A	1400	4/4	0.92	0.17	-0.96	59,62,62,68	0
3	BME	B	1400	4/4	0.85	0.26	-	56,57,57,57	0
2	ZN	A	1399	1/1	0.97	0.11	-	72,72,72,72	0
2	ZN	C	1406	1/1	0.87	0.15	-	154,154,154,154	0
2	ZN	B	1399	1/1	0.96	0.06	-	67,67,67,67	0
2	ZN	D	1405	1/1	0.97	0.04	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.