



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:12 am GMT

PDB ID : 2NPP  
Title : Structure of the Protein Phosphatase 2A Holoenzyme  
Authors : Xu, Y.; Chen, Y.; Xing, Y.; Chao, Y.; Shi, Y.  
Deposited on : 2006-10-28  
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:

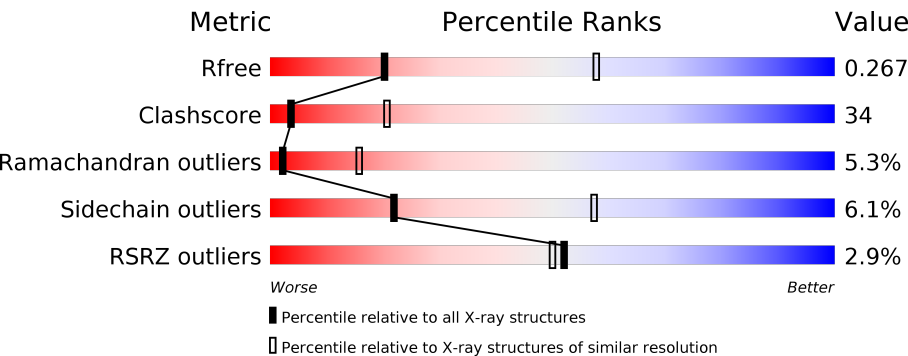
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

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))
$R_{free}$	100719	1034 (3.36-3.24)
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	589	<div><div>3%</div><div><div></div><div>48%</div><div>45%</div><div>5%</div><div></div></div><div></div></div>
1	D	589	<div><div>2%</div><div><div></div><div>52%</div><div>43%</div><div></div><div></div></div><div></div></div>
2	B	449	<div><div>5%</div><div><div></div><div>33%</div><div>46%</div><div>6%</div><div>14%</div><div></div></div><div></div></div>
2	E	449	<div><div>3%</div><div><div></div><div>33%</div><div>45%</div><div>6%</div><div>14%</div><div></div></div><div></div></div>
3	C	309	<div><div>2%</div><div><div></div><div>45%</div><div>47%</div><div>7%</div><div></div></div><div></div></div>
3	F	309	<div><div>2%</div><div><div></div><div>46%</div><div>48%</div><div>6%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain	
4	X	7	<div><div></div></div>	<div><div></div></div>
4	Y	7	<div><div></div></div>	<div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20466 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 Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4535	2881	764	863	27			
1	D	582	Total	C	N	O	S	0	0	0
			4535	2881	764	863	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			3130	2043	513	560	14			
2	E	388	Total	C	N	O	S	0	0	0
			3130	2043	513	560	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	VAL	-	CLONING ARTIFACT	UNP Q13362
B	434	LEU	-	CLONING ARTIFACT	UNP Q13362
B	435	LYS	-	CLONING ARTIFACT	UNP Q13362
B	436	LYS	-	CLONING ARTIFACT	UNP Q13362
B	437	ARG	-	CLONING ARTIFACT	UNP Q13362
B	438	ILE	-	CLONING ARTIFACT	UNP Q13362
B	439	THR	-	CLONING ARTIFACT	UNP Q13362
E	433	VAL	-	CLONING ARTIFACT	UNP Q13362
E	434	LEU	-	CLONING ARTIFACT	UNP Q13362
E	435	LYS	-	CLONING ARTIFACT	UNP Q13362
E	436	LYS	-	CLONING ARTIFACT	UNP Q13362
E	437	ARG	-	CLONING ARTIFACT	UNP Q13362
E	438	ILE	-	CLONING ARTIFACT	UNP Q13362
E	439	THR	-	CLONING ARTIFACT	UNP Q13362

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	308	Total	C	N	O	S	0	0	0
			2497	1579	431	472	15			
3	F	308	Total	C	N	O	S	0	0	0
			2497	1579	431	472	15			

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	X	7	Total	C	N	O	0	0	0
			69	49	10	10			
4	Y	7	Total	C	N	O	0	0	0
			69	49	10	10			

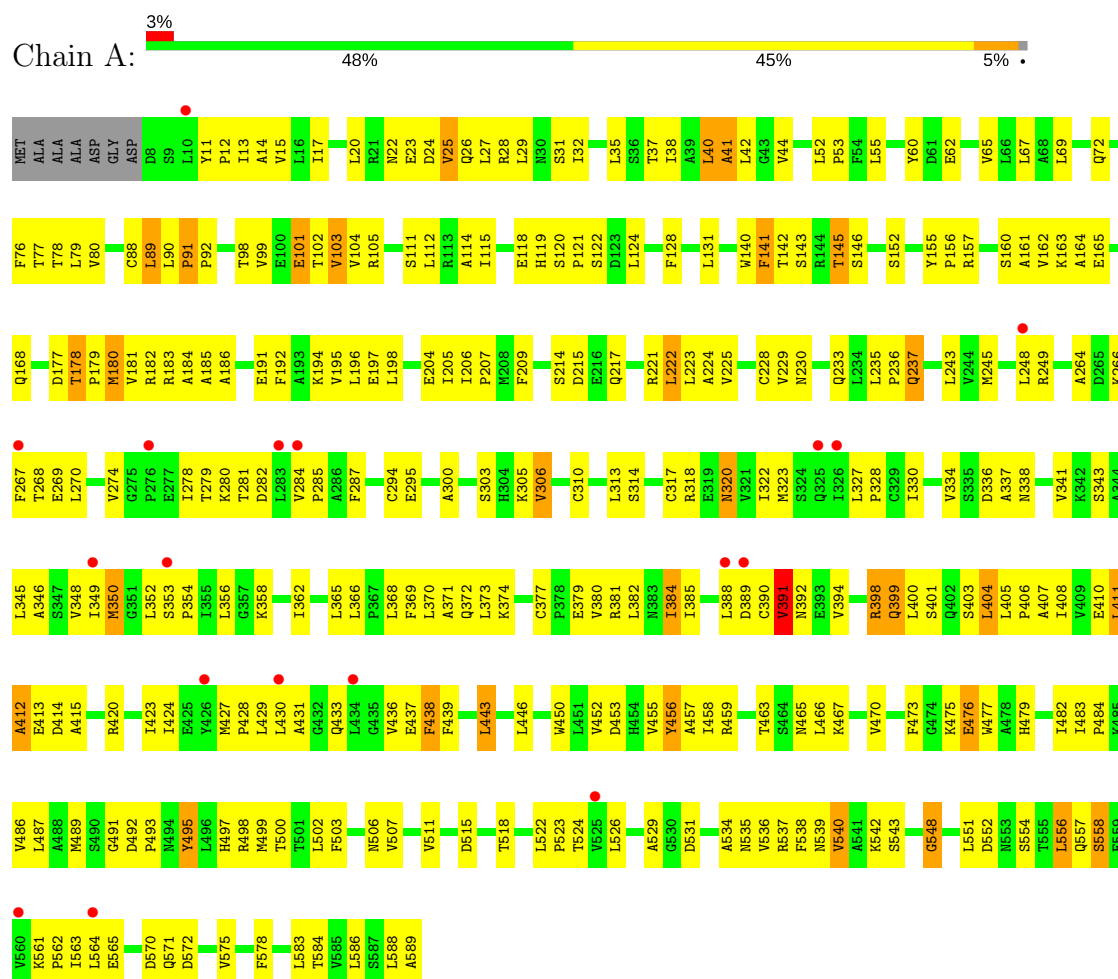
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		

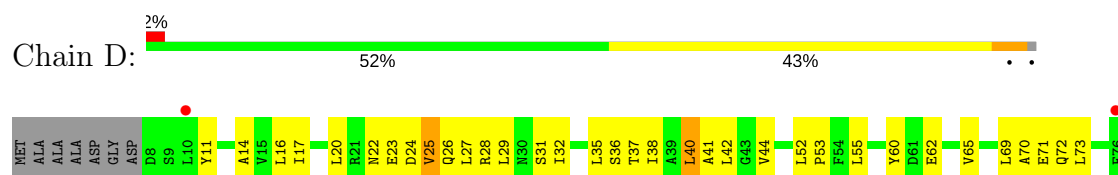
### 3 Residue-property plots

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.

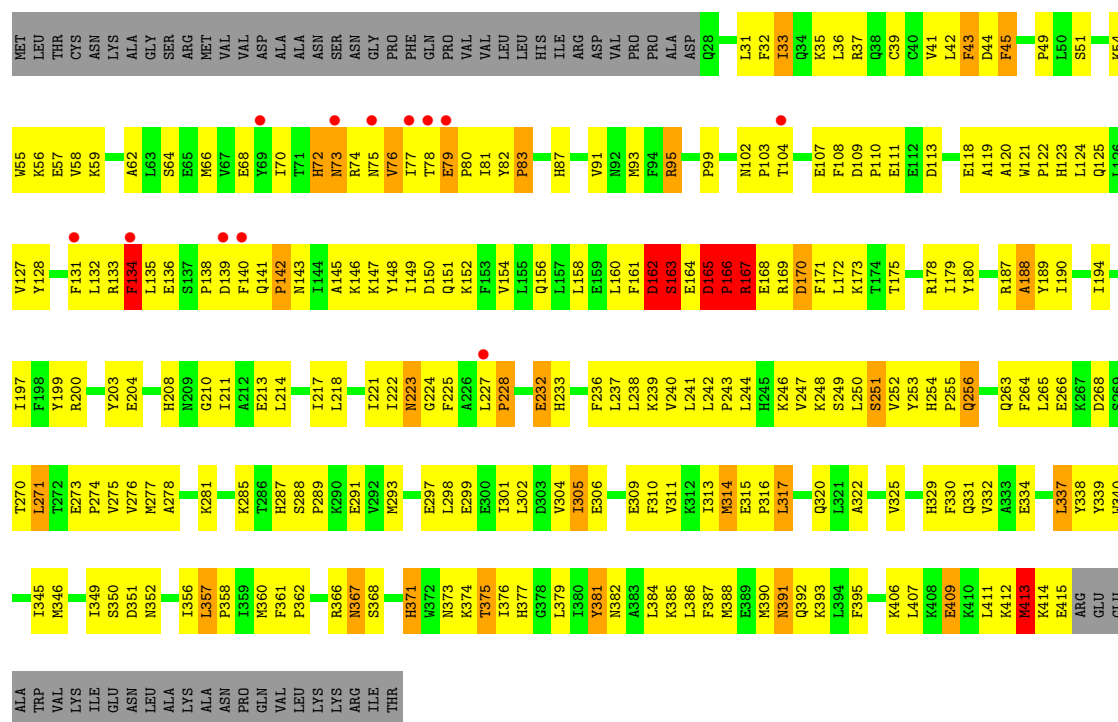
- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform



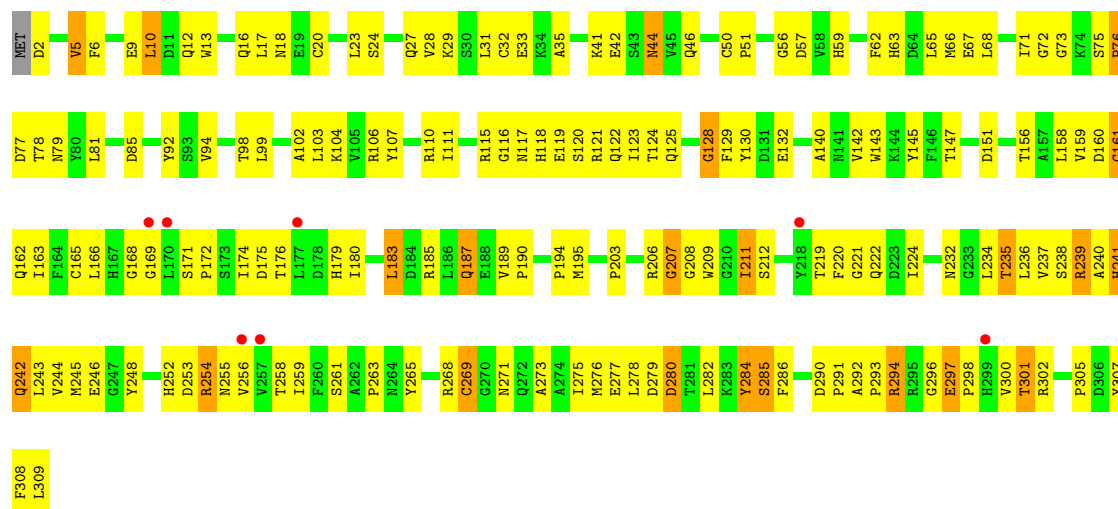
- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform



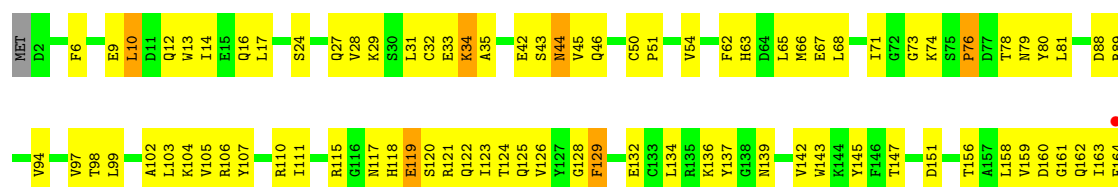




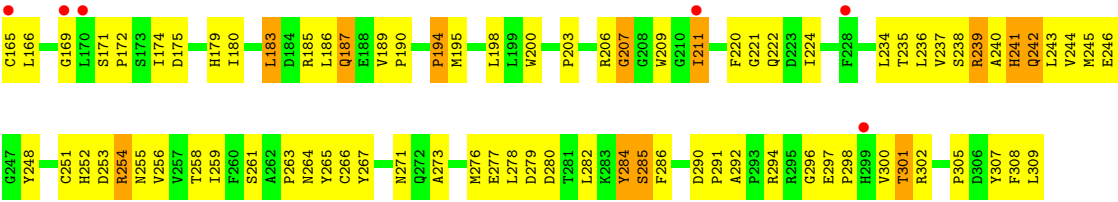
• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform







● Molecule 4: microcystin LR



● Molecule 4: microcystin LR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.26Å 159.05Å 269.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.30 49.33 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.4 (100.00-3.30) 99.3 (49.33-3.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.255 , 0.299 0.225 , 0.267	Depositor DCC
$R_{free}$ test set	3549 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.9	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACB, DAL, DAM, MN, 1ZN, FGA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/4609	0.64	0/6257
1	D	0.45	0/4609	0.66	0/6257
2	B	0.42	0/3212	0.66	2/4359 (0.0%)
2	E	0.42	0/3212	0.66	3/4359 (0.1%)
3	C	0.40	0/2559	0.65	1/3469 (0.0%)
3	F	0.41	0/2559	0.66	0/3469
4	X	0.43	0/17	0.78	0/19
4	Y	0.48	0/17	0.69	0/19
All	All	0.42	0/20794	0.65	6/28208 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	162	ASP	N-CA-C	6.21	127.77	111.00
2	B	162	ASP	N-CA-C	6.08	127.41	111.00
2	B	49	PRO	N-CA-CB	5.29	109.65	103.30
3	C	128	GLY	N-CA-C	5.16	126.01	113.10
2	E	49	PRO	N-CA-CB	5.16	109.50	103.30
2	E	163	SER	N-CA-C	5.08	124.73	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	4535	0	4637	292	0
1	D	4535	0	4637	282	0
2	B	3130	0	3050	258	0
2	E	3130	0	3050	253	0
3	C	2497	0	2393	171	0
3	F	2497	0	2393	161	0
4	X	69	0	68	3	0
4	Y	69	0	68	6	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20466	0	20296	1397	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 34.

All (1397) 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)
3:C:301:THR:HG22	3:C:302:ARG:H	1.27	0.99
3:F:174:ILE:HD13	3:F:180:ILE:HG12	1.48	0.96
3:F:301:THR:HG22	3:F:302:ARG:H	1.30	0.95
2:E:273:GLU:HA	2:E:313:ILE:HD11	1.46	0.93
2:B:322:ALA:HB2	2:B:360:MET:HE1	1.51	0.92
2:B:208:HIS:HD2	2:B:210:GLY:H	1.14	0.92
1:A:455:VAL:HG23	3:C:71:ILE:HA	1.51	0.91
1:A:278:ILE:HD12	1:A:278:ILE:H	1.34	0.91
1:A:102:THR:HG22	1:A:105:ARG:NH2	1.87	0.90
2:B:329:HIS:CD2	2:B:332:VAL:HG23	2.06	0.90
3:C:174:ILE:HD13	3:C:180:ILE:HG12	1.52	0.90
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.54	0.88
3:C:237:VAL:HB	3:C:256:VAL:HG22	1.54	0.88
1:A:178:THR:HB	1:A:180:MET:HG2	1.55	0.87
1:D:537:ARG:O	1:D:540:VAL:HG12	1.74	0.87
2:E:208:HIS:HD2	2:E:210:GLY:H	1.18	0.87
1:A:77:THR:HG21	1:A:118:GLU:HG3	1.57	0.86
2:E:322:ALA:HB2	2:E:360:MET:HE1	1.55	0.86
1:D:401:SER:HA	1:D:405:LEU:HB2	1.57	0.86
2:E:131:PHE:O	2:E:134:PHE:HB3	1.76	0.86
1:A:561:LYS:HB2	1:A:588:LEU:HD13	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:TRP:N	2:B:122:PRO:HD2	1.90	0.85
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.11	0.85
2:E:133:ARG:HA	2:E:136:GLU:HG2	1.56	0.85
1:A:537:ARG:O	1:A:540:VAL:HG12	1.77	0.84
2:E:381:TYR:HE2	2:E:385:LYS:HD2	1.42	0.84
3:C:162:GLN:HB3	3:C:235:THR:CG2	2.07	0.84
1:D:99:VAL:HG21	1:D:104:VAL:HG11	1.59	0.84
2:E:121:TRP:N	2:E:122:PRO:HD2	1.92	0.84
1:D:35:LEU:HD21	1:D:55:LEU:HD11	1.58	0.83
2:B:133:ARG:HA	2:B:136:GLU:HG2	1.60	0.83
2:B:164:GLU:HB3	2:B:168:GLU:HB3	1.60	0.83
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.43	0.82
2:E:208:HIS:CD2	2:E:210:GLY:H	1.96	0.82
2:B:237:LEU:HA	2:B:241:LEU:HB2	1.62	0.82
2:B:330:PHE:CE2	3:C:122:GLN:HG3	2.13	0.82
1:D:362:ILE:HD13	1:D:399:GLN:HG3	1.61	0.82
1:A:385:ILE:HD12	1:A:423:ILE:HD11	1.61	0.81
2:B:131:PHE:O	2:B:134:PHE:HB3	1.79	0.81
2:B:208:HIS:CD2	2:B:210:GLY:H	1.98	0.81
1:A:428:PRO:HD3	1:A:465:ASN:ND2	1.95	0.81
2:B:152:LYS:HG2	2:B:156:GLN:HE21	1.45	0.80
1:D:162:VAL:HA	1:D:165:GLU:OE1	1.80	0.80
1:D:467:LYS:HB2	1:D:507:VAL:HG12	1.63	0.79
2:E:208:HIS:HB3	2:E:211:ILE:CD1	2.13	0.79
1:D:278:ILE:HD12	1:D:278:ILE:H	1.45	0.79
2:E:208:HIS:HB3	2:E:211:ILE:HD11	1.64	0.79
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.65	0.78
2:B:199:TYR:CE2	2:B:240:VAL:HG22	2.19	0.78
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.97	0.78
2:E:175:THR:O	2:E:179:ILE:HG13	1.82	0.78
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.63	0.78
2:E:244:LEU:HD23	2:E:244:LEU:O	1.83	0.78
3:F:54:VAL:HG13	3:F:81:LEU:HD22	1.64	0.78
3:C:162:GLN:HB3	3:C:235:THR:HG22	1.64	0.78
1:D:398:ARG:HB3	1:D:398:ARG:HH11	1.49	0.78
2:E:164:GLU:HB3	2:E:168:GLU:HB3	1.66	0.77
2:B:75:ASN:O	2:B:76:VAL:HG23	1.84	0.77
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.15	0.77
2:E:78:THR:C	2:E:80:PRO:HD2	2.05	0.77
1:D:428:PRO:HD3	1:D:465:ASN:ND2	1.99	0.76
2:B:175:THR:HG22	2:B:179:ILE:HD11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:LYS:HB2	1:D:588:LEU:HD13	1.67	0.76
3:F:175:ASP:H	3:F:179:HIS:HD2	1.34	0.76
3:F:237:VAL:HB	3:F:256:VAL:HG22	1.68	0.76
2:B:340:TRP:HA	2:B:346:MET:HE3	1.68	0.76
2:B:118:GLU:H	2:B:164:GLU:HG2	1.50	0.76
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.66	0.76
1:D:267:PHE:CE2	1:D:287:PHE:HB2	2.20	0.76
3:C:44:ASN:HD22	3:C:44:ASN:N	1.81	0.76
2:E:83:PRO:HG3	2:E:148:TYR:CD2	2.20	0.76
2:E:330:PHE:CE1	2:E:331:GLN:HG2	2.21	0.75
2:B:190:ILE:HD12	2:B:190:ILE:H	1.48	0.75
2:B:288:SER:HB2	2:B:289:PRO:HD3	1.68	0.75
2:B:208:HIS:HB3	2:B:211:ILE:CD1	2.16	0.75
2:E:95:ARG:H	2:E:95:ARG:HD2	1.50	0.75
2:B:164:GLU:O	2:B:165:ASP:O	2.04	0.75
2:E:310:PHE:O	2:E:314:MET:HB2	1.87	0.75
1:D:405:LEU:HD21	1:D:430:LEU:HD11	1.69	0.75
1:D:452:VAL:O	1:D:452:VAL:HG12	1.86	0.75
2:E:75:ASN:O	2:E:76:VAL:HG23	1.87	0.75
2:E:164:GLU:O	2:E:165:ASP:O	2.04	0.74
3:C:104:LYS:N	3:C:111:ILE:HD11	2.01	0.74
2:B:217:ILE:HG22	2:B:221:ILE:HD11	1.70	0.74
1:D:350:MET:SD	1:D:391:VAL:HG13	2.27	0.74
2:E:128:TYR:HB3	2:E:171:PHE:CD2	2.22	0.74
1:D:492:ASP:OD2	1:D:493:PRO:HD2	1.88	0.74
2:B:273:GLU:HA	2:B:313:ILE:HD11	1.69	0.74
3:F:209:TRP:N	3:F:224:ILE:HD11	2.02	0.74
2:B:79:GLU:HG2	2:B:79:GLU:O	1.87	0.73
2:B:83:PRO:HG3	2:B:148:TYR:CD2	2.23	0.73
1:D:334:VAL:HG21	1:D:368:LEU:HD22	1.68	0.73
1:A:222:LEU:HD23	1:A:223:LEU:N	2.04	0.73
3:C:209:TRP:N	3:C:224:ILE:HD11	2.04	0.73
3:C:76:PRO:HB2	3:C:110:ARG:HG3	1.69	0.73
3:F:162:GLN:HB3	3:F:235:THR:HG22	1.68	0.73
3:C:160:ASP:HB3	3:C:282:LEU:HD11	1.70	0.73
3:C:175:ASP:H	3:C:179:HIS:HD2	1.36	0.73
3:F:252:HIS:O	3:F:255:ASN:HB2	1.89	0.73
3:F:290:ASP:HB3	3:F:291:PRO:HD2	1.70	0.73
3:F:44:ASN:HD22	3:F:44:ASN:N	1.86	0.72
1:A:282:ASP:O	1:A:285:PRO:HD2	1.89	0.72
1:A:467:LYS:HB2	1:A:507:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:O	1:A:334:VAL:HG23	1.87	0.72
2:E:118:GLU:H	2:E:164:GLU:HG2	1.52	0.72
3:C:120:SER:O	3:C:124:THR:HG23	1.89	0.72
1:A:334:VAL:HG21	1:A:368:LEU:HD22	1.71	0.72
3:F:171:SER:OG	3:F:174:ILE:HB	1.89	0.71
1:A:392:ASN:HB3	1:A:400:LEU:HD22	1.70	0.71
2:E:123:HIS:O	2:E:127:VAL:HG23	1.90	0.71
1:A:381:ARG:NH1	1:A:414:ASP:OD2	2.22	0.71
1:A:526:LEU:HD22	1:A:563:ILE:HG21	1.70	0.71
2:B:325:VAL:HG22	2:B:337:LEU:HD13	1.73	0.71
2:B:175:THR:O	2:B:179:ILE:HG13	1.90	0.71
2:B:208:HIS:HB3	2:B:211:ILE:HD11	1.72	0.71
1:A:161:ALA:O	1:A:164:ALA:HB3	1.91	0.71
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.71	0.71
2:E:35:LYS:C	2:E:37:ARG:H	1.94	0.71
2:E:329:HIS:CD2	2:E:332:VAL:HG23	2.25	0.71
1:A:401:SER:HA	1:A:405:LEU:HB2	1.72	0.70
1:D:105:ARG:NH1	1:D:142:THR:HG22	2.06	0.70
1:A:385:ILE:HD11	1:A:411:LEU:HG	1.71	0.70
1:D:526:LEU:HD22	1:D:563:ILE:HG21	1.73	0.70
2:B:165:ASP:O	2:B:167:ARG:N	2.24	0.70
3:C:17:LEU:HD21	3:C:23:LEU:HG	1.74	0.70
1:D:109:VAL:HG13	1:D:150:LEU:HD21	1.73	0.70
3:F:120:SER:O	3:F:124:THR:HG23	1.92	0.70
3:F:162:GLN:HB3	3:F:235:THR:CG2	2.21	0.70
3:F:17:LEU:HD11	3:F:98:THR:HG22	1.73	0.70
2:B:78:THR:C	2:B:80:PRO:HD2	2.12	0.69
3:C:308:PHE:O	3:C:309:LEU:HG	1.91	0.69
1:D:408:ILE:HD13	1:D:426:TYR:HE2	1.57	0.69
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.27	0.69
1:D:487:LEU:C	1:D:489:MET:H	1.96	0.69
2:E:165:ASP:O	2:E:167:ARG:N	2.25	0.69
2:E:381:TYR:CE2	2:E:385:LYS:HD2	2.27	0.69
2:E:242:LEU:N	2:E:243:PRO:HD2	2.07	0.69
1:A:452:VAL:HG12	1:A:452:VAL:O	1.92	0.68
2:E:59:LYS:HD3	2:E:123:HIS:CD2	2.27	0.68
3:C:76:PRO:HD3	3:C:107:TYR:CE2	2.27	0.68
2:E:79:GLU:O	2:E:79:GLU:HG2	1.92	0.68
2:B:244:LEU:O	2:B:244:LEU:HD23	1.92	0.68
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.23	0.68
1:D:197:GLU:CD	1:D:197:GLU:H	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:PRO:HB2	3:F:110:ARG:HG3	1.76	0.68
1:D:23:GLU:HA	1:D:28:ARG:HH21	1.58	0.68
3:F:115:ARG:NH1	3:F:151:ASP:HA	2.09	0.68
1:D:377:CYS:SG	1:D:379:GLU:HG2	2.34	0.68
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.56	0.68
1:D:517:THR:HA	1:D:521:MET:HE2	1.74	0.68
1:D:385:ILE:HD12	1:D:423:ILE:HD11	1.75	0.68
2:E:152:LYS:HG2	2:E:156:GLN:HE21	1.58	0.68
2:B:222:ILE:HA	2:B:225:PHE:CE1	2.29	0.67
2:B:310:PHE:O	2:B:314:MET:HB2	1.94	0.67
3:C:244:VAL:O	3:C:246:GLU:N	2.27	0.67
3:F:180:ILE:HA	3:F:183:LEU:HD12	1.76	0.67
1:A:390:CYS:O	1:A:392:ASN:N	2.26	0.67
2:E:346:MET:CE	2:E:349:ILE:HD12	2.25	0.67
2:E:409:GLU:O	2:E:413:MET:HB2	1.95	0.67
2:B:165:ASP:O	2:B:166:PRO:C	2.33	0.67
3:F:243:LEU:HD11	3:F:271:ASN:CG	2.15	0.67
2:B:83:PRO:HG3	2:B:148:TYR:CE2	2.30	0.67
2:B:80:PRO:HG2	2:B:82:TYR:CD2	2.29	0.67
1:A:140:TRP:CZ2	2:B:239:LYS:HD2	2.30	0.67
2:B:59:LYS:HD3	2:B:123:HIS:CD2	2.30	0.67
2:E:217:ILE:HG22	2:E:221:ILE:HD11	1.77	0.66
1:D:330:ILE:O	1:D:334:VAL:HG23	1.96	0.66
1:A:390:CYS:SG	1:A:391:VAL:N	2.68	0.66
3:C:244:VAL:O	3:C:244:VAL:HG23	1.95	0.66
2:B:123:HIS:O	2:B:127:VAL:HG23	1.96	0.66
1:D:390:CYS:O	1:D:392:ASN:N	2.28	0.66
1:A:152:SER:HB2	1:A:191:GLU:HG3	1.78	0.66
2:B:141:GLN:HB3	2:B:142:PRO:HD2	1.77	0.66
2:B:218:LEU:HA	2:B:221:ILE:HD12	1.78	0.66
3:F:194:PRO:HG2	3:F:195:MET:H	1.59	0.66
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.11	0.66
2:B:169:ARG:HA	2:B:172:LEU:HD12	1.77	0.66
1:D:338:ASN:HD22	1:D:341:VAL:HG23	1.59	0.66
1:D:381:ARG:NH1	1:D:414:ASP:OD2	2.29	0.66
2:E:141:GLN:HB3	2:E:142:PRO:HD2	1.76	0.65
2:E:79:GLU:N	2:E:80:PRO:CD	2.59	0.65
2:B:242:LEU:N	2:B:243:PRO:HD2	2.11	0.65
1:D:22:ASN:ND2	1:D:24:ASP:HB3	2.11	0.65
1:A:350:MET:HA	1:A:350:MET:HE3	1.79	0.65
2:E:340:TRP:HE1	2:E:387:PHE:HE1	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:HIS:O	3:C:255:ASN:HB2	1.96	0.65
1:A:214:SER:HA	1:A:221:ARG:HD2	1.78	0.65
1:D:529:ALA:HA	1:D:540:VAL:HG11	1.79	0.65
1:D:529:ALA:HB3	1:D:563:ILE:HD11	1.78	0.65
2:E:254:HIS:CD2	2:E:293:MET:HB3	2.31	0.65
3:C:62:PHE:O	3:C:65:LEU:HB3	1.97	0.65
1:A:487:LEU:C	1:A:489:MET:H	1.99	0.65
2:B:107:GLU:HG3	2:B:108:PHE:CE1	2.31	0.65
1:D:20:LEU:HD23	1:D:31:SER:HB2	1.79	0.65
2:E:165:ASP:O	2:E:166:PRO:C	2.35	0.65
3:C:180:ILE:HA	3:C:183:LEU:HD12	1.78	0.64
2:E:119:ALA:O	2:E:120:ALA:HB3	1.97	0.64
2:B:152:LYS:O	2:B:156:GLN:HG3	1.97	0.64
2:B:254:HIS:CD2	2:B:293:MET:HB3	2.32	0.64
3:C:301:THR:HG22	3:C:302:ARG:N	2.07	0.64
2:E:237:LEU:HA	2:E:241:LEU:HB2	1.79	0.64
2:B:222:ILE:HA	2:B:225:PHE:CZ	2.33	0.64
2:B:381:TYR:C	2:B:381:TYR:HD2	2.01	0.64
1:D:70:ALA:HB2	1:D:96:LEU:HD13	1.78	0.64
2:E:340:TRP:HA	2:E:346:MET:HE3	1.80	0.64
1:A:403:SER:O	1:A:404:LEU:HD13	1.97	0.64
2:B:287:HIS:CE1	2:B:289:PRO:HB2	2.33	0.64
2:B:35:LYS:C	2:B:37:ARG:H	1.99	0.64
3:C:243:LEU:HD22	4:X:7:DAM:HM3	1.78	0.64
1:D:427:MET:HA	1:D:427:MET:CE	2.26	0.64
1:A:35:LEU:HB3	1:A:72:GLN:HG2	1.80	0.64
1:A:280:LYS:HA	1:A:284:VAL:CG2	2.28	0.64
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.61	0.64
1:A:381:ARG:O	1:A:385:ILE:HG12	1.98	0.64
2:B:128:TYR:HB3	2:B:171:PHE:CD2	2.33	0.64
3:F:104:LYS:N	3:F:111:ILE:HD11	2.12	0.64
2:E:169:ARG:HA	2:E:172:LEU:HD12	1.80	0.64
2:E:298:LEU:HB3	2:E:339:TYR:OH	1.98	0.64
1:A:436:VAL:HB	1:A:473:PHE:CD1	2.32	0.63
2:B:254:HIS:HB2	2:B:293:MET:HE1	1.80	0.63
1:D:446:LEU:HD12	1:D:446:LEU:H	1.62	0.63
3:F:284:TYR:CD2	3:F:284:TYR:N	2.65	0.63
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.79	0.63
2:E:325:VAL:HG22	2:E:337:LEU:HD13	1.79	0.63
3:F:244:VAL:O	3:F:246:GLU:N	2.31	0.63
2:B:273:GLU:N	2:B:274:PRO:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:GLY:C	3:C:298:PRO:HD2	2.18	0.63
2:B:297:GLU:O	2:B:301:ILE:HG13	1.98	0.63
1:D:405:LEU:CD2	1:D:430:LEU:HD11	2.27	0.63
1:D:392:ASN:ND2	1:D:433:GLN:HE22	1.96	0.63
3:F:296:GLY:C	3:F:298:PRO:HD2	2.18	0.63
1:A:52:LEU:HD11	1:A:89:LEU:HD12	1.80	0.63
2:B:218:LEU:O	2:B:222:ILE:HG13	1.99	0.63
2:B:247:VAL:HG12	2:B:249:SER:H	1.64	0.63
2:B:79:GLU:N	2:B:80:PRO:CD	2.62	0.63
2:B:251:SER:HA	2:B:293:MET:CE	2.29	0.63
3:F:172:PRO:HG3	3:F:209:TRP:CE3	2.33	0.63
1:D:452:VAL:HG13	1:D:497:HIS:CD2	2.33	0.62
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.81	0.62
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.81	0.62
2:E:322:ALA:CB	2:E:360:MET:HE1	2.26	0.62
3:F:221:GLY:H	3:F:224:ILE:HD12	1.63	0.62
3:C:175:ASP:H	3:C:179:HIS:CD2	2.17	0.62
3:C:56:GLY:N	3:C:261:SER:OG	2.32	0.62
1:D:274:VAL:CG1	1:D:278:ILE:HB	2.29	0.62
1:D:156:PRO:HG3	1:D:195:VAL:HB	1.81	0.62
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.35	0.62
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.81	0.62
2:B:164:GLU:OE2	2:B:167:ARG:HB2	2.00	0.62
3:C:29:LYS:HB2	3:C:145:TYR:CE1	2.34	0.62
1:D:52:LEU:HB2	1:D:53:PRO:HD3	1.80	0.62
3:F:14:ILE:HD13	3:F:103:LEU:HD23	1.81	0.62
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.81	0.62
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.81	0.62
2:E:152:LYS:O	2:E:156:GLN:HG3	1.99	0.62
1:D:561:LYS:HB3	1:D:562:PRO:HD3	1.82	0.62
2:E:190:ILE:H	2:E:190:ILE:HD12	1.64	0.62
2:E:42:LEU:O	2:E:59:LYS:HE3	2.00	0.62
1:A:156:PRO:HG3	1:A:195:VAL:HB	1.80	0.62
1:A:155:TYR:CZ	1:A:196:LEU:HD23	2.34	0.62
1:D:561:LYS:O	1:D:565:GLU:HG2	1.99	0.62
1:A:502:LEU:HD13	1:A:540:VAL:HA	1.82	0.61
1:D:483:ILE:HB	1:D:484:PRO:HD3	1.82	0.61
1:D:222:LEU:HD23	1:D:223:LEU:H	1.64	0.61
1:D:24:ASP:O	1:D:25:VAL:C	2.39	0.61
3:F:174:ILE:HD13	3:F:180:ILE:CG1	2.27	0.61
1:A:300:ALA:HB2	1:A:341:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HA	1:A:540:VAL:HG11	1.83	0.61
2:B:409:GLU:O	2:B:413:MET:HB2	1.99	0.61
3:F:244:VAL:HG23	3:F:244:VAL:O	1.99	0.61
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.80	0.61
1:D:392:ASN:HD21	1:D:433:GLN:HE22	1.48	0.61
2:E:83:PRO:HG3	2:E:148:TYR:CE2	2.35	0.61
1:D:506:ASN:HD21	1:D:543:SER:HA	1.66	0.61
1:D:101:GLU:HG2	2:E:246:LYS:NZ	2.16	0.61
2:E:388:MET:CE	2:E:392:GLN:HE22	2.13	0.61
2:B:381:TYR:C	2:B:381:TYR:CD2	2.73	0.61
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.82	0.61
1:A:572:ASP:OD2	3:C:110:ARG:NH2	2.34	0.61
3:F:251:CYS:SG	3:F:256:VAL:HB	2.40	0.61
3:F:301:THR:HG22	3:F:302:ARG:N	2.08	0.61
2:B:373:ASN:HD22	2:B:376:ILE:HG23	1.66	0.61
1:D:214:SER:HA	1:D:221:ARG:HD2	1.81	0.61
2:E:227:LEU:HB2	2:E:228:PRO:HD3	1.81	0.60
1:A:215:ASP:H	1:A:221:ARG:HG2	1.66	0.60
3:C:284:TYR:N	3:C:284:TYR:CD2	2.69	0.60
2:E:199:TYR:CE2	2:E:240:VAL:HG22	2.35	0.60
1:A:529:ALA:HB3	1:A:563:ILE:HD11	1.84	0.60
2:E:317:LEU:HD12	2:E:317:LEU:C	2.22	0.60
1:A:437:GLU:CD	1:A:438:PHE:H	2.04	0.60
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.22	0.60
2:B:134:PHE:C	2:B:134:PHE:CD2	2.75	0.60
3:C:239:ARG:HH11	3:C:258:THR:HG23	1.67	0.60
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.17	0.60
1:D:538:PHE:HB2	1:D:578:PHE:HD2	1.65	0.60
1:A:162:VAL:HA	1:A:165:GLU:OE1	2.01	0.60
3:F:174:ILE:CD1	3:F:180:ILE:HG12	2.29	0.60
2:B:59:LYS:HD3	2:B:123:HIS:HD2	1.67	0.60
3:C:117:ASN:CG	3:C:241:HIS:HE1	2.05	0.60
1:D:225:VAL:O	1:D:228:CYS:HB3	2.02	0.60
2:B:119:ALA:O	2:B:120:ALA:HB3	2.02	0.60
2:B:133:ARG:HA	2:B:136:GLU:CG	2.31	0.60
2:B:384:LEU:HD22	2:B:395:PHE:HZ	1.66	0.59
1:D:115:ILE:O	1:D:119:HIS:HD2	1.85	0.59
1:D:399:GLN:HE21	1:D:399:GLN:CA	2.15	0.59
3:F:308:PHE:O	3:F:309:LEU:HG	2.01	0.59
1:A:477:TRP:CH2	1:A:482:ILE:HD11	2.37	0.59
1:A:24:ASP:O	1:A:25:VAL:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:MET:CE	3:C:278:LEU:HD21	2.31	0.59
3:C:57:ASP:O	3:C:261:SER:HB2	2.01	0.59
3:C:42:GLU:HB3	3:C:46:GLN:OE1	2.02	0.59
1:D:179:PRO:HD2	1:D:180:MET:HE3	1.85	0.59
2:E:149:ILE:O	2:E:149:ILE:HG22	2.01	0.59
2:E:376:ILE:HG13	2:E:377:HIS:N	2.17	0.59
2:B:149:ILE:O	2:B:149:ILE:HG22	2.01	0.59
2:E:222:ILE:HA	2:E:225:PHE:CE1	2.37	0.59
3:C:162:GLN:HB3	3:C:235:THR:HG21	1.85	0.59
1:D:350:MET:HE2	1:D:350:MET:HA	1.83	0.59
2:E:255:PRO:HG2	2:E:256:GLN:NE2	2.17	0.59
3:F:243:LEU:HD22	4:Y:7:DAM:HM3	1.84	0.59
3:C:156:THR:HG22	3:C:166:LEU:CB	2.33	0.59
3:C:176:THR:H	3:C:179:HIS:CD2	2.21	0.59
3:C:190:PRO:HD3	3:C:195:MET:CE	2.32	0.59
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.85	0.59
1:D:100:GLU:O	1:D:105:ARG:NH1	2.36	0.59
1:D:564:LEU:HD13	1:D:583:LEU:HD23	1.84	0.59
1:A:23:GLU:O	1:A:23:GLU:HG2	2.03	0.59
1:A:446:LEU:HD12	1:A:446:LEU:N	2.18	0.59
2:B:121:TRP:N	2:B:122:PRO:CD	2.65	0.59
2:B:317:LEU:HD12	2:B:317:LEU:O	2.03	0.59
1:D:398:ARG:CB	1:D:398:ARG:HH11	2.14	0.59
2:E:373:ASN:HD21	2:E:375:THR:HG22	1.67	0.59
1:D:399:GLN:NE2	1:D:399:GLN:HA	2.18	0.59
2:E:346:MET:HE1	2:E:349:ILE:HD12	1.85	0.59
1:A:358:LYS:O	1:A:362:ILE:HG13	2.03	0.58
1:A:564:LEU:HD22	1:A:583:LEU:CD2	2.32	0.58
3:C:115:ARG:NH1	3:C:151:ASP:HA	2.18	0.58
2:E:170:ASP:O	2:E:173:LYS:HB3	2.01	0.58
2:E:87:HIS:O	2:E:91:VAL:HG23	2.03	0.58
2:E:62:ALA:O	2:E:66:MET:HG3	2.03	0.58
2:B:266:GLU:HG2	2:B:304:VAL:HG11	1.85	0.58
2:B:95:ARG:H	2:B:95:ARG:HD2	1.67	0.58
1:D:400:LEU:HD12	1:D:404:LEU:HD23	1.85	0.58
2:E:254:HIS:HB2	2:E:293:MET:HE1	1.85	0.58
2:B:237:LEU:HG	2:B:238:LEU:HD23	1.85	0.58
2:B:80:PRO:O	2:B:82:TYR:HD2	1.87	0.58
1:A:180:MET:HE3	1:A:180:MET:H	1.69	0.58
2:B:190:ILE:N	2:B:190:ILE:HD12	2.16	0.58
2:B:346:MET:CE	2:B:349:ILE:HD12	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:PRO:O	2:B:170:ASP:N	2.35	0.58
2:B:254:HIS:N	2:B:255:PRO:HD2	2.19	0.58
1:D:564:LEU:HD22	1:D:583:LEU:HD21	1.85	0.58
2:E:128:TYR:HB3	2:E:171:PHE:HD2	1.67	0.58
1:A:115:ILE:O	1:A:119:HIS:HD2	1.87	0.58
1:D:28:ARG:HD3	1:D:60:TYR:CE2	2.39	0.58
1:D:62:GLU:H	1:D:62:GLU:CD	2.07	0.58
3:F:124:THR:HB	3:F:129:PHE:HB3	1.84	0.58
3:F:165:CYS:HA	3:F:238:SER:O	2.04	0.58
3:F:240:ALA:CB	3:F:259:ILE:O	2.52	0.58
3:F:297:GLU:N	3:F:298:PRO:HD2	2.18	0.58
1:A:368:LEU:O	1:A:371:ALA:HB3	2.04	0.57
1:A:77:THR:HG21	1:A:118:GLU:CG	2.32	0.57
2:E:59:LYS:HD3	2:E:123:HIS:HD2	1.70	0.57
2:E:388:MET:HE1	2:E:392:GLN:HE22	1.69	0.57
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.69	0.57
2:B:128:TYR:HB3	2:B:171:PHE:HD2	1.68	0.57
2:E:218:LEU:HA	2:E:221:ILE:HD12	1.86	0.57
1:A:225:VAL:O	1:A:228:CYS:HB3	2.05	0.57
1:D:376:GLU:OE2	1:D:376:GLU:N	2.36	0.57
2:E:223:ASN:ND2	2:E:263:GLN:HE21	2.02	0.57
1:A:32:ILE:O	1:A:35:LEU:HB2	2.03	0.57
2:B:376:ILE:HG13	2:B:377:HIS:N	2.18	0.57
2:E:118:GLU:N	2:E:164:GLU:HG2	2.18	0.57
2:E:82:TYR:O	2:E:82:TYR:CG	2.57	0.57
3:C:12:GLN:NE2	3:C:16:GLN:HB2	2.19	0.57
1:D:20:LEU:HD23	1:D:31:SER:CB	2.34	0.57
3:F:183:LEU:HD21	3:F:194:PRO:CG	2.34	0.57
1:A:280:LYS:HA	1:A:284:VAL:HG21	1.86	0.57
2:B:160:LEU:O	2:B:162:ASP:N	2.35	0.57
1:D:350:MET:HE1	1:D:353:SER:CB	2.34	0.57
2:E:134:PHE:C	2:E:134:PHE:CD2	2.74	0.57
1:A:495:TYR:HE2	1:A:535:ASN:ND2	2.02	0.57
1:A:229:VAL:O	1:A:233:GLN:HG3	2.05	0.57
1:A:282:ASP:C	1:A:285:PRO:HD2	2.24	0.57
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.85	0.57
2:B:166:PRO:O	2:B:167:ARG:C	2.42	0.57
2:B:413:MET:O	2:B:414:LYS:HG3	2.05	0.57
3:C:121:ARG:HH11	3:C:121:ARG:HG3	1.70	0.57
1:D:564:LEU:HD22	1:D:583:LEU:CD2	2.35	0.57
2:E:254:HIS:N	2:E:255:PRO:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:94:VAL:HG23	3:F:132:GLU:OE2	2.04	0.57
1:A:99:VAL:O	1:A:105:ARG:HD3	2.04	0.57
2:B:346:MET:HE2	2:B:349:ILE:HD12	1.87	0.57
3:C:169:GLY:HA3	3:C:220:PHE:HE2	1.70	0.57
3:C:297:GLU:N	3:C:298:PRO:HD2	2.20	0.57
3:F:284:TYR:HD2	3:F:284:TYR:N	2.01	0.57
1:A:356:LEU:HD12	1:A:365:LEU:HD11	1.87	0.56
2:E:160:LEU:O	2:E:162:ASP:N	2.34	0.56
2:E:80:PRO:HG2	2:E:82:TYR:CD2	2.39	0.56
3:F:63:HIS:O	3:F:66:MET:HB2	2.05	0.56
2:B:265:LEU:CD1	2:B:301:ILE:HG23	2.34	0.56
1:D:349:ILE:HG23	1:D:350:MET:N	2.19	0.56
2:E:164:GLU:O	2:E:165:ASP:C	2.44	0.56
3:C:221:GLY:H	3:C:224:ILE:HD12	1.70	0.56
3:F:160:ASP:HB3	3:F:282:LEU:HD11	1.86	0.56
3:C:24:SER:OG	3:C:27:GLN:HG3	2.05	0.56
1:D:508:LEU:HD22	1:D:508:LEU:H	1.71	0.56
2:E:190:ILE:O	2:E:194:ILE:HG13	2.06	0.56
2:E:72:HIS:O	2:E:74:ARG:N	2.38	0.56
2:B:376:ILE:HA	2:B:379:LEU:HB2	1.86	0.56
2:E:80:PRO:O	2:E:82:TYR:HD2	1.88	0.56
2:B:164:GLU:O	2:B:165:ASP:C	2.43	0.56
1:D:23:GLU:HA	1:D:28:ARG:NH2	2.20	0.56
2:E:164:GLU:OE2	2:E:167:ARG:HB2	2.05	0.56
1:A:492:ASP:OD2	1:A:493:PRO:HD2	2.03	0.56
3:C:243:LEU:CD2	4:X:7:DAM:HM3	2.36	0.56
3:C:44:ASN:N	3:C:44:ASN:ND2	2.51	0.56
1:D:29:LEU:CD1	1:D:65:VAL:HA	2.36	0.56
2:E:166:PRO:O	2:E:167:ARG:C	2.44	0.56
2:B:152:LYS:HG2	2:B:156:GLN:NE2	2.17	0.56
2:B:190:ILE:O	2:B:194:ILE:HG13	2.05	0.56
2:E:381:TYR:CD2	2:E:381:TYR:C	2.79	0.56
1:A:178:THR:HB	1:A:180:MET:CG	2.34	0.56
1:A:181:VAL:O	1:A:184:ALA:HB3	2.06	0.56
2:B:77:ILE:HG22	2:B:77:ILE:O	2.06	0.56
2:E:317:LEU:O	2:E:317:LEU:HD12	2.04	0.56
2:B:227:LEU:HB2	2:B:228:PRO:HD3	1.87	0.56
1:D:452:VAL:O	1:D:452:VAL:CG1	2.53	0.56
1:D:477:TRP:CH2	1:D:482:ILE:HD11	2.41	0.56
3:F:209:TRP:H	3:F:224:ILE:HD11	1.67	0.56
1:A:483:ILE:HB	1:A:484:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:CD1	2:B:260:CYS:HB3	2.36	0.56
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.88	0.56
1:D:489:MET:HB3	1:D:501:THR:OG1	2.06	0.56
2:E:208:HIS:HD2	2:E:210:GLY:N	1.98	0.56
2:E:298:LEU:HD21	2:E:317:LEU:HD13	1.88	0.56
3:F:117:ASN:CG	3:F:241:HIS:HE1	2.09	0.56
1:D:467:LYS:O	1:D:471:GLU:HG3	2.06	0.55
1:A:538:PHE:HB2	1:A:578:PHE:HD2	1.71	0.55
3:C:190:PRO:HD3	3:C:195:MET:HE1	1.89	0.55
3:C:239:ARG:HD3	3:C:239:ARG:C	2.26	0.55
1:D:403:SER:O	1:D:404:LEU:HB2	2.04	0.55
1:D:405:LEU:N	1:D:406:PRO:CD	2.70	0.55
1:D:40:LEU:C	1:D:40:LEU:HD12	2.26	0.55
2:E:288:SER:O	2:E:291:GLU:HB3	2.05	0.55
3:F:239:ARG:C	3:F:239:ARG:HD3	2.25	0.55
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.87	0.55
1:A:427:MET:CE	1:A:427:MET:HA	2.36	0.55
2:B:247:VAL:HG12	2:B:248:LYS:N	2.20	0.55
3:C:209:TRP:H	3:C:224:ILE:HD11	1.70	0.55
1:D:554:SER:O	1:D:558:SER:HB3	2.07	0.55
3:F:203:PRO:HD2	3:F:242:GLN:OE1	2.06	0.55
1:D:446:LEU:HD12	1:D:446:LEU:N	2.20	0.55
2:E:133:ARG:HA	2:E:136:GLU:CG	2.35	0.55
1:A:362:ILE:HD13	1:A:399:GLN:HG3	1.88	0.55
3:C:79:ASN:OD1	3:C:110:ARG:HD3	2.07	0.55
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.89	0.55
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.88	0.55
1:D:427:MET:HE1	1:D:430:LEU:HD12	1.87	0.55
3:F:62:PHE:O	3:F:65:LEU:HB3	2.06	0.55
1:A:327:LEU:HD12	1:A:327:LEU:O	2.06	0.55
1:A:427:MET:HE3	1:A:427:MET:HA	1.87	0.55
2:B:162:ASP:O	2:B:163:SER:HB2	2.06	0.55
3:C:124:THR:HB	3:C:129:PHE:HB3	1.88	0.55
1:D:350:MET:HE3	1:D:369:PHE:CE1	2.42	0.55
2:E:302:LEU:HA	2:E:305:ILE:HB	1.89	0.55
2:E:357:LEU:HD22	2:E:387:PHE:HD2	1.72	0.55
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.88	0.55
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.42	0.55
1:D:99:VAL:HG21	1:D:104:VAL:CG1	2.35	0.55
3:C:71:ILE:HG22	3:C:275:ILE:HD11	1.87	0.55
1:A:105:ARG:HH12	1:A:142:THR:HG22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLU:N	2:B:164:GLU:HG2	2.22	0.55
2:B:180:TYR:CE1	2:B:187:ARG:HA	2.42	0.55
3:C:163:ILE:HD13	3:C:236:LEU:HD23	1.88	0.55
1:D:155:TYR:CZ	1:D:196:LEU:HD23	2.42	0.55
1:A:557:GLN:HG2	1:A:588:LEU:HD22	1.90	0.54
1:D:427:MET:O	1:D:428:PRO:C	2.45	0.54
2:E:246:LYS:HG3	3:F:307:TYR:HE2	1.73	0.54
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.90	0.54
2:E:265:LEU:CD1	2:E:301:ILE:HG23	2.37	0.54
1:A:197:GLU:CD	1:A:197:GLU:H	2.11	0.54
1:A:405:LEU:CD2	1:A:430:LEU:HD11	2.37	0.54
1:A:522:LEU:O	1:A:526:LEU:HG	2.07	0.54
2:E:373:ASN:HD22	2:E:376:ILE:HG23	1.72	0.54
1:D:222:LEU:HD23	1:D:223:LEU:N	2.22	0.54
1:D:373:LEU:HD13	1:D:384:ILE:CG2	2.37	0.54
2:E:302:LEU:O	2:E:305:ILE:HG22	2.08	0.54
1:A:194:LYS:HD2	1:A:230:ASN:HD22	1.72	0.54
1:A:405:LEU:N	1:A:406:PRO:CD	2.71	0.54
2:E:107:GLU:HG3	2:E:108:PHE:CE1	2.42	0.54
1:D:102:THR:CG2	2:E:203:TYR:HB3	2.37	0.54
2:E:79:GLU:N	2:E:80:PRO:HD2	2.21	0.54
1:A:206:ILE:HD11	1:A:235:LEU:HD11	1.90	0.54
3:C:284:TYR:N	3:C:284:TYR:HD2	2.06	0.54
1:D:11:TYR:O	1:D:14:ALA:HB3	2.07	0.54
2:E:250:LEU:C	2:E:252:VAL:H	2.11	0.54
1:A:437:GLU:CD	1:A:438:PHE:N	2.61	0.54
2:B:277:MET:HE2	2:B:277:MET:HA	1.90	0.54
1:D:538:PHE:O	1:D:542:LYS:HG3	2.08	0.54
2:E:138:PRO:O	2:E:140:PHE:HD1	1.91	0.54
2:E:72:HIS:O	2:E:74:ARG:HG2	2.08	0.54
1:A:385:ILE:HD12	1:A:423:ILE:CD1	2.37	0.54
2:B:133:ARG:CA	2:B:136:GLU:HG2	2.35	0.54
2:B:375:THR:O	2:B:379:LEU:HD12	2.08	0.54
1:A:538:PHE:HB3	1:A:575:VAL:HA	1.90	0.54
1:A:564:LEU:O	1:A:564:LEU:HD23	2.08	0.54
2:B:154:VAL:O	2:B:157:LEU:HB3	2.07	0.54
3:C:176:THR:H	3:C:179:HIS:HD2	1.55	0.54
1:D:94:GLU:HB2	1:D:131:LEU:CD1	2.38	0.54
2:B:62:ALA:O	2:B:66:MET:HG3	2.08	0.53
1:D:274:VAL:HG12	1:D:278:ILE:HB	1.90	0.53
2:E:167:ARG:HH11	2:E:167:ARG:CB	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:LEU:HD23	2:E:271:LEU:HD13	1.90	0.53
2:B:381:TYR:CE2	2:B:385:LYS:HD2	2.44	0.53
1:D:452:VAL:HG13	1:D:497:HIS:HD2	1.73	0.53
2:E:305:ILE:HD13	2:E:306:GLU:N	2.23	0.53
1:A:278:ILE:CD1	1:A:278:ILE:H	2.12	0.53
2:B:43:PHE:O	2:B:44:ASP:C	2.47	0.53
3:C:208:GLY:HA2	3:C:224:ILE:HD11	1.89	0.53
3:C:29:LYS:O	3:C:33:GLU:HG2	2.09	0.53
2:E:376:ILE:HA	2:E:379:LEU:HB2	1.90	0.53
3:F:305:PRO:HB3	3:F:307:TYR:CE2	2.43	0.53
1:A:145:THR:HG22	1:A:146:SER:N	2.22	0.53
2:E:255:PRO:HG2	2:E:256:GLN:H	1.73	0.53
1:A:11:TYR:O	1:A:14:ALA:HB3	2.07	0.53
1:A:407:ALA:O	1:A:410:GLU:N	2.41	0.53
2:B:190:ILE:CD1	2:B:190:ILE:H	2.20	0.53
2:B:287:HIS:HE1	2:B:289:PRO:HB2	1.74	0.53
2:B:87:HIS:O	2:B:91:VAL:HG23	2.09	0.53
3:C:171:SER:OG	3:C:174:ILE:HB	2.08	0.53
3:C:263:PRO:HD3	3:C:273:ALA:HB2	1.90	0.53
1:D:116:SER:O	1:D:119:HIS:HB2	2.09	0.53
1:D:404:LEU:H	1:D:406:PRO:HD2	1.74	0.53
1:A:222:LEU:HD23	1:A:223:LEU:H	1.70	0.53
1:A:561:LYS:O	1:A:565:GLU:HG2	2.08	0.53
1:D:384:ILE:CG2	1:D:385:ILE:N	2.71	0.53
2:E:121:TRP:N	2:E:122:PRO:CD	2.66	0.53
2:E:297:GLU:O	2:E:301:ILE:HG13	2.09	0.53
3:F:297:GLU:N	3:F:298:PRO:CD	2.72	0.53
1:A:482:ILE:O	1:A:486:VAL:HG23	2.09	0.53
3:F:156:THR:HG22	3:F:166:LEU:CB	2.38	0.53
2:B:236:PHE:O	2:B:240:VAL:HB	2.09	0.53
2:B:291:GLU:HG2	2:B:332:VAL:HG13	1.91	0.53
3:C:85:ASP:H	3:C:116:GLY:HA3	1.72	0.53
1:D:192:PHE:O	1:D:195:VAL:HG22	2.09	0.53
1:D:524:THR:O	1:D:528:MET:HG3	2.08	0.53
2:E:218:LEU:HD13	2:E:236:PHE:HZ	1.74	0.53
1:A:40:LEU:O	1:A:42:LEU:N	2.42	0.53
1:D:155:TYR:CE2	1:D:196:LEU:HD23	2.43	0.53
1:D:267:PHE:HE2	1:D:287:PHE:HB2	1.71	0.53
2:E:35:LYS:C	2:E:37:ARG:N	2.62	0.53
2:E:371:HIS:ND1	2:E:376:ILE:HD13	2.24	0.53
3:F:76:PRO:HD3	3:F:107:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:240:ALA:HB1	3:F:259:ILE:O	2.09	0.53
1:A:400:LEU:HD12	1:A:404:LEU:HD23	1.91	0.53
1:A:40:LEU:C	1:A:42:LEU:H	2.13	0.53
2:B:138:PRO:O	2:B:140:PHE:HD1	1.92	0.53
2:B:330:PHE:CE1	2:B:331:GLN:HG2	2.44	0.53
3:C:165:CYS:SG	3:C:238:SER:HB3	2.49	0.53
2:E:247:VAL:HG12	2:E:249:SER:H	1.74	0.53
3:F:169:GLY:HA3	3:F:220:PHE:HE2	1.74	0.53
1:A:487:LEU:C	1:A:489:MET:N	2.61	0.52
1:A:98:THR:O	1:A:98:THR:HG22	2.09	0.52
1:D:102:THR:OG1	1:D:103:VAL:N	2.42	0.52
3:F:10:LEU:HD11	3:F:105:VAL:HG12	1.90	0.52
1:A:411:LEU:C	1:A:413:GLU:H	2.13	0.52
1:D:307:LYS:HB2	1:D:348:VAL:HB	1.91	0.52
1:D:522:LEU:HD22	1:D:551:LEU:CD2	2.39	0.52
1:A:184:ALA:O	1:A:185:ALA:C	2.47	0.52
1:A:35:LEU:HD21	1:A:55:LEU:HD11	1.90	0.52
1:A:369:PHE:O	1:A:373:LEU:HD23	2.10	0.52
2:B:78:THR:HG22	2:B:82:TYR:OH	2.10	0.52
1:D:420:ARG:O	1:D:424:ILE:HG13	2.09	0.52
3:C:12:GLN:HE22	3:C:16:GLN:HB2	1.73	0.52
3:C:263:PRO:HD3	3:C:273:ALA:CB	2.38	0.52
1:D:178:THR:HG22	1:D:180:MET:SD	2.50	0.52
1:D:381:ARG:O	1:D:385:ILE:HG12	2.09	0.52
1:D:399:GLN:NE2	1:D:399:GLN:CA	2.72	0.52
1:D:466:LEU:O	1:D:470:VAL:HG23	2.10	0.52
2:E:375:THR:O	2:E:379:LEU:HD12	2.08	0.52
2:E:330:PHE:CE2	3:F:122:GLN:HG3	2.43	0.52
1:D:194:LYS:HD2	1:D:230:ASN:HD22	1.75	0.52
2:E:277:MET:HA	2:E:277:MET:HE2	1.92	0.52
2:E:350:SER:C	2:E:352:ASN:H	2.13	0.52
3:F:143:TRP:CE2	3:F:147:THR:HG21	2.45	0.52
1:A:152:SER:HB3	1:A:191:GLU:OE1	2.09	0.52
3:C:156:THR:HG22	3:C:166:LEU:HB3	1.92	0.52
3:C:297:GLU:N	3:C:298:PRO:CD	2.73	0.52
1:D:572:ASP:OD2	3:F:110:ARG:NH2	2.40	0.52
1:D:99:VAL:O	1:D:105:ARG:HD3	2.10	0.52
2:E:346:MET:HE2	2:E:349:ILE:HD12	1.90	0.52
3:F:243:LEU:CD2	4:Y:7:DAM:HM3	2.40	0.52
1:A:420:ARG:O	1:A:424:ILE:HG13	2.09	0.52
2:B:255:PRO:HG2	2:B:256:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:384:LEU:HD22	2:E:395:PHE:HZ	1.75	0.52
1:A:128:PHE:O	1:A:131:LEU:HB3	2.10	0.52
3:C:276:MET:HB2	3:C:286:PHE:CE1	2.44	0.52
1:D:322:ILE:HG21	1:D:356:LEU:HD21	1.91	0.52
1:D:437:GLU:CD	1:D:438:PHE:H	2.13	0.52
1:A:40:LEU:C	1:A:40:LEU:HD12	2.29	0.52
1:A:452:VAL:CG1	1:A:452:VAL:O	2.57	0.52
1:A:470:VAL:HG11	1:A:511:VAL:HG23	1.92	0.52
2:B:167:ARG:HH11	2:B:167:ARG:CB	2.22	0.52
2:B:169:ARG:O	2:B:172:LEU:HB2	2.10	0.52
3:C:143:TRP:CE2	3:C:147:THR:HG21	2.45	0.52
1:A:40:LEU:C	1:A:42:LEU:N	2.63	0.52
2:B:208:HIS:HD2	2:B:210:GLY:N	1.96	0.52
2:B:371:HIS:ND1	2:B:376:ILE:HD13	2.25	0.52
3:C:240:ALA:CB	3:C:259:ILE:O	2.57	0.52
1:A:446:LEU:HD12	1:A:446:LEU:H	1.74	0.51
1:A:554:SER:O	1:A:558:SER:HB3	2.10	0.51
2:B:42:LEU:O	2:B:59:LYS:HE3	2.10	0.51
3:C:68:LEU:HD23	3:C:68:LEU:C	2.30	0.51
3:F:185:ARG:O	3:F:187:GLN:N	2.43	0.51
1:A:456:TYR:C	1:A:456:TYR:CD1	2.84	0.51
2:B:251:SER:HA	2:B:293:MET:HE1	1.92	0.51
3:F:261:SER:HA	3:F:273:ALA:HB1	1.91	0.51
2:B:244:LEU:CD2	2:B:253:TYR:CE1	2.93	0.51
2:B:79:GLU:N	2:B:80:PRO:HD2	2.24	0.51
3:C:165:CYS:HA	3:C:238:SER:O	2.11	0.51
1:D:77:THR:HG21	1:D:118:GLU:CG	2.36	0.51
2:E:91:VAL:O	2:E:91:VAL:HG12	2.11	0.51
1:A:345:LEU:HD21	1:A:349:ILE:HD12	1.90	0.51
1:D:350:MET:HE1	1:D:353:SER:HB2	1.92	0.51
1:D:405:LEU:HD13	1:D:405:LEU:O	2.09	0.51
2:E:247:VAL:HG12	2:E:248:LYS:N	2.25	0.51
2:E:289:PRO:O	2:E:293:MET:HG3	2.11	0.51
2:B:320:GLN:O	2:B:323:LYS:N	2.43	0.51
3:C:276:MET:HE2	3:C:278:LEU:HD21	1.92	0.51
1:D:120:SER:O	1:D:121:PRO:C	2.48	0.51
1:D:11:TYR:O	1:D:14:ALA:N	2.43	0.51
3:C:305:PRO:HB3	3:C:307:TYR:CE2	2.45	0.51
1:D:109:VAL:HG13	1:D:150:LEU:CD2	2.38	0.51
2:B:373:ASN:HD21	2:B:375:THR:HG22	1.76	0.51
2:B:108:PHE:HB3	3:C:268:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ILE:HD11	1:D:433:GLN:HB3	1.92	0.51
2:E:340:TRP:NE1	2:E:387:PHE:HE1	2.09	0.51
2:E:406:LYS:O	2:E:406:LYS:HD3	2.11	0.51
1:A:529:ALA:CB	1:A:563:ILE:HD11	2.41	0.51
3:C:31:LEU:HD11	3:C:102:ALA:HA	1.93	0.51
3:F:42:GLU:HB3	3:F:46:GLN:OE1	2.09	0.51
1:A:502:LEU:HD21	1:A:540:VAL:HG23	1.92	0.51
2:E:373:ASN:ND2	2:E:375:THR:HG22	2.26	0.51
2:E:43:PHE:O	2:E:44:ASP:C	2.48	0.51
3:F:24:SER:O	3:F:28:VAL:HG23	2.11	0.51
3:F:263:PRO:HD3	3:F:273:ALA:HB2	1.92	0.51
1:A:105:ARG:NH1	1:A:142:THR:HG22	2.24	0.51
1:A:192:PHE:O	1:A:195:VAL:HG22	2.11	0.51
1:A:280:LYS:HA	1:A:284:VAL:HG23	1.93	0.51
1:A:506:ASN:HD21	1:A:543:SER:CB	2.24	0.51
1:A:556:LEU:O	1:A:558:SER:N	2.43	0.51
2:B:373:ASN:ND2	2:B:375:THR:HG22	2.26	0.51
3:C:51:PRO:HB3	3:C:279:ASP:C	2.31	0.51
1:D:180:MET:HE2	1:D:180:MET:H	1.76	0.51
1:A:489:MET:C	1:A:491:GLY:N	2.64	0.50
3:C:63:HIS:O	3:C:66:MET:HB2	2.11	0.50
1:D:412:ALA:HB1	1:D:450:TRP:HZ2	1.75	0.50
2:E:322:ALA:HB2	2:E:360:MET:CE	2.36	0.50
3:F:44:ASN:ND2	3:F:44:ASN:N	2.58	0.50
1:A:165:GLU:O	1:A:168:GLN:HB3	2.11	0.50
1:A:456:TYR:HA	1:A:459:ARG:NH1	2.26	0.50
2:B:175:THR:HG22	2:B:179:ILE:CD1	2.39	0.50
2:B:205:THR:O	2:B:207:HIS:N	2.41	0.50
2:B:350:SER:O	2:B:352:ASN:N	2.44	0.50
2:B:375:THR:HG23	2:B:379:LEU:HD12	1.94	0.50
3:C:32:CYS:O	3:C:35:ALA:HB3	2.11	0.50
2:B:302:LEU:HA	2:B:305:ILE:HB	1.93	0.50
1:D:373:LEU:HD22	1:D:384:ILE:HG21	1.94	0.50
1:D:487:LEU:C	1:D:489:MET:N	2.60	0.50
1:A:343:SER:HA	1:A:380:VAL:HG22	1.94	0.50
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.11	0.50
3:C:159:VAL:HG11	3:C:278:LEU:HD12	1.94	0.50
1:D:463:THR:HG22	1:D:507:VAL:HG21	1.93	0.50
2:B:107:GLU:HG3	2:B:108:PHE:CD1	2.47	0.50
1:A:102:THR:O	1:A:105:ARG:HG2	2.11	0.50
1:A:489:MET:C	1:A:491:GLY:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HD12	2:B:317:LEU:C	2.32	0.50
2:B:315:GLU:O	2:B:319:ARG:HB2	2.11	0.50
3:C:172:PRO:HG3	3:C:209:TRP:CE3	2.47	0.50
2:E:304:VAL:HG12	2:E:304:VAL:O	2.12	0.50
1:A:303:SER:HB3	1:A:345:LEU:HB2	1.94	0.50
1:A:362:ILE:HG23	1:A:366:LEU:HD23	1.94	0.50
2:B:110:PRO:HA	2:B:113:ASP:OD2	2.12	0.50
2:B:205:THR:C	2:B:207:HIS:H	2.15	0.50
2:B:255:PRO:HG2	2:B:256:GLN:H	1.75	0.50
2:E:350:SER:O	2:E:352:ASN:N	2.45	0.50
2:E:381:TYR:HD2	2:E:381:TYR:C	2.14	0.50
2:E:44:ASP:O	2:E:45:PHE:C	2.49	0.50
2:E:180:TYR:CE1	2:E:187:ARG:HA	2.47	0.50
2:E:287:HIS:CE1	2:E:289:PRO:HB2	2.47	0.50
2:E:322:ALA:N	2:E:360:MET:HE1	2.26	0.50
1:A:25:VAL:CG2	1:A:62:GLU:HG2	2.42	0.49
3:C:189:VAL:HA	3:C:195:MET:HE2	1.94	0.49
1:D:522:LEU:O	1:D:526:LEU:HG	2.11	0.49
1:D:71:GLU:HG3	1:D:107:LYS:CE	2.42	0.49
2:E:39:CYS:O	2:E:42:LEU:N	2.45	0.49
3:F:103:LEU:C	3:F:111:ILE:HD11	2.32	0.49
1:A:570:ASP:OD2	1:A:571:GLN:N	2.44	0.49
3:C:44:ASN:ND2	3:C:185:ARG:HH11	2.11	0.49
1:D:40:LEU:C	1:D:42:LEU:H	2.16	0.49
3:F:156:THR:HG22	3:F:166:LEU:HB3	1.93	0.49
3:F:166:LEU:HD23	3:F:239:ARG:HB3	1.94	0.49
3:C:194:PRO:HG2	3:C:195:MET:H	1.77	0.49
3:C:240:ALA:HB1	3:C:259:ILE:O	2.12	0.49
1:D:98:THR:HG22	1:D:98:THR:O	2.10	0.49
1:A:91:PRO:HB2	1:A:92:PRO:CD	2.42	0.49
2:B:142:PRO:HG2	2:B:143:ASN:H	1.77	0.49
2:B:145:ALA:O	2:B:148:TYR:N	2.42	0.49
2:B:35:LYS:C	2:B:37:ARG:N	2.65	0.49
1:D:436:VAL:HB	1:D:473:PHE:CD1	2.48	0.49
1:D:91:PRO:HB2	1:D:92:PRO:CD	2.43	0.49
1:A:24:ASP:O	1:A:26:GLN:N	2.46	0.49
2:B:388:MET:C	2:B:390:MET:H	2.16	0.49
3:F:29:LYS:HB2	3:F:145:TYR:CE1	2.47	0.49
1:A:411:LEU:O	1:A:413:GLU:N	2.45	0.49
3:C:44:ASN:ND2	3:C:185:ARG:NH1	2.61	0.49
2:E:242:LEU:N	2:E:243:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:SER:HA	2:B:390:MET:SD	2.53	0.49
1:D:330:ILE:HD13	1:D:352:LEU:HD11	1.94	0.49
2:E:166:PRO:O	2:E:170:ASP:N	2.43	0.49
3:F:51:PRO:HB3	3:F:279:ASP:C	2.33	0.49
1:A:267:PHE:CE2	1:A:287:PHE:HB2	2.47	0.49
3:C:277:GLU:HB2	3:C:285:SER:OG	2.13	0.49
1:D:437:GLU:CD	1:D:438:PHE:N	2.66	0.49
2:E:103:PRO:HG3	2:E:108:PHE:CD2	2.48	0.49
2:E:273:GLU:N	2:E:274:PRO:HD2	2.28	0.49
3:C:59:HIS:HE1	3:C:118:HIS:CD2	2.31	0.49
1:D:23:GLU:HG2	1:D:23:GLU:O	2.13	0.49
2:E:119:ALA:O	2:E:120:ALA:CB	2.61	0.49
1:A:11:TYR:O	1:A:14:ALA:N	2.45	0.48
1:A:427:MET:HE1	1:A:443:LEU:HD21	1.95	0.48
2:B:59:LYS:O	2:B:63:LEU:HG	2.12	0.48
2:B:94:PHE:CE1	2:B:156:GLN:HB2	2.48	0.48
3:F:137:TYR:CD2	3:F:142:VAL:HG21	2.48	0.48
3:F:248:TYR:CE2	3:F:286:PHE:CD2	3.01	0.48
1:A:330:ILE:HD13	1:A:352:LEU:HD11	1.95	0.48
1:A:588:LEU:O	1:A:589:ALA:HB2	2.13	0.48
2:B:242:LEU:HD11	2:B:275:VAL:HG22	1.95	0.48
2:E:223:ASN:ND2	2:E:263:GLN:NE2	2.60	0.48
2:E:329:HIS:HA	3:F:125:GLN:OE1	2.13	0.48
2:B:170:ASP:O	2:B:173:LYS:HB3	2.13	0.48
2:B:70:ILE:O	2:B:70:ILE:HG22	2.14	0.48
3:C:158:LEU:HD12	3:C:163:ILE:O	2.13	0.48
3:C:73:GLY:HA3	3:C:78:THR:HG21	1.95	0.48
3:F:118:HIS:HA	3:F:123:ILE:HG21	1.96	0.48
1:A:155:TYR:CE1	1:A:163:LYS:HB3	2.48	0.48
1:A:492:ASP:O	1:A:498:ARG:HD3	2.13	0.48
3:C:94:VAL:HG23	3:C:132:GLU:OE2	2.14	0.48
1:D:29:LEU:HD12	1:D:65:VAL:HG22	1.95	0.48
2:E:238:LEU:O	2:E:243:PRO:HD3	2.13	0.48
2:E:407:LEU:HD23	2:E:411:LEU:HB2	1.94	0.48
3:F:244:VAL:C	3:F:246:GLU:H	2.17	0.48
1:A:111:SER:O	1:A:112:LEU:C	2.52	0.48
1:A:118:GLU:HA	1:A:118:GLU:OE2	2.14	0.48
1:A:399:GLN:NE2	1:A:399:GLN:HA	2.28	0.48
1:D:101:GLU:HG2	2:E:246:LYS:HZ1	1.79	0.48
1:D:140:TRP:HH2	2:E:199:TYR:HH	1.60	0.48
2:E:78:THR:O	2:E:140:PHE:CE2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:242:LEU:HD11	2:E:275:VAL:HA	1.96	0.48
2:E:299:GLU:O	2:E:302:LEU:N	2.46	0.48
2:E:31:LEU:C	2:E:33:ILE:H	2.15	0.48
2:E:77:ILE:HG22	2:E:77:ILE:O	2.14	0.48
3:F:79:ASN:OD1	3:F:110:ARG:HD3	2.13	0.48
3:F:264:ASN:ND2	3:F:267:TYR:HA	2.28	0.48
2:B:93:MET:SD	2:B:124:LEU:HD22	2.53	0.48
2:B:384:LEU:O	2:B:387:PHE:HB2	2.14	0.48
2:B:44:ASP:O	2:B:45:PHE:C	2.51	0.48
3:C:166:LEU:O	3:C:239:ARG:HA	2.14	0.48
3:C:203:PRO:HD2	3:C:242:GLN:OE1	2.13	0.48
1:D:350:MET:CE	1:D:353:SER:HB2	2.43	0.48
1:D:35:LEU:HB3	1:D:72:GLN:HG2	1.96	0.48
1:D:385:ILE:HD11	1:D:411:LEU:HG	1.96	0.48
3:F:266:CYS:O	3:F:267:TYR:HB2	2.14	0.48
1:A:102:THR:CG2	2:B:203:TYR:HB3	2.44	0.48
1:D:415:ALA:O	1:D:420:ARG:NH1	2.46	0.48
1:D:446:LEU:CD1	1:D:446:LEU:H	2.26	0.48
2:E:382:ASN:O	2:E:386:LEU:HD12	2.12	0.48
3:F:12:GLN:HE22	3:F:16:GLN:HB2	1.79	0.48
3:F:239:ARG:NH1	3:F:258:THR:HG23	2.28	0.48
2:B:304:VAL:HG12	2:B:304:VAL:O	2.13	0.48
3:C:56:GLY:HA3	3:C:259:ILE:O	2.14	0.48
1:D:25:VAL:HG22	1:D:62:GLU:HG2	1.95	0.48
1:D:356:LEU:HD12	1:D:365:LEU:HD11	1.94	0.48
1:A:11:TYR:N	1:A:12:PRO:HD2	2.28	0.48
1:A:320:ASN:O	1:A:323:MET:N	2.46	0.48
1:A:475:LYS:HG3	1:A:476:GLU:N	2.29	0.48
1:A:452:VAL:HG13	1:A:497:HIS:CD2	2.49	0.48
3:C:308:PHE:O	3:C:309:LEU:CG	2.60	0.48
1:D:119:HIS:O	1:D:157:ARG:NH2	2.38	0.48
2:E:384:LEU:HD22	2:E:395:PHE:CZ	2.49	0.48
2:B:91:VAL:O	2:B:91:VAL:HG12	2.14	0.48
1:D:129:VAL:HB	1:D:130:PRO:HD3	1.96	0.48
1:D:52:LEU:HD11	1:D:89:LEU:HD12	1.95	0.48
2:E:133:ARG:CA	2:E:136:GLU:HG2	2.38	0.48
3:F:190:PRO:HD3	3:F:195:MET:CE	2.44	0.48
1:D:184:ALA:O	1:D:185:ALA:C	2.52	0.47
1:D:427:MET:CE	1:D:430:LEU:HD12	2.43	0.47
1:D:570:ASP:OD2	1:D:571:GLN:N	2.46	0.47
1:A:155:TYR:CE2	1:A:196:LEU:HD23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:VAL:CB	3:C:256:VAL:HG22	2.36	0.47
1:D:345:LEU:HD23	1:D:345:LEU:C	2.35	0.47
2:E:313:ILE:O	2:E:316:PRO:HD2	2.14	0.47
2:E:381:TYR:HE2	2:E:385:LYS:CD	2.22	0.47
3:F:126:VAL:O	3:F:126:VAL:HG12	2.14	0.47
1:A:358:LYS:HA	1:A:394:VAL:HG12	1.95	0.47
1:A:399:GLN:HE21	1:A:399:GLN:CA	2.26	0.47
1:D:25:VAL:O	1:D:26:GLN:C	2.53	0.47
1:D:479:HIS:CG	1:D:479:HIS:O	2.67	0.47
1:D:504:CYS:O	1:D:507:VAL:N	2.43	0.47
1:D:78:THR:O	1:D:80:VAL:N	2.47	0.47
2:E:142:PRO:HG2	2:E:143:ASN:H	1.79	0.47
3:F:132:GLU:HG3	3:F:136:LYS:HE3	1.94	0.47
3:F:189:VAL:HA	3:F:195:MET:HE2	1.96	0.47
1:A:373:LEU:HD22	1:A:384:ILE:HG21	1.97	0.47
2:B:244:LEU:HD21	2:B:253:TYR:CE1	2.50	0.47
2:B:276:VAL:HG11	2:B:313:ILE:CG2	2.44	0.47
1:D:443:LEU:HA	1:D:446:LEU:HD13	1.97	0.47
1:D:483:ILE:O	1:D:487:LEU:HG	2.13	0.47
2:E:150:ASP:CG	2:E:151:GLN:N	2.68	0.47
2:B:381:TYR:HE2	2:B:385:LYS:HD2	1.80	0.47
1:D:486:VAL:O	1:D:486:VAL:HG12	2.14	0.47
2:E:150:ASP:CG	2:E:151:GLN:H	2.18	0.47
2:E:222:ILE:HA	2:E:225:PHE:CZ	2.49	0.47
3:F:159:VAL:HB	3:F:163:ILE:HB	1.96	0.47
2:B:72:HIS:O	2:B:74:ARG:N	2.47	0.47
2:B:90:ALA:O	2:B:94:PHE:HB2	2.14	0.47
3:C:104:LYS:CA	3:C:111:ILE:HD11	2.44	0.47
1:D:408:ILE:HD13	1:D:426:TYR:CE2	2.45	0.47
2:E:236:PHE:O	2:E:240:VAL:HB	2.15	0.47
2:E:357:LEU:N	2:E:358:PRO:HD2	2.30	0.47
1:A:264:ALA:O	1:A:267:PHE:HB2	2.15	0.47
1:A:350:MET:HE1	1:A:391:VAL:HG11	1.96	0.47
1:A:522:LEU:N	1:A:523:PRO:CD	2.78	0.47
1:D:109:VAL:O	1:D:113:ARG:HG3	2.14	0.47
2:E:93:MET:SD	2:E:124:LEU:HD22	2.54	0.47
3:F:237:VAL:CB	3:F:256:VAL:HG22	2.42	0.47
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.49	0.47
1:A:349:ILE:HG23	1:A:350:MET:N	2.30	0.47
2:B:262:VAL:O	2:B:265:LEU:N	2.47	0.47
1:D:353:SER:HB3	1:D:354:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:GLU:H	2:E:164:GLU:CG	2.22	0.47
2:E:223:ASN:HD22	2:E:263:GLN:NE2	2.13	0.47
2:E:254:HIS:CB	2:E:293:MET:HE1	2.44	0.47
3:F:12:GLN:NE2	3:F:16:GLN:HB2	2.30	0.47
2:B:298:LEU:HD21	2:B:317:LEU:HD13	1.97	0.47
3:C:121:ARG:HG3	3:C:121:ARG:NH1	2.29	0.47
1:D:517:THR:HA	1:D:521:MET:CE	2.44	0.47
2:E:142:PRO:HG2	2:E:143:ASN:N	2.29	0.47
2:E:266:GLU:HG2	2:E:304:VAL:HG11	1.96	0.47
2:B:118:GLU:H	2:B:164:GLU:CG	2.25	0.47
2:B:239:LYS:O	2:B:243:PRO:HG3	2.14	0.47
3:C:294:ARG:HH11	3:C:294:ARG:HG2	1.78	0.47
3:C:2:ASP:O	3:C:5:VAL:HB	2.15	0.47
1:D:155:TYR:CZ	1:D:196:LEU:CD2	2.98	0.47
1:D:368:LEU:O	1:D:371:ALA:HB3	2.15	0.47
1:D:564:LEU:HD23	1:D:564:LEU:O	2.15	0.47
2:E:244:LEU:CD2	2:E:253:TYR:CE1	2.98	0.47
3:F:65:LEU:O	3:F:68:LEU:HB3	2.15	0.47
1:A:105:ARG:NH1	1:A:142:THR:CG2	2.78	0.47
1:A:323:MET:HE2	1:A:356:LEU:HD22	1.97	0.47
1:A:438:PHE:O	1:A:439:PHE:C	2.52	0.47
2:B:82:TYR:CG	2:B:82:TYR:O	2.68	0.47
1:D:503:PHE:O	1:D:506:ASN:HB2	2.16	0.47
2:E:107:GLU:HG3	2:E:108:PHE:CD1	2.50	0.47
2:E:189:TYR:O	2:E:190:ILE:C	2.53	0.47
2:E:371:HIS:HB2	2:E:376:ILE:HD11	1.97	0.47
1:A:25:VAL:HG22	1:A:62:GLU:HG2	1.98	0.46
1:A:350:MET:HE2	1:A:391:VAL:HG13	1.97	0.46
1:A:377:CYS:SG	1:A:379:GLU:HG2	2.55	0.46
2:B:85:VAL:HG11	2:B:134:PHE:CD1	2.50	0.46
2:E:164:GLU:OE2	2:E:164:GLU:C	2.54	0.46
2:E:322:ALA:CA	2:E:360:MET:HE1	2.44	0.46
1:A:196:LEU:HD12	1:A:205:ILE:HD11	1.96	0.46
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.50	0.46
1:D:17:ILE:HG12	1:D:38:ILE:HG23	1.97	0.46
1:D:502:LEU:HD13	1:D:540:VAL:HA	1.96	0.46
2:E:70:ILE:O	2:E:70:ILE:HG22	2.14	0.46
2:E:78:THR:HG22	2:E:78:THR:O	2.15	0.46
3:F:169:GLY:O	3:F:198:LEU:HA	2.15	0.46
3:F:71:ILE:HD12	3:F:71:ILE:N	2.31	0.46
1:A:405:LEU:O	1:A:405:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HB3	1:A:428:PRO:CD	2.45	0.46
1:A:498:ARG:NE	1:A:531:ASP:OD2	2.48	0.46
1:A:98:THR:HG23	1:A:143:SER:OG	2.15	0.46
3:C:190:PRO:HD3	3:C:195:MET:HE2	1.98	0.46
3:F:276:MET:HG3	3:F:286:PHE:CE1	2.50	0.46
2:B:357:LEU:N	2:B:358:PRO:HD2	2.30	0.46
3:C:239:ARG:NH1	3:C:258:THR:HG23	2.29	0.46
1:D:291:MET:HB3	1:D:333:LEU:HD11	1.98	0.46
2:E:124:LEU:O	2:E:125:GLN:C	2.53	0.46
2:E:330:PHE:CD1	2:E:331:GLN:N	2.84	0.46
2:E:35:LYS:O	2:E:37:ARG:N	2.47	0.46
2:E:407:LEU:HD21	2:E:411:LEU:HD12	1.98	0.46
3:F:203:PRO:HA	3:F:220:PHE:CE1	2.51	0.46
1:A:206:ILE:HG21	1:A:243:LEU:HB3	1.97	0.46
2:B:247:VAL:CG1	2:B:248:LYS:N	2.78	0.46
2:B:305:ILE:HD13	2:B:306:GLU:N	2.30	0.46
2:B:384:LEU:HD22	2:B:395:PHE:CZ	2.50	0.46
3:C:308:PHE:O	3:C:309:LEU:CB	2.62	0.46
1:D:245:MET:O	1:D:249:ARG:HG3	2.16	0.46
1:D:40:LEU:C	1:D:42:LEU:N	2.69	0.46
2:E:250:LEU:O	2:E:252:VAL:N	2.48	0.46
2:E:242:LEU:HD11	2:E:275:VAL:HG22	1.97	0.46
2:E:288:SER:HB2	2:E:289:PRO:HD3	1.97	0.46
3:F:67:GLU:O	3:F:71:ILE:HD13	2.16	0.46
1:A:407:ALA:O	1:A:408:ILE:C	2.54	0.46
2:B:283:TRP:O	2:B:285:LYS:HE3	2.16	0.46
1:D:267:PHE:CZ	1:D:287:PHE:HB2	2.51	0.46
1:D:411:LEU:C	1:D:413:GLU:H	2.18	0.46
3:F:183:LEU:HD21	3:F:194:PRO:HG3	1.97	0.46
1:A:214:SER:HA	1:A:221:ARG:CD	2.46	0.46
2:B:366:ARG:O	2:B:367:ASN:C	2.54	0.46
1:D:25:VAL:CG2	1:D:62:GLU:HG2	2.46	0.46
3:F:13:TRP:HE1	3:F:27:GLN:HE21	1.64	0.46
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.15	0.46
2:B:298:LEU:HB3	2:B:339:TYR:OH	2.16	0.46
2:B:31:LEU:C	2:B:33:ILE:H	2.19	0.46
2:B:357:LEU:HD12	2:B:357:LEU:O	2.16	0.46
2:B:412:LYS:O	2:B:414:LYS:N	2.42	0.46
3:C:103:LEU:C	3:C:111:ILE:HD11	2.36	0.46
1:D:470:VAL:HG21	1:D:508:LEU:HD12	1.98	0.46
2:E:136:GLU:HG3	2:E:136:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:317:LEU:O	2:E:320:GLN:HB3	2.16	0.46
2:B:173:LYS:HA	2:B:217:ILE:HD11	1.98	0.46
1:D:35:LEU:HD21	1:D:55:LEU:CD1	2.37	0.46
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.98	0.46
1:D:94:GLU:HB2	1:D:131:LEU:HD12	1.97	0.46
2:E:350:SER:C	2:E:352:ASN:N	2.68	0.46
3:F:117:ASN:ND2	3:F:241:HIS:HE1	2.12	0.46
3:F:128:GLY:O	3:F:129:PHE:C	2.54	0.46
2:B:151:GLN:HB3	2:B:189:TYR:CE2	2.51	0.46
1:D:482:ILE:O	1:D:483:ILE:C	2.53	0.46
1:D:140:TRP:CZ2	2:E:239:LYS:HD2	2.51	0.46
1:A:327:LEU:HB3	1:A:328:PRO:HD3	1.98	0.45
1:A:456:TYR:O	1:A:457:ALA:C	2.54	0.45
2:B:373:ASN:O	2:B:375:THR:N	2.45	0.45
2:B:86:VAL:HG12	2:B:87:HIS:N	2.31	0.45
1:D:146:SER:O	1:D:147:ALA:C	2.55	0.45
1:D:350:MET:CE	1:D:369:PHE:CZ	2.99	0.45
1:D:427:MET:HA	1:D:427:MET:HE3	1.96	0.45
1:D:456:TYR:O	1:D:457:ALA:C	2.54	0.45
2:E:121:TRP:CD1	2:E:167:ARG:NH1	2.84	0.45
2:E:407:LEU:CD2	2:E:411:LEU:HD12	2.45	0.45
2:E:246:LYS:HE3	3:F:307:TYR:OH	2.16	0.45
1:A:327:LEU:HA	1:A:330:ILE:HD12	1.98	0.45
1:A:353:SER:HB3	1:A:354:PRO:HD3	1.97	0.45
2:B:83:PRO:CG	2:B:148:TYR:CD2	2.98	0.45
1:D:353:SER:HB3	1:D:354:PRO:HD3	1.98	0.45
1:D:522:LEU:HD22	1:D:551:LEU:HD22	1.99	0.45
2:E:373:ASN:O	2:E:375:THR:N	2.49	0.45
1:A:429:LEU:O	1:A:433:GLN:HG3	2.16	0.45
1:A:438:PHE:CD1	1:A:438:PHE:C	2.89	0.45
3:C:232:ASN:HB2	3:C:234:LEU:HG	1.99	0.45
1:D:24:ASP:O	1:D:26:GLN:N	2.49	0.45
1:D:385:ILE:HD12	1:D:423:ILE:CD1	2.46	0.45
3:F:137:TYR:CE2	3:F:142:VAL:HG21	2.52	0.45
1:A:404:LEU:H	1:A:406:PRO:HD2	1.82	0.45
2:B:120:ALA:C	2:B:122:PRO:HD2	2.36	0.45
2:E:278:ALA:O	2:E:281:LYS:HB3	2.15	0.45
2:E:54:LYS:O	2:E:56:LYS:N	2.48	0.45
4:Y:6:FGA:HG3	4:Y:7:DAM:HM1	1.76	0.45
1:A:561:LYS:N	1:A:562:PRO:CD	2.80	0.45
2:B:238:LEU:O	2:B:243:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:MET:HE1	2:B:280:LEU:HD12	1.99	0.45
3:C:71:ILE:CG2	3:C:275:ILE:HD11	2.47	0.45
3:C:99:LEU:O	3:C:99:LEU:HD12	2.17	0.45
1:D:427:MET:HG2	1:D:447:CYS:SG	2.56	0.45
2:E:138:PRO:C	2:E:140:PHE:H	2.20	0.45
3:F:97:VAL:HG13	3:F:98:THR:N	2.31	0.45
1:A:119:HIS:O	1:A:157:ARG:NH2	2.43	0.45
1:A:534:ALA:O	1:A:537:ARG:N	2.50	0.45
2:B:276:VAL:HG11	2:B:313:ILE:HG21	1.99	0.45
2:B:288:SER:O	2:B:291:GLU:HB3	2.17	0.45
2:B:72:HIS:O	2:B:74:ARG:HG2	2.17	0.45
1:D:71:GLU:HG3	1:D:107:LYS:HE3	1.97	0.45
1:D:28:ARG:HD3	1:D:60:TYR:HE2	1.81	0.45
1:D:16:LEU:HB3	1:D:38:ILE:HD11	1.98	0.45
1:D:29:LEU:CD1	1:D:65:VAL:HG22	2.47	0.45
3:F:239:ARG:O	3:F:258:THR:HA	2.17	0.45
1:A:245:MET:O	1:A:249:ARG:HG3	2.17	0.45
3:C:71:ILE:HG22	3:C:72:GLY:N	2.31	0.45
2:E:337:LEU:O	2:E:340:TRP:HE3	1.99	0.45
1:A:209:PHE:CZ	1:A:228:CYS:HB2	2.52	0.45
2:B:93:MET:O	2:B:160:LEU:HD21	2.16	0.45
2:B:350:SER:C	2:B:352:ASN:N	2.70	0.45
3:C:76:PRO:HB3	3:C:107:TYR:CG	2.52	0.45
1:D:398:ARG:O	1:D:402:GLN:N	2.50	0.45
2:E:287:HIS:HE1	2:E:289:PRO:HB2	1.81	0.45
1:A:141:PHE:CD1	1:A:141:PHE:C	2.90	0.45
1:A:372:GLN:C	1:A:374:LYS:N	2.70	0.45
1:A:538:PHE:HB2	1:A:578:PHE:CD2	2.51	0.45
3:C:118:HIS:ND1	3:C:123:ILE:HG21	2.32	0.45
3:C:128:GLY:O	3:C:129:PHE:C	2.54	0.45
3:C:244:VAL:C	3:C:246:GLU:H	2.21	0.45
2:E:361:PHE:N	2:E:362:PRO:HD2	2.32	0.45
2:E:76:VAL:O	2:E:76:VAL:CG1	2.64	0.45
3:F:134:LEU:HD12	3:F:139:ASN:O	2.17	0.45
3:F:32:CYS:O	3:F:35:ALA:HB3	2.17	0.45
1:A:162:VAL:O	1:A:163:LYS:C	2.54	0.45
1:A:322:ILE:CG2	1:A:356:LEU:HD21	2.47	0.45
2:B:134:PHE:C	2:B:134:PHE:HD2	2.18	0.45
2:B:329:HIS:HA	3:C:125:GLN:OE1	2.16	0.45
3:C:51:PRO:HA	3:C:278:LEU:O	2.17	0.45
1:D:538:PHE:HB2	1:D:578:PHE:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:GLU:C	2:E:165:ASP:O	2.55	0.45
2:E:227:LEU:HB2	2:E:228:PRO:CD	2.45	0.45
2:E:250:LEU:C	2:E:252:VAL:N	2.70	0.45
2:E:273:GLU:CA	2:E:313:ILE:HD11	2.32	0.45
2:B:145:ALA:O	2:B:147:LYS:N	2.49	0.44
2:B:350:SER:C	2:B:352:ASN:H	2.21	0.44
2:E:145:ALA:O	2:E:147:LYS:N	2.50	0.44
3:F:132:GLU:CG	3:F:136:LYS:HE3	2.47	0.44
1:A:38:ILE:O	1:A:42:LEU:HB2	2.17	0.44
3:C:211:ILE:HG22	3:C:211:ILE:O	2.17	0.44
3:C:253:ASP:O	3:C:254:ARG:C	2.55	0.44
1:D:155:TYR:HB3	1:D:156:PRO:HD3	1.99	0.44
2:E:384:LEU:O	2:E:387:PHE:HB2	2.17	0.44
1:A:99:VAL:HG21	1:A:104:VAL:HG11	1.99	0.44
1:A:183:ARG:O	1:A:186:ALA:HB3	2.18	0.44
2:B:164:GLU:HB3	2:B:168:GLU:CB	2.39	0.44
2:B:382:ASN:O	2:B:386:LEU:HD12	2.17	0.44
1:D:196:LEU:HD12	1:D:205:ILE:HD11	1.99	0.44
1:D:28:ARG:NH1	1:D:62:GLU:OE1	2.50	0.44
1:D:453:ASP:OD1	1:D:454:HIS:N	2.49	0.44
1:D:475:LYS:HG2	1:D:476:GLU:OE2	2.18	0.44
1:D:522:LEU:N	1:D:523:PRO:CD	2.80	0.44
1:D:529:ALA:CB	1:D:563:ILE:HD11	2.47	0.44
2:E:345:ILE:O	2:E:349:ILE:HG13	2.18	0.44
1:A:248:LEU:HD11	1:A:270:LEU:HD13	1.99	0.44
1:A:28:ARG:HD3	1:A:60:TYR:CE2	2.53	0.44
1:A:479:HIS:CG	1:A:479:HIS:O	2.70	0.44
1:A:503:PHE:O	1:A:506:ASN:HB2	2.18	0.44
2:B:138:PRO:C	2:B:140:PHE:H	2.20	0.44
2:B:242:LEU:HD11	2:B:275:VAL:HA	2.00	0.44
2:E:102:ASN:ND2	2:E:113:ASP:HB3	2.31	0.44
3:F:119:GLU:N	3:F:119:GLU:OE1	2.50	0.44
3:F:252:HIS:O	3:F:253:ASP:C	2.56	0.44
1:A:492:ASP:OD2	1:A:493:PRO:CD	2.65	0.44
3:C:18:ASN:C	3:C:20:CYS:H	2.20	0.44
1:D:408:ILE:CD1	1:D:426:TYR:HE2	2.29	0.44
2:E:315:GLU:HB2	2:E:316:PRO:CD	2.48	0.44
3:F:117:ASN:HB2	3:F:200:TRP:CE2	2.53	0.44
3:F:276:MET:CG	3:F:286:PHE:CE1	3.00	0.44
1:A:365:LEU:HB3	1:A:369:PHE:CZ	2.52	0.44
2:B:71:THR:O	2:B:73:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ASP:H	1:D:221:ARG:HG2	1.81	0.44
2:E:314:MET:HG3	2:E:356:ILE:HD11	1.99	0.44
1:A:25:VAL:O	1:A:26:GLN:C	2.55	0.44
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.84	0.44
2:B:76:VAL:CG1	2:B:76:VAL:O	2.65	0.44
3:C:118:HIS:HA	3:C:123:ILE:HG21	2.00	0.44
1:D:162:VAL:O	1:D:163:LYS:C	2.55	0.44
1:D:322:ILE:CG2	1:D:356:LEU:HD21	2.48	0.44
1:D:429:LEU:O	1:D:433:GLN:HG3	2.17	0.44
3:F:308:PHE:O	3:F:309:LEU:CB	2.66	0.44
1:A:268:THR:HG23	1:A:305:LYS:HD2	2.00	0.44
1:A:420:ARG:HH21	1:A:453:ASP:CG	2.22	0.44
1:A:489:MET:O	1:A:491:GLY:N	2.51	0.44
2:B:283:TRP:O	2:B:285:LYS:CE	2.66	0.44
2:B:309:GLU:C	2:B:311:VAL:N	2.70	0.44
1:D:218:ASP:OD1	1:D:219:SER:N	2.51	0.44
1:D:492:ASP:OD2	1:D:493:PRO:CD	2.62	0.44
1:D:521:MET:C	1:D:523:PRO:HD2	2.37	0.44
1:D:506:ASN:ND2	1:D:543:SER:HA	2.32	0.44
1:D:70:ALA:CB	1:D:96:LEU:HD13	2.45	0.44
1:A:266:LYS:O	1:A:269:GLU:HB2	2.18	0.44
1:A:411:LEU:C	1:A:413:GLU:N	2.71	0.44
1:A:427:MET:O	1:A:431:ALA:N	2.47	0.44
3:C:140:ALA:O	3:C:143:TRP:HB3	2.17	0.44
3:C:143:TRP:CZ2	3:C:147:THR:HG21	2.53	0.44
1:D:427:MET:O	1:D:431:ALA:N	2.42	0.44
2:E:254:HIS:CE1	2:E:297:GLU:HB2	2.53	0.44
2:E:330:PHE:CG	2:E:331:GLN:N	2.86	0.44
2:E:56:LYS:O	2:E:58:VAL:HG23	2.18	0.44
1:A:229:VAL:HG22	1:A:270:LEU:HD23	2.00	0.43
1:A:350:MET:HE3	1:A:369:PHE:CZ	2.53	0.43
1:A:502:LEU:CD2	1:A:540:VAL:HG23	2.48	0.43
1:A:538:PHE:O	1:A:542:LYS:HG3	2.17	0.43
2:B:330:PHE:CZ	3:C:122:GLN:HG3	2.53	0.43
3:C:301:THR:CG2	3:C:302:ARG:H	2.09	0.43
1:D:279:THR:O	1:D:284:VAL:HG23	2.18	0.43
1:D:476:GLU:H	1:D:476:GLU:CD	2.21	0.43
2:E:109:ASP:OD1	2:E:111:GLU:HB2	2.18	0.43
3:F:200:TRP:HZ3	4:Y:5:1ZN:H20	1.83	0.43
3:F:253:ASP:O	3:F:254:ARG:C	2.56	0.43
3:F:46:GLN:O	3:F:158:LEU:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:PHE:O	3:F:9:GLU:N	2.50	0.43
1:A:209:PHE:HE1	1:A:224:ALA:O	2.01	0.43
1:A:314:SER:HB3	1:A:317:CYS:SG	2.58	0.43
2:B:230:LYS:HB2	2:B:233:HIS:HD2	1.83	0.43
2:E:164:GLU:OE1	2:E:167:ARG:NH1	2.51	0.43
3:F:163:ILE:HD13	3:F:236:LEU:HD23	2.01	0.43
1:A:102:THR:HA	1:A:105:ARG:NE	2.33	0.43
1:A:346:ALA:HB2	1:A:380:VAL:HG13	1.99	0.43
2:B:366:ARG:O	2:B:368:SER:N	2.52	0.43
2:B:64:SER:O	2:B:68:GLU:HG3	2.18	0.43
3:C:12:GLN:O	3:C:13:TRP:C	2.56	0.43
3:C:243:LEU:HD21	3:C:269:CYS:HB3	2.00	0.43
1:D:556:LEU:O	1:D:558:SER:N	2.45	0.43
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.31	0.43
1:A:412:ALA:HB1	1:A:450:TRP:CZ2	2.50	0.43
1:A:502:LEU:HD13	1:A:540:VAL:CA	2.47	0.43
2:B:251:SER:HA	2:B:293:MET:HE3	1.99	0.43
2:B:257:LEU:O	2:B:258:ALA:C	2.56	0.43
3:C:278:LEU:HB3	3:C:282:LEU:HD23	2.00	0.43
2:E:136:GLU:CD	2:E:178:ARG:NH1	2.72	0.43
2:E:388:MET:C	2:E:390:MET:H	2.21	0.43
3:F:24:SER:OG	3:F:27:GLN:HG3	2.19	0.43
3:F:277:GLU:HB2	3:F:285:SER:OG	2.17	0.43
1:A:548:GLY:HA3	1:A:586:LEU:HD21	2.00	0.43
1:A:217:GLN:HE22	2:B:155:LEU:HD11	1.83	0.43
2:E:407:LEU:C	2:E:407:LEU:HD23	2.39	0.43
3:F:121:ARG:HH11	3:F:121:ARG:HG3	1.82	0.43
3:F:183:LEU:HD21	3:F:194:PRO:HG2	2.00	0.43
1:A:182:ARG:NE	1:A:215:ASP:OD2	2.46	0.43
1:A:90:LEU:HD11	1:A:119:HIS:HE1	1.84	0.43
2:B:164:GLU:C	2:B:165:ASP:O	2.56	0.43
2:B:218:LEU:O	2:B:219:GLY:C	2.57	0.43
1:D:392:ASN:HB3	1:D:400:LEU:HD22	2.01	0.43
2:E:110:PRO:HA	2:E:113:ASP:OD2	2.18	0.43
3:F:164:PHE:HB2	3:F:234:LEU:HD13	2.01	0.43
3:F:276:MET:CE	3:F:278:LEU:HD21	2.48	0.43
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.89	0.43
2:B:278:ALA:O	2:B:281:LYS:HB3	2.19	0.43
2:B:329:HIS:HD2	2:B:332:VAL:H	1.67	0.43
2:B:362:PRO:O	2:B:366:ARG:HB2	2.18	0.43
1:D:398:ARG:CB	1:D:398:ARG:NH1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:160:ASP:C	3:F:162:GLN:H	2.22	0.43
1:A:475:LYS:CG	1:A:476:GLU:N	2.81	0.43
2:B:315:GLU:HB2	2:B:316:PRO:CD	2.49	0.43
2:B:361:PHE:HB3	2:B:362:PRO:CD	2.49	0.43
3:C:118:HIS:ND1	3:C:123:ILE:CG2	2.82	0.43
3:C:292:ALA:HB1	3:C:293:PRO:HD2	2.01	0.43
1:D:349:ILE:CG2	1:D:350:MET:N	2.80	0.43
2:E:217:ILE:HG22	2:E:221:ILE:CD1	2.48	0.43
3:F:211:ILE:O	3:F:211:ILE:HG22	2.18	0.43
1:A:77:THR:CG2	1:A:118:GLU:HG3	2.37	0.43
1:A:120:SER:O	1:A:121:PRO:C	2.57	0.43
2:B:277:MET:CE	2:B:280:LEU:HD12	2.49	0.43
2:B:313:ILE:HD12	2:B:313:ILE:N	2.34	0.43
2:B:373:ASN:HD21	2:B:375:THR:CG2	2.32	0.43
2:B:80:PRO:HG2	2:B:82:TYR:CE2	2.54	0.43
2:B:329:HIS:HE1	3:C:125:GLN:O	2.01	0.43
3:C:174:ILE:HD13	3:C:180:ILE:CG1	2.36	0.43
1:D:313:LEU:HD13	1:D:321:VAL:CG2	2.49	0.43
1:D:403:SER:O	1:D:404:LEU:CB	2.67	0.43
1:D:29:LEU:HD12	1:D:65:VAL:HA	2.00	0.43
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.84	0.43
3:C:156:THR:HG22	3:C:166:LEU:HB2	2.00	0.43
2:E:93:MET:HE1	2:E:128:TYR:CE1	2.54	0.43
2:E:188:ALA:O	2:E:189:TYR:C	2.57	0.43
2:E:194:ILE:HG23	2:E:214:LEU:HD22	1.99	0.43
3:F:301:THR:CG2	3:F:302:ARG:H	2.12	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.88	0.42
2:B:237:LEU:CA	2:B:241:LEU:HB2	2.42	0.42
2:B:277:MET:HA	2:B:277:MET:CE	2.49	0.42
2:B:388:MET:O	2:B:390:MET:N	2.46	0.42
2:B:408:LYS:C	2:B:410:LYS:H	2.23	0.42
3:C:183:LEU:HD21	3:C:194:PRO:CG	2.49	0.42
3:C:276:MET:HE3	3:C:278:LEU:HD21	2.00	0.42
1:D:40:LEU:O	1:D:42:LEU:N	2.52	0.42
1:D:546:LYS:C	1:D:548:GLY:H	2.21	0.42
2:E:78:THR:HG22	2:E:82:TYR:OH	2.19	0.42
3:F:240:ALA:HA	3:F:258:THR:HG23	2.01	0.42
1:A:336:ASP:OD1	1:A:337:ALA:N	2.51	0.42
2:B:376:ILE:HD12	2:B:380:ILE:HD11	2.00	0.42
2:B:408:LYS:O	2:B:410:LYS:N	2.53	0.42
3:C:240:ALA:O	3:C:241:HIS:HB2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASN:ND2	1:D:433:GLN:NE2	2.64	0.42
1:D:438:PHE:C	1:D:438:PHE:CD1	2.91	0.42
2:E:268:ASP:OD1	2:E:270:THR:N	2.52	0.42
2:E:64:SER:O	2:E:68:GLU:HG3	2.19	0.42
3:F:160:ASP:O	3:F:162:GLN:N	2.52	0.42
3:F:163:ILE:HG12	3:F:236:LEU:HB3	2.01	0.42
3:F:239:ARG:HH11	3:F:258:THR:HG23	1.83	0.42
1:A:388:LEU:C	1:A:390:CYS:N	2.73	0.42
1:A:78:THR:O	1:A:80:VAL:N	2.53	0.42
3:C:208:GLY:CA	3:C:224:ILE:HD11	2.48	0.42
1:D:408:ILE:HG22	1:D:408:ILE:O	2.19	0.42
2:E:103:PRO:HB2	2:E:108:PHE:CE1	2.54	0.42
2:E:154:VAL:HG11	2:E:190:ILE:HG13	2.01	0.42
3:F:120:SER:OG	3:F:123:ILE:HB	2.19	0.42
3:F:17:LEU:HD13	3:F:99:LEU:N	2.34	0.42
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.49	0.42
1:A:399:GLN:NE2	1:A:399:GLN:CA	2.81	0.42
1:A:486:VAL:O	1:A:486:VAL:HG12	2.19	0.42
1:A:55:LEU:HD13	1:A:69:LEU:HD11	2.00	0.42
2:B:313:ILE:O	2:B:314:MET:C	2.57	0.42
1:D:278:ILE:O	1:D:282:ASP:N	2.40	0.42
1:D:455:VAL:O	1:D:455:VAL:HG13	2.19	0.42
1:D:525:VAL:HG11	1:D:544:LEU:CD2	2.49	0.42
2:E:309:GLU:C	2:E:311:VAL:N	2.72	0.42
1:A:67:LEU:HD13	1:A:103:VAL:HG12	2.01	0.42
1:A:13:ILE:O	1:A:17:ILE:HG13	2.19	0.42
1:A:91:PRO:HB2	1:A:92:PRO:HD3	2.00	0.42
3:C:62:PHE:HB2	3:C:92:TYR:HB2	2.01	0.42
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.74	0.42
1:D:412:ALA:HB1	1:D:450:TRP:CZ2	2.53	0.42
2:E:232:GLU:HG3	2:E:233:HIS:N	2.34	0.42
2:E:276:VAL:HG11	2:E:313:ILE:CG2	2.50	0.42
2:E:366:ARG:O	2:E:367:ASN:C	2.58	0.42
2:E:373:ASN:ND2	2:E:376:ILE:HG23	2.34	0.42
3:F:263:PRO:HD3	3:F:273:ALA:CB	2.50	0.42
1:A:12:PRO:O	1:A:15:VAL:HB	2.20	0.42
1:A:204:GLU:C	1:A:207:PRO:HD2	2.39	0.42
1:A:236:PRO:O	1:A:237:GLN:C	2.58	0.42
1:A:443:LEU:HA	1:A:446:LEU:HD13	2.02	0.42
1:A:28:ARG:CD	1:A:60:TYR:CE2	3.02	0.42
2:B:97:LEU:HD13	2:B:162:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:LEU:O	2:B:261:VAL:HG23	2.18	0.42
2:B:371:HIS:HB2	2:B:376:ILE:HD11	2.01	0.42
2:B:380:ILE:O	2:B:383:ALA:HB3	2.20	0.42
3:C:185:ARG:O	3:C:187:GLN:N	2.53	0.42
3:C:237:VAL:O	3:C:256:VAL:HG13	2.19	0.42
3:F:266:CYS:SG	4:Y:2:LEU:HD12	2.59	0.42
1:A:278:ILE:HA	1:A:281:THR:HB	2.02	0.42
1:A:438:PHE:HD1	1:A:438:PHE:C	2.22	0.42
1:D:257:TRP:CE2	2:E:99:PRO:HD3	2.54	0.42
1:D:321:VAL:CG2	1:D:322:ILE:N	2.81	0.42
1:D:350:MET:CA	1:D:350:MET:HE2	2.50	0.42
1:D:526:LEU:HA	1:D:563:ILE:HD13	2.02	0.42
2:E:158:LEU:HB3	2:E:197:ILE:HD11	2.02	0.42
2:E:412:LYS:O	2:E:414:LYS:N	2.45	0.42
1:A:269:GLU:OE2	1:A:305:LYS:NZ	2.53	0.42
1:A:392:ASN:ND2	1:A:433:GLN:OE1	2.53	0.42
2:B:142:PRO:C	2:B:144:ILE:H	2.22	0.42
2:B:402:PHE:O	2:B:406:LYS:HB2	2.19	0.42
2:B:78:THR:HG22	2:B:78:THR:O	2.20	0.42
1:D:330:ILE:CD1	1:D:352:LEU:HD11	2.49	0.42
2:E:199:TYR:CZ	2:E:240:VAL:HG22	2.54	0.42
3:F:190:PRO:HD3	3:F:195:MET:HE2	2.02	0.42
3:F:6:PHE:CE2	3:F:34:LYS:HE3	2.54	0.42
3:F:76:PRO:HB3	3:F:107:TYR:CG	2.55	0.42
4:X:5:1ZN:H17	4:X:5:1ZN:H21	1.91	0.42
1:A:303:SER:O	1:A:306:VAL:HG23	2.19	0.42
3:C:278:LEU:HD13	3:C:282:LEU:CD2	2.49	0.42
1:A:535:ASN:ND2	3:C:77:ASP:O	2.49	0.42
2:E:288:SER:O	2:E:289:PRO:C	2.58	0.42
3:F:143:TRP:CZ2	3:F:147:THR:HG21	2.55	0.42
3:F:31:LEU:HD11	3:F:102:ALA:HA	2.01	0.42
1:A:111:SER:O	1:A:114:ALA:N	2.53	0.42
2:B:381:TYR:O	2:B:381:TYR:HD2	2.02	0.42
3:C:10:LEU:HD23	3:C:13:TRP:HE3	1.85	0.42
1:D:102:THR:O	1:D:103:VAL:C	2.58	0.42
1:D:111:SER:O	1:D:112:LEU:C	2.58	0.42
1:D:52:LEU:CD1	1:D:88:CYS:HB3	2.50	0.42
2:E:162:ASP:O	2:E:163:SER:HB2	2.20	0.42
2:E:180:TYR:CE2	2:E:221:ILE:HG23	2.55	0.42
3:F:137:TYR:CG	3:F:142:VAL:HG21	2.55	0.42
3:F:187:GLN:HE21	3:F:187:GLN:HB2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:5:1ZN:H17	4:Y:5:1ZN:H21	1.95	0.42
1:A:323:MET:CE	1:A:356:LEU:HD22	2.50	0.41
1:A:437:GLU:CG	1:A:438:PHE:N	2.83	0.41
1:A:446:LEU:CD1	1:A:446:LEU:H	2.32	0.41
2:B:318:PHE:O	2:B:360:MET:CE	2.67	0.41
1:D:198:LEU:O	1:D:201:VAL:HB	2.20	0.41
1:D:537:ARG:HG3	1:D:537:ARG:HH11	1.85	0.41
2:E:244:LEU:HD23	2:E:244:LEU:C	2.40	0.41
3:F:74:LYS:HB3	3:F:74:LYS:HE2	1.86	0.41
3:F:88:ASP:O	3:F:89:ARG:HB2	2.19	0.41
1:A:13:ILE:HG21	1:A:41:ALA:HB3	2.02	0.41
2:B:76:VAL:HG12	2:B:76:VAL:O	2.20	0.41
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.89	0.41
3:C:189:VAL:HA	3:C:195:MET:CE	2.50	0.41
3:C:17:LEU:CD1	3:C:98:THR:HG22	2.50	0.41
1:D:20:LEU:CD2	1:D:31:SER:HB3	2.49	0.41
1:D:69:LEU:O	1:D:73:LEU:HG	2.19	0.41
2:E:169:ARG:O	2:E:172:LEU:HB2	2.20	0.41
2:E:169:ARG:HB3	2:E:213:GLU:HG2	2.03	0.41
3:F:45:VAL:HG22	3:F:156:THR:OG1	2.20	0.41
1:A:101:GLU:OE1	1:A:101:GLU:C	2.59	0.41
1:A:77:THR:O	1:A:80:VAL:HG12	2.20	0.41
3:C:117:ASN:CG	3:C:241:HIS:CE1	2.90	0.41
3:C:203:PRO:HA	3:C:220:PHE:CE1	2.55	0.41
3:C:76:PRO:HD3	3:C:107:TYR:CZ	2.53	0.41
2:E:251:SER:HA	2:E:293:MET:CE	2.50	0.41
2:B:142:PRO:HG2	2:B:143:ASN:N	2.36	0.41
2:B:294:PHE:O	2:B:295:LEU:C	2.58	0.41
1:A:536:VAL:O	1:A:540:VAL:HB	2.20	0.41
2:B:136:GLU:O	2:B:136:GLU:HG3	2.21	0.41
2:B:164:GLU:C	2:B:164:GLU:OE2	2.58	0.41
2:B:222:ILE:O	2:B:224:GLY:N	2.52	0.41
3:C:130:TYR:HA	3:C:143:TRP:CD1	2.56	0.41
1:D:214:SER:HA	1:D:221:ARG:CD	2.50	0.41
1:D:398:ARG:O	1:D:402:GLN:HB2	2.21	0.41
2:E:39:CYS:C	2:E:41:VAL:N	2.74	0.41
3:F:12:GLN:O	3:F:13:TRP:C	2.58	0.41
3:F:163:ILE:HD12	3:F:278:LEU:HD13	2.03	0.41
1:A:284:VAL:N	1:A:285:PRO:CD	2.83	0.41
1:A:436:VAL:HG13	1:A:437:GLU:N	2.35	0.41
1:A:29:LEU:CD1	1:A:65:VAL:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:CD1	1:A:65:VAL:HG22	2.50	0.41
3:C:117:ASN:ND2	3:C:241:HIS:HE1	2.19	0.41
3:C:222:GLN:HA	3:C:252:HIS:CG	2.55	0.41
3:C:81:LEU:C	3:C:81:LEU:HD23	2.41	0.41
1:D:121:PRO:O	1:D:124:LEU:HB2	2.20	0.41
2:E:141:GLN:HB3	2:E:142:PRO:CD	2.46	0.41
2:E:72:HIS:O	2:E:73:ASN:C	2.59	0.41
2:E:79:GLU:O	2:E:80:PRO:C	2.59	0.41
3:F:17:LEU:HD13	3:F:99:LEU:CA	2.50	0.41
1:A:105:ARG:HH11	1:A:142:THR:HB	1.86	0.41
1:A:221:ARG:O	1:A:224:ALA:HB3	2.20	0.41
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.78	0.41
2:B:310:PHE:CZ	2:B:318:PHE:HE1	2.39	0.41
2:B:368:SER:HB2	2:B:377:HIS:CD2	2.56	0.41
2:B:381:TYR:O	2:B:382:ASN:C	2.59	0.41
1:D:350:MET:HE2	1:D:369:PHE:CZ	2.56	0.41
1:D:489:MET:C	1:D:491:GLY:H	2.24	0.41
1:D:514:GLN:HG3	1:D:550:ILE:O	2.20	0.41
2:E:329:HIS:CD2	2:E:331:GLN:HB2	2.56	0.41
3:F:115:ARG:HH12	3:F:151:ASP:HA	1.85	0.41
3:F:44:ASN:ND2	3:F:185:ARG:HH11	2.18	0.41
1:A:353:SER:HB3	1:A:354:PRO:CD	2.51	0.41
1:A:499:MET:O	1:A:500:THR:C	2.59	0.41
1:A:518:THR:OG1	1:A:551:LEU:HD23	2.21	0.41
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.86	0.41
2:B:154:VAL:HG11	2:B:190:ILE:HG13	2.02	0.41
2:B:356:ILE:O	2:B:359:ILE:HB	2.21	0.41
3:C:158:LEU:CD2	3:C:161:GLY:HA2	2.50	0.41
3:C:207:GLY:HA2	3:C:221:GLY:HA3	2.03	0.41
3:C:206:ARG:O	3:C:207:GLY:O	2.39	0.41
3:C:248:TYR:CE2	3:C:286:PHE:CD2	3.09	0.41
3:C:29:LYS:HB2	3:C:145:TYR:HE1	1.83	0.41
1:D:155:TYR:CE1	1:D:163:LYS:HB3	2.56	0.41
1:D:296:ALA:O	1:D:297:GLU:C	2.58	0.41
1:D:463:THR:HG23	1:D:504:CYS:HA	2.03	0.41
1:D:98:THR:O	1:D:99:VAL:C	2.59	0.41
2:E:247:VAL:CG1	2:E:248:LYS:N	2.84	0.41
3:F:110:ARG:HA	3:F:110:ARG:HD3	1.93	0.41
3:F:206:ARG:O	3:F:207:GLY:O	2.39	0.41
3:F:29:LYS:O	3:F:33:GLU:HG2	2.20	0.41
1:A:405:LEU:HD23	1:A:430:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:C	1:A:431:ALA:N	2.75	0.41
1:A:502:LEU:HB3	1:A:543:SER:OG	2.20	0.41
3:C:103:LEU:CB	3:C:111:ILE:HD13	2.50	0.41
1:D:230:ASN:O	1:D:234:LEU:HG	2.21	0.41
1:D:327:LEU:HB3	1:D:328:PRO:HD3	2.01	0.41
1:D:398:ARG:H	1:D:398:ARG:HG2	1.67	0.41
2:E:366:ARG:O	2:E:368:SER:N	2.53	0.41
3:F:73:GLY:HA3	3:F:78:THR:HG21	2.03	0.41
1:A:424:ILE:CD1	1:A:458:ILE:HG23	2.51	0.41
2:B:227:LEU:HB2	2:B:228:PRO:CD	2.51	0.41
2:B:313:ILE:O	2:B:316:PRO:HD2	2.21	0.41
2:B:79:GLU:O	2:B:80:PRO:C	2.58	0.41
3:C:239:ARG:O	3:C:258:THR:HA	2.21	0.41
1:D:155:TYR:CZ	1:D:163:LYS:HB3	2.56	0.41
2:E:221:ILE:H	2:E:221:ILE:HG13	1.66	0.41
2:B:39:CYS:O	2:B:42:LEU:N	2.54	0.41
3:C:244:VAL:C	3:C:246:GLU:N	2.74	0.41
1:D:248:LEU:HD11	1:D:270:LEU:HD13	2.03	0.41
1:D:350:MET:HE3	1:D:369:PHE:CZ	2.56	0.41
1:D:424:ILE:CD1	1:D:458:ILE:HG23	2.51	0.41
1:D:483:ILE:N	1:D:484:PRO:CD	2.84	0.41
1:D:86:VAL:HG13	1:D:87:HIS:N	2.36	0.41
2:E:175:THR:HG22	2:E:179:ILE:HD11	2.03	0.41
2:E:200:ARG:HG3	2:E:204:GLU:OE1	2.20	0.41
2:E:31:LEU:O	2:E:33:ILE:N	2.46	0.41
2:E:390:MET:O	2:E:391:ASN:HB2	2.21	0.41
2:E:54:LYS:C	2:E:56:LYS:H	2.23	0.41
3:F:278:LEU:HB3	3:F:282:LEU:HD23	2.02	0.41
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.48	0.40
1:A:384:ILE:HD13	1:A:384:ILE:O	2.21	0.40
1:A:535:ASN:O	1:A:539:ASN:HB2	2.20	0.40
2:B:244:LEU:HD21	2:B:253:TYR:CZ	2.56	0.40
2:B:254:HIS:HE1	2:B:297:GLU:OE1	2.04	0.40
3:C:244:VAL:CG2	3:C:244:VAL:O	2.66	0.40
3:C:6:PHE:O	3:C:9:GLU:N	2.54	0.40
3:F:28:VAL:HG11	3:F:142:VAL:HG13	2.03	0.40
3:F:240:ALA:HB2	3:F:259:ILE:H	1.85	0.40
1:A:178:THR:HA	1:A:179:PRO:HD3	1.89	0.40
1:A:411:LEU:HB3	1:A:423:ILE:HG13	2.03	0.40
1:A:463:THR:O	1:A:466:LEU:HB2	2.22	0.40
2:B:205:THR:C	2:B:207:HIS:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:LYS:O	2:B:231:GLU:C	2.59	0.40
2:B:318:PHE:O	2:B:319:ARG:C	2.60	0.40
2:B:329:HIS:CD2	2:B:331:GLN:HB2	2.56	0.40
3:C:263:PRO:CD	3:C:273:ALA:HB2	2.51	0.40
1:D:343:SER:HA	1:D:380:VAL:HG22	2.03	0.40
1:D:557:GLN:HG2	1:D:588:LEU:HD22	2.03	0.40
1:A:279:THR:O	1:A:284:VAL:HG23	2.22	0.40
1:A:392:ASN:HD21	1:A:433:GLN:HE22	1.70	0.40
1:A:456:TYR:HD1	1:A:457:ALA:N	2.19	0.40
1:D:131:LEU:C	1:D:131:LEU:HD23	2.41	0.40
3:F:222:GLN:HA	3:F:252:HIS:CG	2.57	0.40
1:A:583:LEU:O	1:A:586:LEU:N	2.55	0.40
1:A:90:LEU:HB2	1:A:91:PRO:HD3	2.03	0.40
2:B:121:TRP:CD1	2:B:167:ARG:NH1	2.90	0.40
1:D:182:ARG:O	1:D:183:ARG:C	2.59	0.40
1:D:32:ILE:O	1:D:35:LEU:HB2	2.22	0.40
3:F:165:CYS:SG	3:F:238:SER:HB3	2.62	0.40
1:A:28:ARG:CD	1:A:60:TYR:HE2	2.35	0.40
2:B:268:ASP:OD1	2:B:268:ASP:C	2.60	0.40
3:C:76:PRO:CB	3:C:110:ARG:HG3	2.46	0.40
3:C:212:SER:HA	3:C:219:THR:CG2	2.52	0.40
1:D:282:ASP:O	1:D:285:PRO:HD2	2.22	0.40
3:F:309:LEU:HA	3:F:309:LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/589 (98%)	469 (81%)	94 (16%)	17 (3%)	5	31
1	D	580/589 (98%)	481 (83%)	85 (15%)	14 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	386/449 (86%)	273 (71%)	78 (20%)	35 (9%)	1	6
2	E	386/449 (86%)	277 (72%)	72 (19%)	37 (10%)	1	5
3	C	306/309 (99%)	245 (80%)	44 (14%)	17 (6%)	2	14
3	F	306/309 (99%)	250 (82%)	42 (14%)	14 (5%)	3	19
4	X	1/7 (14%)	1 (100%)	0	0	100	100
4	Y	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2546/2708 (94%)	1997 (78%)	415 (16%)	134 (5%)	2	16

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	391	VAL
2	B	43	PHE
2	B	45	PHE
2	B	55	TRP
2	B	57	GLU
2	B	73	ASN
2	B	76	VAL
2	B	134	PHE
2	B	165	ASP
2	B	314	MET
2	B	367	ASN
3	C	183	LEU
3	C	245	MET
1	D	25	VAL
1	D	391	VAL
1	D	404	LEU
2	E	43	PHE
2	E	45	PHE
2	E	55	TRP
2	E	57	GLU
2	E	73	ASN
2	E	76	VAL
2	E	165	ASP
2	E	314	MET
2	E	367	ASN
3	F	245	MET
1	A	318	ARG
1	A	404	LEU

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Mol	Chain	Res	Type
1	A	412	ALA
1	A	415	ALA
1	A	443	LEU
1	A	558	SER
2	B	33	ILE
2	B	72	HIS
2	B	146	LYS
2	B	161	PHE
2	B	223	ASN
2	B	393	LYS
3	C	106	ARG
3	C	207	GLY
3	C	241	HIS
3	C	254	ARG
3	C	265	TYR
3	C	269	CYS
3	C	301	THR
1	D	79	LEU
1	D	318	ARG
1	D	558	SER
2	E	33	ILE
2	E	36	LEU
2	E	72	HIS
2	E	134	PHE
2	E	146	LYS
2	E	161	PHE
2	E	251	SER
2	E	391	ASN
3	F	183	LEU
3	F	186	LEU
3	F	207	GLY
3	F	265	TYR
3	F	285	SER
3	F	301	THR
1	A	41	ALA
1	A	76	PHE
1	A	79	LEU
1	A	103	VAL
1	A	556	LEU
2	B	104	THR
2	B	142	PRO
2	B	163	SER

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Mol	Chain	Res	Type
2	B	166	PRO
2	B	351	ASP
2	B	374	LYS
2	B	391	ASN
2	B	409	GLU
3	C	285	SER
1	D	415	ALA
1	D	443	LEU
1	D	556	LEU
2	E	51	SER
2	E	104	THR
2	E	142	PRO
2	E	166	PRO
2	E	188	ALA
2	E	351	ASP
2	E	393	LYS
3	F	106	ARG
3	F	129	PHE
3	F	241	HIS
3	F	254	ARG
1	A	320	ASN
2	B	167	ARG
2	B	187	ARG
3	C	280	ASP
1	D	103	VAL
2	E	167	ARG
2	E	271	LEU
2	E	334	GLU
2	E	413	MET
2	B	413	MET
3	C	41	LYS
3	C	161	GLY
1	D	41	ALA
2	E	163	SER
2	E	223	ASN
2	E	224	GLY
2	E	374	LYS
3	F	161	GLY
1	A	584	THR
2	B	36	LEU
2	B	81	ILE
2	B	143	ASN

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Mol	Chain	Res	Type
2	B	188	ALA
2	B	224	GLY
2	B	389	GLU
1	D	412	ALA
2	E	32	PHE
2	E	409	GLU
1	D	484	PRO
3	F	300	VAL
1	A	306	VAL
2	B	79	GLU
2	B	103	PRO
2	E	79	GLU
2	E	228	PRO
1	A	548	GLY
3	C	5	VAL
3	C	300	VAL
2	E	81	ILE
3	F	194	PRO
3	C	168	GLY
3	C	297	GLU
1	D	104	VAL

### 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	509/512 (99%)	474 (93%)	35 (7%)	18	53
1	D	509/512 (99%)	480 (94%)	29 (6%)	24	60
2	B	331/414 (80%)	309 (93%)	22 (7%)	19	54
2	E	331/414 (80%)	306 (92%)	25 (8%)	15	47
3	C	273/274 (100%)	260 (95%)	13 (5%)	30	65
3	F	273/274 (100%)	260 (95%)	13 (5%)	30	65
4	X	2/2 (100%)	2 (100%)	0	100	100
4	Y	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2230/2404 (93%)	2093 (94%)	137 (6%)	22 57

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	40	LEU
1	A	44	VAL
1	A	88	CYS
1	A	89	LEU
1	A	91	PRO
1	A	101	GLU
1	A	122	SER
1	A	141	PHE
1	A	145	THR
1	A	160	SER
1	A	177	ASP
1	A	178	THR
1	A	180	MET
1	A	198	LEU
1	A	222	LEU
1	A	237	GLN
1	A	294	CYS
1	A	295	GLU
1	A	348	VAL
1	A	350	MET
1	A	370	LEU
1	A	382	LEU
1	A	384	ILE
1	A	389	ASP
1	A	391	VAL
1	A	398	ARG
1	A	399	GLN
1	A	411	LEU
1	A	438	PHE
1	A	456	TYR
1	A	476	GLU
1	A	495	TYR
1	A	515	ASP
1	A	540	VAL
2	B	95	ARG
2	B	134	PHE

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Mol	Chain	Res	Type
2	B	135	LEU
2	B	139	ASP
2	B	162	ASP
2	B	165	ASP
2	B	166	PRO
2	B	167	ARG
2	B	170	ASP
2	B	256	GLN
2	B	264	PHE
2	B	285	LYS
2	B	305	ILE
2	B	317	LEU
2	B	337	LEU
2	B	338	TYR
2	B	357	LEU
2	B	371	HIS
2	B	375	THR
2	B	381	TYR
2	B	413	MET
2	B	415	GLU
3	C	10	LEU
3	C	44	ASN
3	C	75	SER
3	C	76	PRO
3	C	119	GLU
3	C	187	GLN
3	C	211	ILE
3	C	235	THR
3	C	239	ARG
3	C	242	GLN
3	C	280	ASP
3	C	284	TYR
3	C	294	ARG
1	D	36	SER
1	D	37	THR
1	D	40	LEU
1	D	44	VAL
1	D	95	SER
1	D	101	GLU
1	D	122	SER
1	D	177	ASP
1	D	178	THR

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Mol	Chain	Res	Type
1	D	180	MET
1	D	210	SER
1	D	222	LEU
1	D	237	GLN
1	D	294	CYS
1	D	295	GLU
1	D	321	VAL
1	D	350	MET
1	D	370	LEU
1	D	382	LEU
1	D	384	ILE
1	D	398	ARG
1	D	399	GLN
1	D	403	SER
1	D	414	ASP
1	D	438	PHE
1	D	476	GLU
1	D	495	TYR
1	D	515	ASP
1	D	540	VAL
2	E	83	PRO
2	E	95	ARG
2	E	132	LEU
2	E	134	PHE
2	E	135	LEU
2	E	139	ASP
2	E	162	ASP
2	E	165	ASP
2	E	166	PRO
2	E	167	ARG
2	E	170	ASP
2	E	232	GLU
2	E	256	GLN
2	E	264	PHE
2	E	285	LYS
2	E	305	ILE
2	E	317	LEU
2	E	337	LEU
2	E	338	TYR
2	E	357	LEU
2	E	371	HIS
2	E	375	THR

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Mol	Chain	Res	Type
2	E	381	TYR
2	E	413	MET
2	E	415	GLU
3	F	10	LEU
3	F	34	LYS
3	F	43	SER
3	F	44	ASN
3	F	76	PRO
3	F	119	GLU
3	F	187	GLN
3	F	211	ILE
3	F	239	ARG
3	F	242	GLN
3	F	280	ASP
3	F	284	TYR
3	F	294	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	72	GLN
1	A	119	HIS
1	A	200	ASN
1	A	217	GLN
1	A	230	ASN
1	A	271	GLN
1	A	338	ASN
1	A	387	ASN
1	A	392	ASN
1	A	399	GLN
1	A	433	GLN
1	A	465	ASN
1	A	506	ASN
1	A	580	GLN
2	B	123	HIS
2	B	156	GLN
2	B	208	HIS
2	B	233	HIS
2	B	254	HIS
2	B	329	HIS
2	B	373	ASN

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Mol	Chain	Res	Type
2	B	377	HIS
2	B	382	ASN
2	B	392	GLN
3	C	12	GLN
3	C	16	GLN
3	C	44	ASN
3	C	179	HIS
3	C	187	GLN
1	D	22	ASN
1	D	72	GLN
1	D	119	HIS
1	D	200	ASN
1	D	217	GLN
1	D	230	ASN
1	D	271	GLN
1	D	338	ASN
1	D	392	ASN
1	D	399	GLN
1	D	433	GLN
1	D	465	ASN
1	D	506	ASN
1	D	571	GLN
1	D	580	GLN
2	E	92	ASN
2	E	123	HIS
2	E	156	GLN
2	E	208	HIS
2	E	223	ASN
2	E	254	HIS
2	E	329	HIS
2	E	373	ASN
2	E	377	HIS
2	E	382	ASN
2	E	392	GLN
3	F	12	GLN
3	F	44	ASN
3	F	179	HIS
3	F	187	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	DAL	X	1	4	4,4,5	3.05	1 (25%)	1,4,6	0.28	0
4	ACB	X	3	4	4,8,9	3.79	2 (50%)	3,10,12	0.81	0
4	1ZN	X	5	4	22,23,24	1.12	2 (9%)	24,29,31	0.90	0
4	FGA	X	6	4	6,6,9	1.42	1 (16%)	5,6,11	0.53	0
4	DAM	X	7	3,4	5,5,6	2.48	2 (40%)	3,5,7	3.36	2 (66%)
4	DAL	Y	1	4	4,4,5	2.39	1 (25%)	1,4,6	0.15	0
4	ACB	Y	3	4	4,8,9	3.22	2 (50%)	3,10,12	0.91	0
4	1ZN	Y	5	4	22,23,24	1.16	2 (9%)	24,29,31	0.87	0
4	FGA	Y	6	4	6,6,9	1.37	1 (16%)	5,6,11	0.75	0
4	DAM	Y	7	3,4	5,5,6	2.28	2 (40%)	3,5,7	3.07	1 (33%)

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
4	DAL	X	1	4	-	0/0/2/4	0/0/0/0
4	ACB	X	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	X	5	4	-	0/22/25/27	0/1/1/1
4	FGA	X	6	4	-	0/3/4/9	0/0/0/0
4	DAM	X	7	3,4	-	0/0/4/6	0/0/0/0
4	DAL	Y	1	4	-	0/0/2/4	0/0/0/0
4	ACB	Y	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	Y	5	4	-	0/22/25/27	0/1/1/1
4	FGA	Y	6	4	-	0/3/4/9	0/0/0/0
4	DAM	Y	7	3,4	-	0/0/4/6	0/0/0/0

All (16) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	6	FGA	CB-CA	-2.06	1.50	1.53
4	Y	5	1ZN	C9-C4	2.15	1.43	1.38
4	X	6	FGA	CG-CD	2.20	1.55	1.49
4	X	5	1ZN	C3-C2	2.21	1.55	1.52
4	Y	5	1ZN	C3-C2	2.27	1.55	1.52
4	X	5	1ZN	C9-C4	2.29	1.43	1.38
4	Y	3	ACB	CB-CA	2.55	1.57	1.55
4	Y	7	DAM	C-CA	2.61	1.49	1.45
4	X	7	DAM	C-CA	3.19	1.50	1.45
4	Y	7	DAM	CA-N	3.97	1.44	1.34
4	X	7	DAM	CA-N	4.11	1.45	1.34
4	X	3	ACB	CB-CA	4.21	1.59	1.55
4	Y	1	DAL	CA-C	4.68	1.56	1.50
4	Y	3	ACB	CA-N	5.84	1.59	1.47
4	X	1	DAL	CA-C	6.01	1.58	1.50
4	X	3	ACB	CA-N	6.21	1.60	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	7	DAM	O-C-CA	-5.39	118.41	125.07
4	Y	7	DAM	O-C-CA	-4.94	118.97	125.07
4	X	7	DAM	CB-CA-N	-2.17	120.35	125.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	5	1ZN	1	0
4	X	7	DAM	2	0
4	Y	5	1ZN	2	0
4	Y	6	FGA	1	0
4	Y	7	DAM	3	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	582/589 (98%)	-0.11	18 (3%) 49 48	25, 65, 112, 147	0
1	D	582/589 (98%)	-0.03	9 (1%) 74 70	22, 53, 109, 145	0
2	B	388/449 (86%)	0.12	22 (5%) 24 23	31, 81, 140, 155	0
2	E	388/449 (86%)	-0.01	12 (3%) 49 48	28, 75, 136, 155	0
3	C	308/309 (99%)	0.04	7 (2%) 61 58	26, 68, 110, 168	0
3	F	308/309 (99%)	0.03	7 (2%) 61 58	27, 64, 109, 169	0
4	X	2/7 (28%)	0.46	0 100 100	91, 91, 91, 103	0
4	Y	2/7 (28%)	-0.12	0 100 100	76, 76, 76, 96	0
All	All	2560/2708 (94%)	-0.01	75 (2%) 52 50	22, 65, 127, 169	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	73	ASN	5.3
2	B	130	PHE	4.9
2	B	71	THR	4.4
3	F	170	LEU	4.2
2	B	77	ILE	3.9
1	A	349	ILE	3.8
1	D	589	ALA	3.8
1	D	447	CYS	3.4
3	C	170	LEU	3.4
2	E	79	GLU	3.4
2	B	131	PHE	3.4
2	B	78	THR	3.3
2	E	134	PHE	3.3
1	A	560	VAL	3.3
2	E	77	ILE	3.1
1	D	588	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	73	ASN	3.1
2	B	79	GLU	3.0
1	A	326	ILE	2.9
2	B	67	VAL	2.9
2	E	140	PHE	2.9
1	A	430	LEU	2.8
1	D	10	LEU	2.8
2	B	140	PHE	2.7
2	B	134	PHE	2.7
2	B	72	HIS	2.7
2	B	82	TYR	2.7
2	B	85	VAL	2.6
1	D	352	LEU	2.6
3	C	256	VAL	2.5
2	E	131	PHE	2.5
2	E	78	THR	2.5
2	E	104	THR	2.5
1	A	426	TYR	2.5
2	E	227	LEU	2.5
1	D	345	LEU	2.5
1	A	434	LEU	2.5
1	A	283	LEU	2.4
2	B	126	LEU	2.4
2	E	75	ASN	2.4
1	A	267	PHE	2.4
3	F	299	HIS	2.4
3	C	169	GLY	2.4
2	B	139	ASP	2.4
2	B	69	TYR	2.4
1	A	388	LEU	2.3
2	E	69	TYR	2.3
1	D	586	LEU	2.3
1	A	248	LEU	2.3
2	E	139	ASP	2.2
3	F	164	PHE	2.2
1	A	525	VAL	2.2
1	A	353	SER	2.2
1	D	76	PHE	2.2
3	F	211	ILE	2.2
3	C	299	HIS	2.2
2	B	63	LEU	2.2
1	A	389	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	217	ILE	2.1
2	B	92	ASN	2.1
2	B	153	PHE	2.1
2	B	74	ARG	2.1
1	A	276	PRO	2.1
3	C	177	LEU	2.1
3	F	228	PHE	2.1
2	B	123	HIS	2.1
3	F	169	GLY	2.1
3	C	257	VAL	2.1
3	F	165	CYS	2.0
1	A	10	LEU	2.0
1	D	544	LEU	2.0
1	A	325	GLN	2.0
3	C	218	TYR	2.0
1	A	284	VAL	2.0
1	A	564	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
4	DAL	Y	1	5/6	0.97	0.14	-	72,72,73,74	0
4	DAM	Y	7	6/7	0.95	0.16	-	72,77,79,81	0
4	1ZN	X	5	23/24	0.92	0.48	-	64,70,89,93	0
4	FGA	X	6	7/10	0.79	0.24	-	81,88,93,97	0
4	DAL	X	1	5/6	0.94	0.20	-	77,77,80,80	0
4	ACB	X	3	9/10	0.93	0.25	-	93,97,99,101	0
4	ACB	Y	3	9/10	0.94	0.25	-	80,85,92,93	0
4	DAM	X	7	6/7	0.96	0.22	-	76,80,81,82	0
4	FGA	Y	6	7/10	0.85	0.24	-	77,81,87,93	0
4	1ZN	Y	5	23/24	0.93	0.32	-	64,74,82,84	0

## 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(Å <sup>2</sup> )	Q<0.9
5	MN	F	502	1/1	0.97	0.20	0.14	56,56,56,56	0
5	MN	C	501	1/1	0.97	0.18	0.05	46,46,46,46	0
5	MN	C	502	1/1	0.94	0.16	-0.78	65,65,65,65	0
5	MN	F	501	1/1	0.98	0.15	-1.08	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.