



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DW8  
Title : Structure of a Protein Phosphatase 2A Holoenzyme with B55 subunit  
Authors : Xu, Y.; Chen, Y.; Zhang, P.; Jeffrey, P.D.; Shi, Y.  
Deposited on : 2008-07-21  
Resolution : 2.85 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

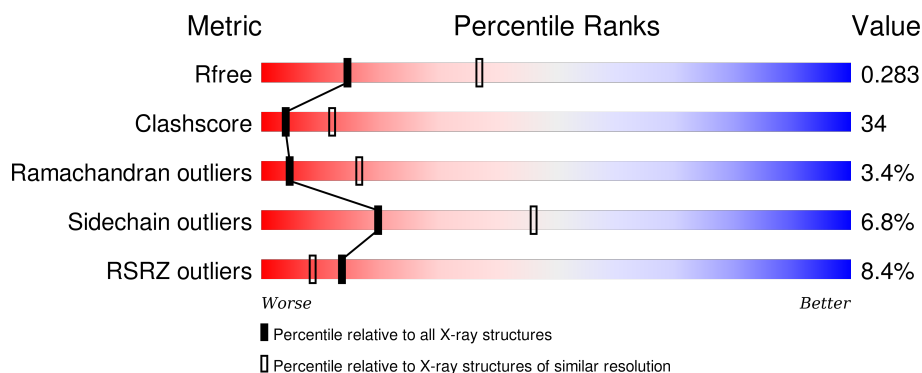
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	582	
1	D	582	
2	B	447	
2	E	447	
3	C	309	

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Mol	Chain	Length	Quality of chain
3	F	309	
4	G	7	
4	H	7	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20717 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4535	2882	764	861	28			
1	D	582	Total	C	N	O	S	0	0	0
			4535	2882	764	861	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	EXPRESSION TAG	UNP P30153
D	8	MET	-	EXPRESSION TAG	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3429	2158	595	658	18			
2	E	421	Total	C	N	O	S	0	0	0
			3428	2157	595	658	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	VAL	ILE	ENGINEERED	UNP P63151
E	310	VAL	ILE	ENGINEERED	UNP P63151

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			
3	F	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	H	7	Total	C	N	O	0	0	0
			71	49	10	12			

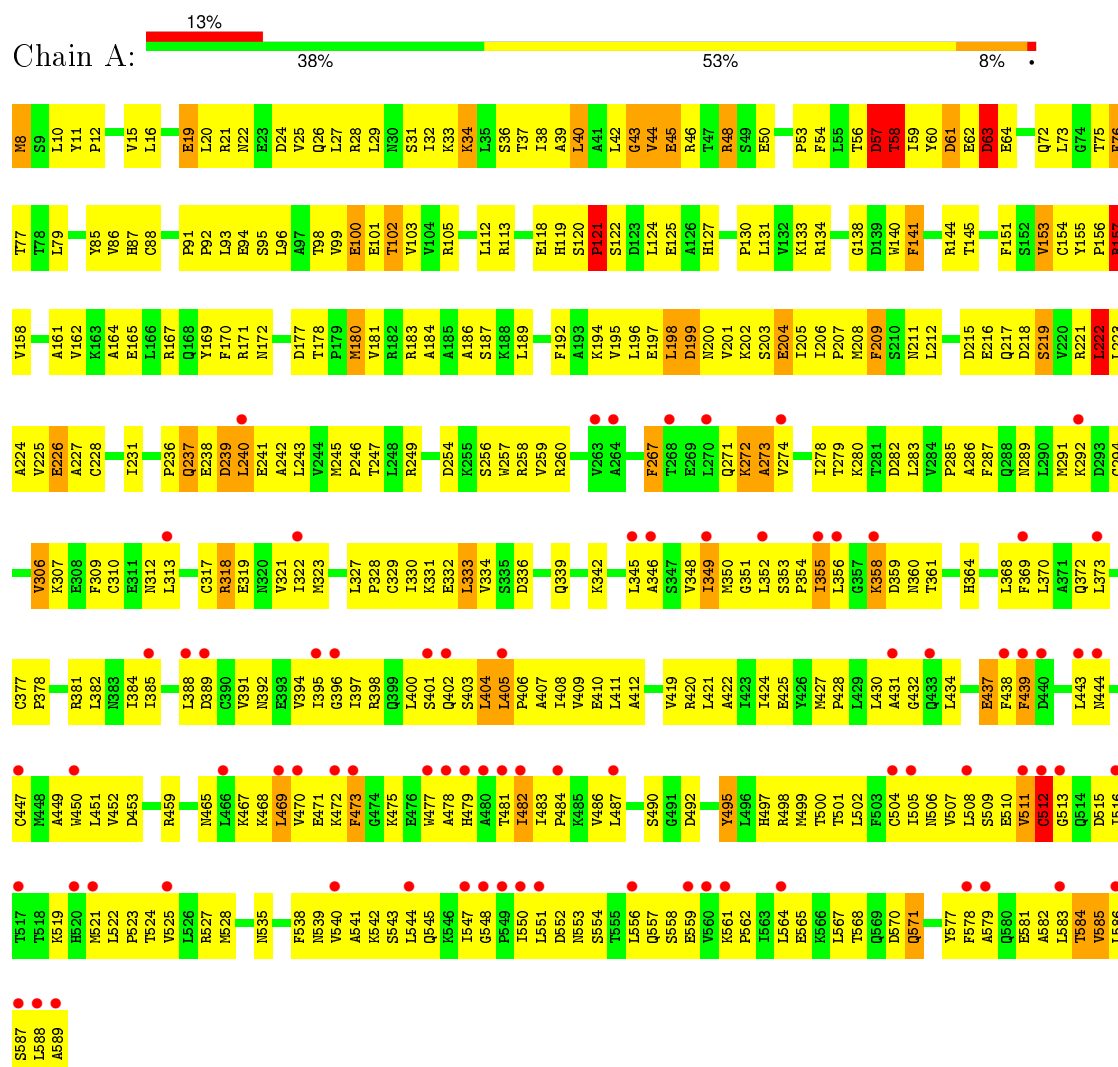
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

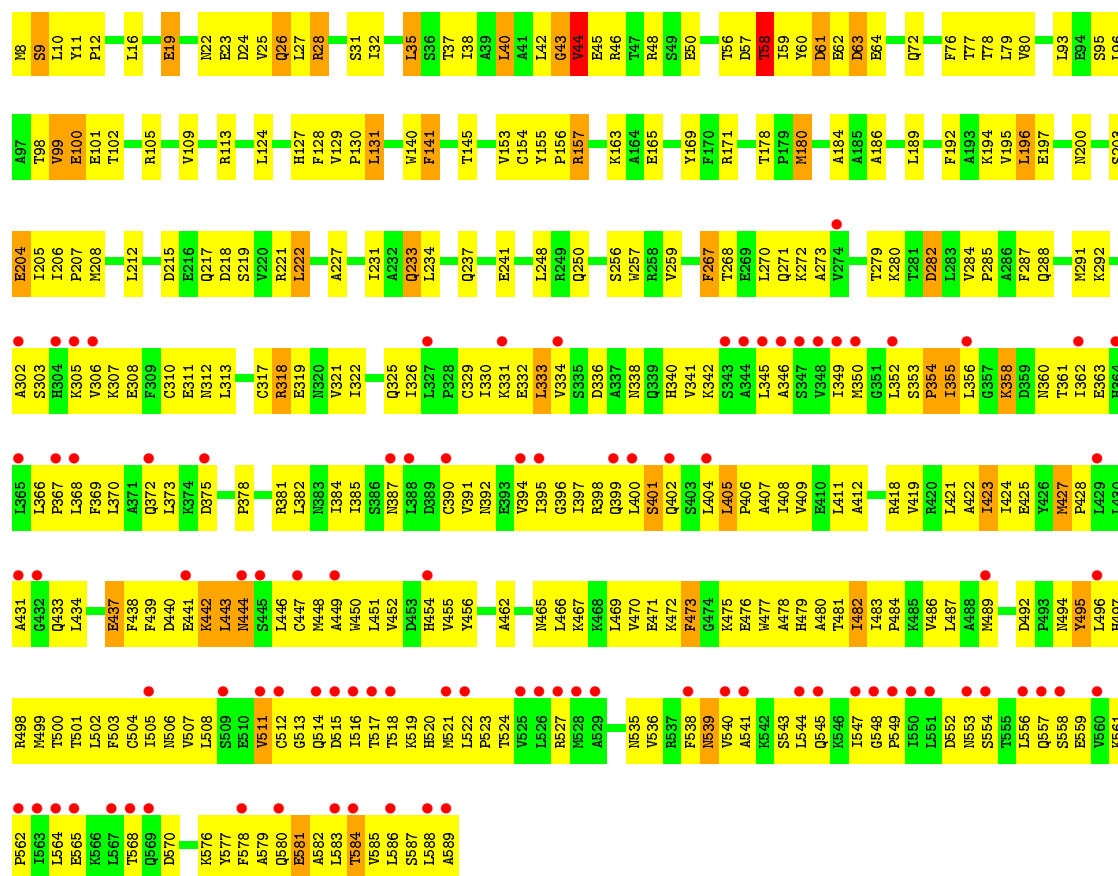
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

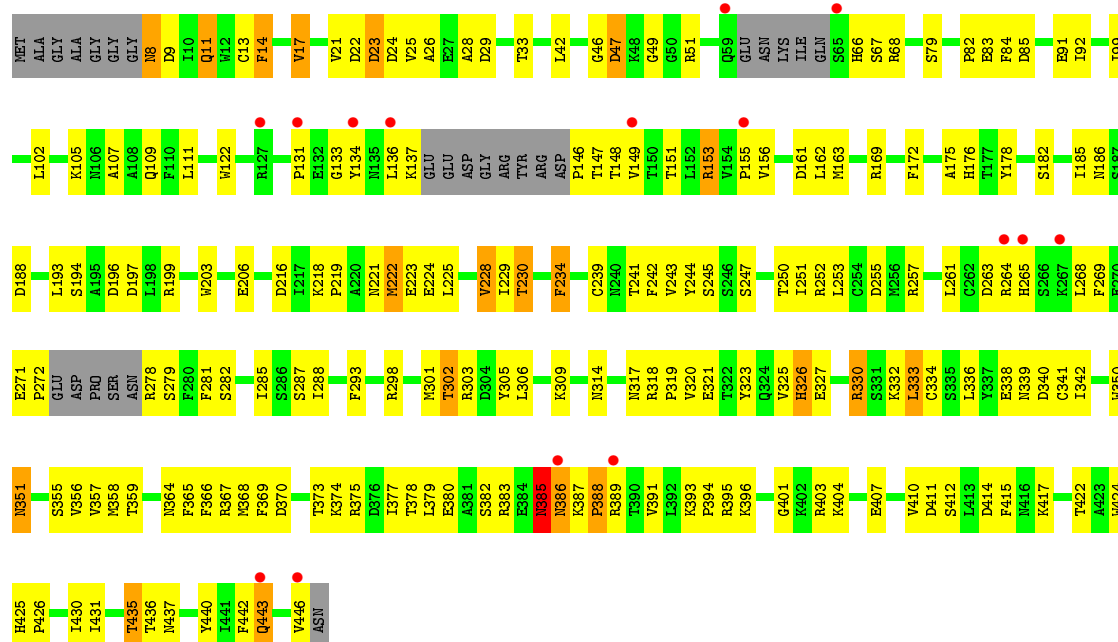


- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

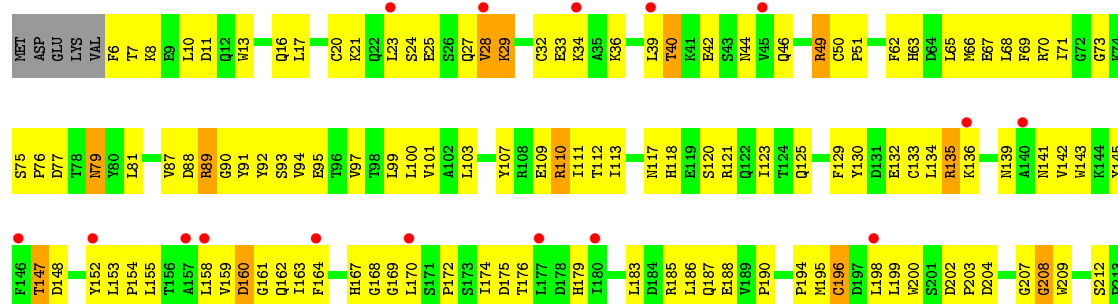




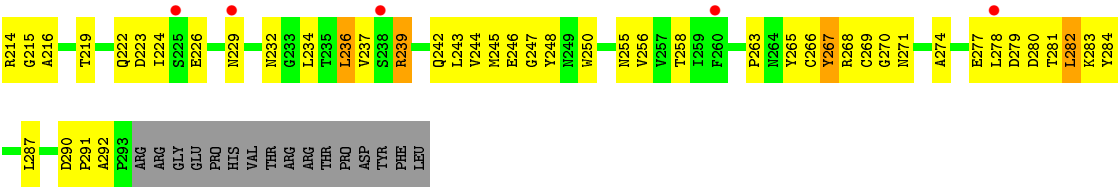
• Molecule 2: Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform



- Chain E:  2% 55% 34% 6%







● Molecule 4: microcystin LR



● Molecule 4: microcystin LR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.34Å 121.39Å 172.48Å 90.00° 132.60° 90.00°	Depositor
Resolution (Å)	49.63 – 2.85 49.63 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.85) 99.3 (49.63-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.228 , 0.285 0.227 , 0.283	Depositor DCC
$R_{free}$ test set	4180 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.5	EDS
Estimated twinning fraction	0.010 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 83615 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

### 5.1 Standard geometry

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	0.42	0/4609	0.65	1/6256 (0.0%)
1	D	0.44	0/4609	0.66	1/6256 (0.0%)
2	B	0.55	0/3501	0.76	2/4730 (0.0%)
2	E	0.59	1/3500 (0.0%)	0.80	2/4728 (0.0%)
3	C	0.43	0/2379	0.68	0/3227
3	F	0.42	0/2379	0.65	0/3227
4	G	0.43	0/17	0.60	0/19
4	H	0.43	0/17	0.50	0/19
All	All	0.48	1/21011 (0.0%)	0.70	6/28462 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	CYS	CB-SG	-6.12	1.71	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	VAL	N-CA-C	-6.37	93.79	111.00
2	B	146	PRO	N-CA-CB	5.70	110.13	103.30
2	B	85	ASP	N-CA-C	-5.68	95.67	111.00
2	E	146	PRO	N-CA-CB	5.65	110.08	103.30
1	A	222	LEU	CA-CB-CG	5.62	128.24	115.30
2	E	100	ARG	NE-CZ-NH1	-5.32	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4642	402	0
1	D	4535	0	4642	368	0
2	B	3429	0	3323	209	0
2	E	3428	0	3322	178	0
3	C	2322	0	2223	113	0
3	F	2322	0	2223	165	0
4	G	71	0	67	4	0
4	H	71	0	67	2	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20717	0	20509	1392	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 (1392) 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:A:208:MET:SD	1:A:208:MET:CE	2.01	1.49
3:C:38:ILE:HG12	3:C:108:ARG:HH21	1.10	1.11
1:A:478:ALA:HA	1:A:482:ILE:HD12	1.30	1.10
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.69	1.08
2:E:370:ASP:HB3	2:E:373:THR:HG22	1.37	1.04
1:A:373:LEU:HD21	1:A:404:LEU:HB3	1.39	1.04
2:B:199:ARG:HH21	2:B:218:LYS:HD3	1.24	1.03
1:D:378:PRO:O	1:D:382:LEU:HB2	1.57	1.03
1:D:100:GLU:HG3	2:E:106:ASN:HD21	1.25	1.02
2:E:373:THR:HG23	2:E:375:ARG:H	1.22	1.01
2:E:25:VAL:HG13	2:E:437:ASN:HB3	1.44	0.99
1:D:506:ASN:HD21	1:D:543:SER:HA	1.26	0.99
1:D:59:ILE:HD13	1:D:95:SER:HB3	1.42	0.98
1:A:307:LYS:HE2	1:A:351:GLY:HA3	1.44	0.97
2:B:199:ARG:NH2	2:B:218:LYS:HD3	1.79	0.97
1:D:478:ALA:HA	1:D:482:ILE:HD12	1.46	0.96
1:A:11:TYR:HB3	1:A:12:PRO:HD3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:28:VAL:HG11	3:F:142:VAL:HG13	1.45	0.96
2:B:278:ARG:HG3	2:B:279:SER:H	1.29	0.95
1:D:405:LEU:HB2	1:D:406:PRO:HD3	1.49	0.94
1:A:378:PRO:O	1:A:382:LEU:HB2	1.68	0.92
3:C:81:LEU:HD13	3:C:112:THR:HB	1.52	0.92
1:D:178:THR:HG22	1:D:180:MET:H	1.35	0.92
2:E:399:ALA:HB3	2:E:402:LYS:HE2	1.48	0.91
2:B:325:VAL:HG23	2:B:367:ARG:HG3	1.53	0.90
1:A:178:THR:HG22	1:A:180:MET:H	1.36	0.90
2:B:330:ARG:HG3	2:B:330:ARG:HH11	1.35	0.90
1:A:432:GLY:HA3	1:A:472:LYS:HE3	1.51	0.90
1:A:479:HIS:HB2	1:A:516:ILE:HD13	1.53	0.89
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.55	0.89
3:F:100:LEU:HA	3:F:103:LEU:HD12	1.54	0.89
2:B:21:VAL:HA	2:B:383:ARG:HH12	1.36	0.88
1:A:186:ALA:HB2	1:A:212:LEU:HD13	1.56	0.88
2:B:334:CYS:O	2:B:338:GLU:HG2	1.74	0.88
2:B:251:ILE:HD12	2:B:251:ILE:H	1.39	0.87
1:A:21:ARG:O	1:A:21:ARG:HG2	1.72	0.87
2:B:21:VAL:HA	2:B:383:ARG:NH1	1.88	0.87
1:D:124:LEU:HD11	1:D:154:CYS:HB2	1.57	0.87
3:C:125:GLN:HA	3:C:130:TYR:HB2	1.56	0.86
2:E:393:LYS:HB3	2:E:395:ARG:NH2	1.91	0.86
1:A:404:LEU:HD12	1:A:408:ILE:HD11	1.56	0.86
3:C:34:LYS:HA	3:C:34:LYS:HE2	1.57	0.86
1:D:396:GLY:O	1:D:400:LEU:HD13	1.75	0.86
1:D:141:PHE:HE1	1:D:180:MET:SD	1.98	0.86
1:D:452:VAL:HG22	1:D:497:HIS:CE1	2.11	0.85
1:A:59:ILE:HG12	1:A:95:SER:HB3	1.56	0.85
2:E:395:ARG:HA	2:E:395:ARG:NH1	1.91	0.85
2:B:25:VAL:HG13	2:B:437:ASN:HB3	1.59	0.84
1:D:56:THR:O	1:D:59:ILE:HD12	1.76	0.84
1:A:15:VAL:HG22	2:B:136:LEU:HD21	1.58	0.84
1:D:443:LEU:HD12	1:D:443:LEU:H	1.42	0.84
2:B:351:ASN:HD21	2:B:355:SER:H	1.24	0.84
2:B:25:VAL:HG22	2:B:437:ASN:HD22	1.42	0.84
1:D:318:ARG:HG2	1:D:319:GLU:N	1.92	0.83
2:B:250:THR:HB	2:B:268:LEU:HD11	1.60	0.83
2:E:396:LYS:HB3	2:E:407:GLU:HG2	1.60	0.81
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.61	0.81
3:C:38:ILE:HG12	3:C:108:ARG:NH2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG22	1:A:28:ARG:HH12	1.45	0.81
3:C:103:LEU:HB3	3:C:111:ILE:CD1	2.10	0.81
1:A:141:PHE:CE2	2:B:105:LYS:HA	2.16	0.81
1:D:409:VAL:HG22	1:D:446:LEU:HD21	1.63	0.81
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.62	0.80
2:B:8:ASN:N	2:B:8:ASN:HD22	1.75	0.80
3:F:16:GLN:HG2	3:F:21:LYS:HB2	1.62	0.80
3:F:266:CYS:O	3:F:268:ARG:HG2	1.82	0.80
1:A:236:PRO:HG2	1:A:239:ASP:OD2	1.81	0.80
1:A:113:ARG:HG2	1:A:153:VAL:HG11	1.62	0.80
2:E:221:ASN:HD21	2:E:224:GLU:HG3	1.45	0.80
1:D:58:THR:HG23	1:D:59:ILE:H	1.45	0.79
1:D:391:VAL:O	1:D:395:ILE:HG12	1.81	0.79
3:F:125:GLN:HA	3:F:130:TYR:CB	2.13	0.79
3:F:109:GLU:HB2	3:F:110:ARG:HH21	1.47	0.79
2:E:309:LYS:HD3	2:E:319:PRO:HG3	1.65	0.78
1:D:431:ALA:HB1	1:D:473:PHE:HE2	1.48	0.78
1:D:392:ASN:HD21	1:D:397:ILE:HG12	1.49	0.78
3:F:76:PRO:HB2	3:F:110:ARG:HD2	1.66	0.78
1:A:197:GLU:CD	1:A:197:GLU:H	1.88	0.78
1:A:223:LEU:O	1:A:226:GLU:HG3	1.84	0.78
1:A:59:ILE:HG22	1:A:59:ILE:O	1.83	0.78
1:A:43:GLY:HA3	1:A:45:GLU:OE1	1.83	0.78
2:E:8:ASN:N	2:E:8:ASN:HD22	1.80	0.77
1:A:141:PHE:HE1	1:A:180:MET:SD	2.08	0.77
2:E:370:ASP:CB	2:E:373:THR:HG22	2.13	0.77
1:A:46:ARG:HH12	2:B:153:ARG:NH1	1.82	0.77
1:A:392:ASN:OD1	1:A:397:ILE:HG12	1.85	0.77
2:B:387:LYS:HE2	2:B:387:LYS:HA	1.65	0.77
2:B:162:LEU:HD23	2:B:163:MET:N	2.00	0.77
3:F:79:ASN:ND2	3:F:110:ARG:HA	1.99	0.76
3:C:115:ARG:NH1	3:C:151:ASP:HA	1.99	0.76
1:D:543:SER:O	1:D:547:ILE:HG12	1.84	0.76
2:E:393:LYS:HB3	2:E:395:ARG:HH21	1.51	0.76
1:D:439:PHE:HA	1:D:443:LEU:HD13	1.68	0.76
2:E:25:VAL:CG1	2:E:437:ASN:HB3	2.16	0.76
2:E:251:ILE:N	2:E:251:ILE:HD12	2.01	0.76
1:D:577:TYR:O	1:D:581:GLU:HB3	1.86	0.76
3:F:125:GLN:HA	3:F:130:TYR:HB2	1.66	0.76
3:C:125:GLN:HA	3:C:130:TYR:CB	2.15	0.75
3:F:237:VAL:HB	3:F:256:VAL:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ILE:HA	1:D:35:LEU:HD22	1.68	0.75
1:D:321:VAL:HA	1:D:325:GLN:HG2	1.69	0.75
1:D:479:HIS:HB2	1:D:516:ILE:HD13	1.68	0.75
1:A:553:ASN:O	1:A:557:GLN:HG2	1.86	0.75
1:A:178:THR:HG22	1:A:180:MET:N	2.01	0.75
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.69	0.75
1:A:385:ILE:HG21	1:A:430:LEU:HD11	1.68	0.75
2:B:436:THR:HG23	2:B:437:ASN:N	2.02	0.75
1:D:155:TYR:HB3	1:D:156:PRO:HD3	1.69	0.74
1:A:12:PRO:O	1:A:16:LEU:HD13	1.87	0.74
1:A:267:PHE:CE2	1:A:287:PHE:HB2	2.23	0.74
2:B:327:GLU:OE2	2:B:330:ARG:HG3	1.87	0.74
3:F:76:PRO:HB2	3:F:110:ARG:CD	2.17	0.74
2:B:396:LYS:HD3	2:B:407:GLU:OE2	1.87	0.74
1:D:102:THR:HG22	1:D:105:ARG:HH22	1.52	0.74
1:D:561:LYS:HD2	1:D:588:LEU:HD22	1.69	0.74
2:E:87:LEU:HD12	2:E:87:LEU:H	1.53	0.73
1:D:192:PHE:O	1:D:196:LEU:HD23	1.88	0.73
1:A:45:GLU:H	1:A:45:GLU:CD	1.91	0.73
1:D:22:ASN:HD21	1:D:27:LEU:HD12	1.52	0.73
1:D:284:VAL:O	1:D:288:GLN:HG3	1.88	0.73
1:D:544:LEU:HD12	1:D:564:LEU:HD21	1.69	0.73
3:F:117:ASN:HB3	3:F:199:LEU:O	1.89	0.73
3:C:266:CYS:SG	4:G:2:LEU:HD13	2.29	0.72
2:E:395:ARG:HA	2:E:395:ARG:HH11	1.53	0.72
1:A:571:GLN:CD	1:A:571:GLN:H	1.93	0.72
1:D:506:ASN:ND2	1:D:543:SER:HA	2.01	0.72
2:E:271:GLU:HG3	2:E:318:ARG:HG2	1.71	0.72
1:A:561:LYS:O	1:A:565:GLU:HG3	1.90	0.72
1:A:217:GLN:OE1	2:B:239:CYS:HB3	1.90	0.72
1:A:421:LEU:O	1:A:425:GLU:HG2	1.89	0.72
2:B:373:THR:O	2:B:374:LYS:HB2	1.89	0.72
3:F:154:PRO:HA	3:F:185:ARG:NH1	2.04	0.72
1:A:396:GLY:O	1:A:400:LEU:HD13	1.90	0.71
2:E:251:ILE:HD12	2:E:251:ILE:H	1.55	0.71
3:C:204:ASP:OD2	3:C:219:THR:HB	1.90	0.71
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.20	0.71
1:D:349:ILE:HG23	1:D:350:MET:HE2	1.72	0.71
1:D:405:LEU:H	1:D:405:LEU:HD12	1.53	0.71
2:E:178:TYR:HB2	2:E:196:ASP:HB3	1.72	0.71
3:F:121:ARG:O	3:F:125:GLN:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:ARG:CG	2:B:330:ARG:HH11	2.02	0.71
1:A:141:PHE:CZ	2:B:105:LYS:HG3	2.25	0.71
1:A:543:SER:O	1:A:547:ILE:HG12	1.89	0.71
1:A:127:HIS:C	1:A:130:PRO:HD2	2.11	0.71
3:F:121:ARG:HG2	3:F:147:THR:CG2	2.21	0.71
1:D:59:ILE:HD13	1:D:95:SER:CB	2.20	0.70
2:B:21:VAL:CA	2:B:383:ARG:HH12	2.03	0.70
1:D:392:ASN:ND2	1:D:397:ILE:HG12	2.05	0.70
3:F:121:ARG:NH2	3:F:148:ASP:HA	2.06	0.70
1:A:545:GLN:OE1	1:A:582:ALA:HA	1.90	0.70
1:D:178:THR:HG22	1:D:180:MET:N	2.06	0.70
1:A:271:GLN:HA	1:A:274:VAL:HG12	1.73	0.70
1:D:492:ASP:OD2	1:D:497:HIS:HB2	1.90	0.70
1:D:363:GLU:HG2	1:D:363:GLU:O	1.91	0.70
1:D:346:ALA:HA	1:D:349:ILE:HG22	1.73	0.70
2:B:25:VAL:HG22	2:B:437:ASN:ND2	2.07	0.70
1:A:559:GLU:C	1:A:562:PRO:HD2	2.12	0.69
3:F:174:ILE:HD11	3:F:183:LEU:HD11	1.74	0.69
1:D:24:ASP:HB3	1:D:27:LEU:HG	1.73	0.69
1:D:100:GLU:HG2	2:E:110:PHE:CZ	2.27	0.69
3:C:38:ILE:CG1	3:C:108:ARG:HH21	1.98	0.69
1:D:570:ASP:O	1:D:576:LYS:HE2	1.93	0.69
2:E:271:GLU:HG2	2:E:272:PRO:HD2	1.74	0.69
1:D:19:GLU:HB3	1:D:31:SER:OG	1.93	0.69
2:E:373:THR:CG2	2:E:375:ARG:H	2.04	0.69
3:C:81:LEU:CD1	3:C:112:THR:HB	2.23	0.69
1:D:287:PHE:HE1	1:D:291:MET:SD	2.15	0.69
1:D:77:THR:O	1:D:80:VAL:HG12	1.93	0.69
1:A:169:TYR:O	1:A:172:ASN:HB2	1.92	0.69
2:B:11:GLN:HA	2:B:11:GLN:HE21	1.57	0.68
1:D:217:GLN:OE1	2:E:239:CYS:HB3	1.93	0.68
1:D:59:ILE:HG23	1:D:96:LEU:HD23	1.74	0.68
1:A:282:ASP:O	1:A:285:PRO:HD2	1.94	0.68
1:D:366:LEU:HB3	1:D:367:PRO:HD3	1.75	0.68
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.29	0.68
1:A:46:ARG:HD2	1:A:50:GLU:OE2	1.94	0.68
1:D:11:TYR:HB3	1:D:12:PRO:HD3	1.76	0.68
2:B:197:ASP:HB3	2:B:228:VAL:HG22	1.74	0.68
2:E:14:PHE:HZ	2:E:17:VAL:HG22	1.57	0.68
3:C:24:SER:OG	3:C:27:GLN:HG3	1.93	0.68
2:E:241:THR:HG23	2:E:253:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:O	1:A:568:THR:HG23	1.93	0.68
1:A:402:GLN:O	1:A:405:LEU:HD11	1.93	0.68
1:A:279:THR:HA	1:A:283:LEU:HG	1.74	0.67
1:A:577:TYR:O	1:A:581:GLU:HB3	1.94	0.67
1:D:141:PHE:CE1	1:D:180:MET:SD	2.85	0.67
2:E:14:PHE:CZ	2:E:17:VAL:HG22	2.28	0.67
3:C:44:ASN:OD1	3:C:185:ARG:HD3	1.94	0.67
1:D:381:ARG:O	1:D:385:ILE:HG12	1.93	0.67
1:D:395:ILE:HD12	1:D:400:LEU:HD11	1.77	0.67
2:E:85:ASP:HB3	2:E:90:LEU:HB3	1.75	0.67
1:D:545:GLN:OE1	1:D:582:ALA:HA	1.94	0.67
1:A:475:LYS:HB2	1:A:512:CYS:HA	1.76	0.67
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.24	0.67
2:B:14:PHE:C	2:B:14:PHE:CD1	2.68	0.67
1:A:431:ALA:HB1	1:A:473:PHE:HE2	1.58	0.67
1:D:22:ASN:HD22	1:D:27:LEU:HD12	1.56	0.67
2:E:25:VAL:HG11	2:E:436:THR:HG22	1.76	0.67
1:A:382:LEU:HD21	1:A:422:ALA:HB1	1.77	0.67
3:F:79:ASN:HD21	3:F:110:ARG:HA	1.58	0.67
3:F:174:ILE:CD1	3:F:194:PRO:HB2	2.25	0.66
1:D:427:MET:N	1:D:428:PRO:HD2	2.10	0.66
2:B:351:ASN:HD21	2:B:355:SER:N	1.93	0.66
1:D:516:ILE:HA	1:D:519:LYS:HD2	1.77	0.66
1:A:8:MET:N	1:A:8:MET:SD	2.69	0.66
3:C:214:ARG:NH2	3:C:242:GLN:HG2	2.11	0.66
1:A:427:MET:N	1:A:428:PRO:HD2	2.11	0.66
2:B:234:PHE:CD1	2:B:242:PHE:HB3	2.31	0.66
1:D:405:LEU:HB2	1:D:406:PRO:CD	2.23	0.66
2:B:8:ASN:HD21	2:B:375:ARG:NH2	1.94	0.66
1:D:427:MET:HA	1:D:427:MET:HE3	1.77	0.65
1:A:246:PRO:HA	1:A:249:ARG:NH1	2.11	0.65
3:F:163:ILE:HG23	3:F:236:LEU:HD23	1.78	0.65
1:D:467:LYS:HB2	1:D:507:VAL:HG12	1.76	0.65
2:B:196:ASP:HB2	2:B:199:ARG:H	1.62	0.65
1:A:453:ASP:O	1:A:459:ARG:HD3	1.96	0.65
1:D:267:PHE:CE2	1:D:287:PHE:HB2	2.31	0.65
1:D:23:GLU:OE1	1:D:23:GLU:HA	1.94	0.65
1:D:59:ILE:O	1:D:59:ILE:HG22	1.97	0.65
1:A:11:TYR:HB3	1:A:12:PRO:CD	2.26	0.65
2:B:320:VAL:HG12	2:B:321:GLU:HG3	1.79	0.65
2:E:387:LYS:O	2:E:390:THR:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ARG:HH12	3:C:151:ASP:HA	1.62	0.65
1:A:330:ILE:O	1:A:334:VAL:HG23	1.97	0.65
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.17	0.65
3:F:222:GLN:O	3:F:226:GLU:HG3	1.96	0.65
1:A:75:THR:O	1:A:76:PHE:HD1	1.80	0.65
1:A:15:VAL:HG22	2:B:136:LEU:CD2	2.27	0.65
1:D:282:ASP:O	1:D:285:PRO:HD2	1.96	0.65
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.12	0.65
1:A:93:LEU:HD13	1:A:112:LEU:HD23	1.78	0.65
1:D:441:GLU:O	1:D:442:LYS:HG2	1.97	0.65
1:A:515:ASP:O	1:A:519:LYS:HB2	1.97	0.65
2:E:219:PRO:HG2	2:E:222:MET:CE	2.27	0.65
1:A:208:MET:CB	1:A:208:MET:CE	2.75	0.64
1:A:548:GLY:HA3	1:A:586:LEU:HD22	1.79	0.64
1:A:405:LEU:HD12	1:A:405:LEU:H	1.61	0.64
3:C:209:TRP:CE2	3:C:224:ILE:HD13	2.32	0.64
1:A:209:PHE:CE1	1:A:247:THR:HG21	2.32	0.64
2:B:298:ARG:HH21	2:B:314:ASN:HD21	1.46	0.64
1:D:373:LEU:HD21	1:D:404:LEU:HB3	1.80	0.64
1:A:75:THR:OG1	1:A:75:THR:O	2.16	0.64
1:A:192:PHE:O	1:A:195:VAL:HG22	1.97	0.64
2:E:373:THR:O	2:E:374:LYS:HB2	1.96	0.64
2:E:47:ASP:HB2	2:E:51:ARG:H	1.63	0.64
1:D:556:LEU:O	1:D:588:LEU:HD11	1.96	0.64
1:A:19:GLU:HB3	1:A:31:SER:OG	1.97	0.63
2:B:336:LEU:HD21	2:B:415:PHE:CE2	2.33	0.63
2:E:373:THR:HG23	2:E:375:ARG:N	2.03	0.63
1:A:391:VAL:O	1:A:391:VAL:HG12	1.98	0.63
1:D:131:LEU:O	1:D:131:LEU:HD12	1.98	0.63
1:A:395:ILE:HD12	1:A:400:LEU:HD11	1.80	0.63
3:F:109:GLU:HB2	3:F:110:ARG:NH2	2.14	0.63
1:A:58:THR:HA	1:A:60:TYR:CD1	2.34	0.63
2:B:436:THR:CG2	2:B:437:ASN:H	2.12	0.63
1:A:204:GLU:O	1:A:207:PRO:HD2	1.99	0.63
1:D:267:PHE:CE2	1:D:287:PHE:HD2	2.17	0.63
1:A:38:ILE:O	1:A:42:LEU:HD23	1.98	0.63
1:A:211:ASN:HA	1:D:8:MET:HE3	1.79	0.63
3:F:87:VAL:O	3:F:88:ASP:HB2	1.96	0.63
1:A:59:ILE:HG12	1:A:95:SER:CB	2.27	0.63
1:A:553:ASN:HA	1:A:556:LEU:HD12	1.79	0.63
2:E:373:THR:HG23	2:E:375:ARG:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:THR:CG2	2:B:437:ASN:N	2.62	0.63
1:A:373:LEU:HD11	1:A:385:ILE:HD11	1.81	0.62
1:A:127:HIS:O	1:A:130:PRO:HD2	1.99	0.62
2:E:241:THR:CG2	2:E:253:LEU:HD21	2.28	0.62
2:B:272:PRO:HG2	2:B:318:ARG:HE	1.64	0.62
1:A:208:MET:HB2	1:A:208:MET:CE	2.29	0.62
3:F:103:LEU:HB3	3:F:111:ILE:CD1	2.30	0.62
1:A:287:PHE:HE1	1:A:291:MET:SD	2.22	0.62
1:D:57:ASP:HB3	2:E:129:LYS:NZ	2.14	0.62
1:D:373:LEU:HD11	1:D:385:ILE:HD11	1.81	0.62
1:D:405:LEU:H	1:D:405:LEU:CD1	2.13	0.62
1:D:127:HIS:C	1:D:130:PRO:HD2	2.20	0.62
3:F:246:GLU:HA	3:F:246:GLU:OE1	1.98	0.62
1:D:350:MET:HB3	1:D:391:VAL:CG2	2.30	0.62
1:D:318:ARG:O	1:D:321:VAL:HG22	2.00	0.62
1:D:145:THR:HG23	1:D:184:ALA:HB2	1.82	0.62
1:A:59:ILE:CG2	1:A:59:ILE:O	2.48	0.62
2:E:302:THR:HG22	2:E:309:LYS:HG2	1.82	0.62
2:E:387:LYS:HB3	2:E:388:PRO:HD2	1.80	0.62
2:E:278:ARG:HG3	2:E:279:SER:H	1.64	0.62
3:F:158:LEU:HD21	3:F:161:GLY:HA2	1.80	0.61
1:A:350:MET:HB3	1:A:391:VAL:HG23	1.82	0.61
1:D:483:ILE:O	1:D:487:LEU:HG	2.00	0.61
2:B:278:ARG:HG3	2:B:279:SER:N	2.09	0.61
1:A:15:VAL:CG2	2:B:136:LEU:HD21	2.28	0.61
2:B:387:LYS:HB3	2:B:388:PRO:HD2	1.82	0.61
1:D:287:PHE:CE1	1:D:291:MET:SD	2.93	0.61
1:A:209:PHE:CD2	1:A:231:ILE:HD12	2.35	0.61
1:A:400:LEU:O	1:A:404:LEU:HD23	2.00	0.61
3:C:266:CYS:C	3:C:267:TYR:HD1	2.03	0.61
3:F:199:LEU:N	3:F:199:LEU:HD12	2.15	0.61
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.29	0.61
3:F:248:TYR:HA	3:F:258:THR:O	2.01	0.61
1:A:385:ILE:CG2	1:A:430:LEU:HD11	2.31	0.61
1:D:536:VAL:O	1:D:540:VAL:HG23	2.00	0.61
1:A:200:ASN:HA	1:A:203:SER:OG	2.00	0.61
2:E:222:MET:CE	2:E:222:MET:HA	2.30	0.61
3:F:281:THR:OG1	3:F:283:LYS:HG2	2.00	0.61
1:A:120:SER:O	1:A:122:SER:N	2.34	0.61
1:A:24:ASP:OD1	1:A:26:GLN:N	2.33	0.61
3:C:248:TYR:HA	3:C:258:THR:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HD11	1:A:430:LEU:HD23	1.83	0.61
1:A:25:VAL:HA	1:A:28:ARG:NH1	2.15	0.61
1:A:524:THR:HG23	1:A:527:ARG:NH2	2.14	0.61
1:D:227:ALA:O	1:D:231:ILE:HG13	2.00	0.61
2:B:404:LYS:HD2	2:B:407:GLU:OE1	2.00	0.60
1:A:452:VAL:HG23	1:A:497:HIS:ND1	2.15	0.60
1:A:196:LEU:HB2	1:A:201:VAL:CG2	2.31	0.60
1:D:319:GLU:HG3	1:D:356:LEU:CD2	2.32	0.60
3:F:121:ARG:HG3	3:F:188:GLU:OE2	2.01	0.60
2:E:197:ASP:HB3	2:E:228:VAL:HG22	1.83	0.60
1:A:211:ASN:OD1	1:D:8:MET:CE	2.50	0.60
1:A:405:LEU:HB2	1:A:406:PRO:HD3	1.83	0.60
2:B:264:ARG:HG2	2:B:265:HIS:N	2.16	0.60
2:B:330:ARG:NH1	2:B:330:ARG:CG	2.61	0.60
2:B:436:THR:HG23	2:B:437:ASN:H	1.64	0.60
1:A:94:GLU:HG3	1:A:131:LEU:HD11	1.82	0.60
3:F:121:ARG:HG2	3:F:147:THR:HB	1.83	0.60
1:D:561:LYS:HE3	1:D:588:LEU:O	2.01	0.60
1:D:561:LYS:HB2	1:D:588:LEU:HD13	1.83	0.60
2:B:373:THR:HG21	2:B:375:ARG:HB2	1.83	0.60
1:D:392:ASN:HD21	1:D:397:ILE:CG1	2.15	0.60
3:F:195:MET:O	3:F:199:LEU:HD13	2.02	0.60
1:A:544:LEU:HD12	1:A:564:LEU:HD21	1.82	0.60
2:E:358:MET:CE	2:E:431:ILE:HD13	2.32	0.60
3:F:75:SER:OG	3:F:111:ILE:HD11	2.02	0.60
2:E:317:ASN:O	2:E:318:ARG:HG3	2.02	0.60
1:D:194:LYS:HD3	1:D:234:LEU:HD21	1.83	0.60
3:C:174:ILE:HD13	3:C:180:ILE:HG12	1.84	0.60
3:F:239:ARG:O	3:F:258:THR:HA	2.02	0.60
2:B:47:ASP:HB2	2:B:51:ARG:H	1.67	0.60
3:F:164:PHE:HB2	3:F:234:LEU:HD13	1.84	0.60
1:D:59:ILE:CD1	1:D:95:SER:HB3	2.26	0.59
2:E:214:ILE:O	2:E:215:VAL:HG23	2.02	0.59
2:E:92:ILE:HD13	2:E:117:LYS:HG3	1.84	0.59
1:D:338:ASN:OD1	1:D:340:HIS:N	2.33	0.59
1:D:578:PHE:O	1:D:582:ALA:HB2	2.03	0.59
3:C:243:LEU:HD11	3:C:271:ASN:ND2	2.16	0.59
3:C:135:ARG:HH11	3:C:135:ARG:HG2	1.66	0.59
3:F:123:ILE:HD11	3:F:200:TRP:CH2	2.36	0.59
1:A:405:LEU:HB2	1:A:406:PRO:CD	2.31	0.59
1:D:548:GLY:HA3	1:D:586:LEU:CD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:MET:HG2	2:E:161:ASP:N	2.16	0.59
1:D:421:LEU:O	1:D:425:GLU:HG2	2.02	0.59
3:F:190:PRO:O	3:F:196:CYS:HB2	2.02	0.59
2:E:8:ASN:ND2	2:E:8:ASN:N	2.50	0.59
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.83	0.59
1:A:373:LEU:HD13	1:A:384:ILE:CG2	2.32	0.59
1:A:58:THR:HA	1:A:60:TYR:HD1	1.66	0.59
1:A:492:ASP:O	1:A:498:ARG:HD3	2.02	0.59
1:D:358:LYS:O	1:D:362:ILE:HG13	2.00	0.59
2:B:8:ASN:N	2:B:8:ASN:ND2	2.48	0.59
1:D:267:PHE:CD2	1:D:287:PHE:HD2	2.21	0.59
1:A:208:MET:CG	1:A:208:MET:CE	2.80	0.59
2:E:389:ARG:HG3	2:E:389:ARG:HH11	1.67	0.59
1:D:456:TYR:CG	3:F:73:GLY:HA2	2.38	0.59
2:B:230:THR:HG21	2:B:288:ILE:O	2.03	0.59
3:C:97:VAL:O	3:C:101:VAL:HG23	2.02	0.59
2:B:305:TYR:CE1	2:B:342:ILE:HA	2.37	0.59
1:D:331:LYS:HD3	1:D:368:LEU:HD21	1.84	0.59
2:B:221:ASN:HD21	2:B:224:GLU:HG3	1.66	0.59
1:A:478:ALA:O	1:A:482:ILE:HB	2.03	0.59
1:A:382:LEU:HD12	1:A:411:LEU:HD13	1.84	0.59
2:B:47:ASP:HB3	2:B:49:GLY:H	1.68	0.59
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.38	0.59
1:D:63:ASP:OD1	1:D:101:GLU:HG3	2.03	0.58
1:A:196:LEU:HB2	1:A:201:VAL:HG22	1.85	0.58
2:B:373:THR:CG2	2:B:375:ARG:HB2	2.33	0.58
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.84	0.58
3:F:236:LEU:HD12	3:F:250:TRP:HZ3	1.68	0.58
1:D:428:PRO:HD3	1:D:465:ASN:ND2	2.19	0.58
3:F:16:GLN:CG	3:F:21:LYS:HB2	2.32	0.58
1:A:508:LEU:O	1:A:512:CYS:HB2	2.02	0.58
1:A:548:GLY:HA3	1:A:586:LEU:CD2	2.34	0.58
2:B:365:PHE:HA	2:B:379:LEU:O	2.02	0.58
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.85	0.58
1:D:448:MET:HA	1:D:451:LEU:HD12	1.86	0.58
2:E:234:PHE:CD1	2:E:242:PHE:HB3	2.38	0.58
1:A:93:LEU:HB3	1:A:112:LEU:HD21	1.83	0.58
2:B:14:PHE:CZ	2:B:17:VAL:HG22	2.39	0.58
1:A:140:TRP:CH2	2:B:107:ALA:HB2	2.39	0.58
1:D:101:GLU:OE2	2:E:170:ARG:NH2	2.35	0.58
1:D:194:LYS:CD	1:D:234:LEU:HD21	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:TYR:CD1	3:C:267:TYR:N	2.71	0.58
3:F:76:PRO:O	3:F:110:ARG:HG2	2.04	0.58
3:F:117:ASN:HB2	3:F:200:TRP:CE2	2.39	0.58
1:A:161:ALA:O	1:A:164:ALA:HB3	2.04	0.58
2:B:333:LEU:H	2:B:333:LEU:HD23	1.69	0.58
1:A:346:ALA:HB1	1:A:384:ILE:HD11	1.86	0.57
1:D:405:LEU:N	1:D:405:LEU:HD12	2.18	0.57
2:B:306:LEU:O	2:B:325:VAL:HG12	2.03	0.57
2:B:317:ASN:O	2:B:318:ARG:HG3	2.04	0.57
1:A:102:THR:HB	1:A:105:ARG:NH2	2.19	0.57
3:F:95:GLU:H	3:F:95:GLU:CD	2.06	0.57
2:B:251:ILE:HD12	2:B:251:ILE:N	2.14	0.57
1:D:515:ASP:O	1:D:519:LYS:HB2	2.04	0.57
1:D:22:ASN:O	1:D:28:ARG:HD3	2.04	0.57
1:A:373:LEU:HD21	1:A:404:LEU:CB	2.25	0.57
1:D:353:SER:O	1:D:355:ILE:N	2.37	0.57
3:C:121:ARG:HG2	3:C:147:THR:HB	1.84	0.57
1:A:307:LYS:HD2	1:A:348:VAL:HB	1.85	0.57
1:D:407:ALA:O	1:D:411:LEU:HG	2.04	0.57
2:E:36:PHE:CD1	2:E:43:LEU:HD13	2.39	0.57
1:A:323:MET:HE2	1:A:356:LEU:HD13	1.85	0.57
1:A:350:MET:SD	1:A:369:PHE:CD1	2.98	0.57
2:E:272:PRO:HG2	2:E:318:ARG:HE	1.69	0.57
1:D:494:ASN:HA	3:F:280:ASP:OD1	2.05	0.57
1:D:484:PRO:HA	1:D:487:LEU:HD12	1.85	0.57
1:D:431:ALA:HB1	1:D:473:PHE:CE2	2.36	0.57
1:A:291:MET:O	1:A:333:LEU:HD21	2.05	0.57
1:A:318:ARG:HG2	1:A:319:GLU:N	2.19	0.57
1:A:19:GLU:HG3	1:A:27:LEU:HB3	1.85	0.57
1:D:189:LEU:HD11	1:D:208:MET:HE3	1.87	0.57
1:A:157:ARG:CB	1:A:157:ARG:HH11	2.17	0.57
2:E:403:ARG:C	2:E:404:LYS:HG3	2.26	0.57
2:B:8:ASN:ND2	2:B:375:ARG:HH21	2.03	0.57
3:F:236:LEU:HG	3:F:237:VAL:N	2.20	0.57
2:B:11:GLN:HA	2:B:11:GLN:NE2	2.20	0.56
1:A:394:VAL:O	1:A:394:VAL:HG12	2.05	0.56
2:B:268:LEU:HD12	2:B:269:PHE:N	2.21	0.56
1:D:292:LYS:HE2	1:D:329:CYS:SG	2.45	0.56
1:A:294:CYS:SG	2:B:264:ARG:NH1	2.79	0.56
1:A:492:ASP:O	1:A:498:ARG:CD	2.54	0.56
1:A:538:PHE:O	1:A:542:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:81:LEU:HD13	3:F:112:THR:HB	1.86	0.56
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.87	0.56
1:A:88:CYS:O	1:A:91:PRO:HD2	2.06	0.56
1:A:346:ALA:HB1	1:A:384:ILE:CD1	2.35	0.56
1:D:350:MET:HG3	1:D:369:PHE:CE1	2.41	0.56
1:A:178:THR:CG2	1:A:180:MET:H	2.13	0.56
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.69	0.56
1:D:561:LYS:HB2	1:D:588:LEU:HD22	1.88	0.56
1:A:579:ALA:O	1:A:583:LEU:HG	2.05	0.56
2:E:42:LEU:HD12	2:E:109:GLN:HG2	1.86	0.56
1:A:286:ALA:O	1:A:289:ASN:N	2.39	0.56
1:A:171:ARG:HA	1:A:208:MET:SD	2.46	0.56
1:D:57:ASP:HB2	2:E:157:PHE:CE2	2.41	0.56
1:D:131:LEU:C	1:D:131:LEU:HD12	2.25	0.56
2:B:446:VAL:HG13	2:B:446:VAL:O	2.05	0.56
1:A:381:ARG:O	1:A:385:ILE:HG12	2.06	0.56
1:A:385:ILE:HG23	1:A:430:LEU:HD21	1.87	0.56
2:B:385:ASN:HB3	2:B:386:ASN:OD1	2.06	0.56
1:A:431:ALA:HB1	1:A:473:PHE:CE2	2.39	0.56
3:F:103:LEU:HB3	3:F:111:ILE:HD13	1.87	0.56
2:E:386:ASN:O	2:E:387:LYS:HE2	2.04	0.56
1:A:34:LYS:O	1:A:38:ILE:HD13	2.06	0.56
1:A:186:ALA:CB	1:A:212:LEU:HD13	2.34	0.56
3:F:266:CYS:C	3:F:267:TYR:CD1	2.79	0.56
1:D:544:LEU:HD12	1:D:564:LEU:CD2	2.35	0.56
3:F:123:ILE:HD11	3:F:200:TRP:HH2	1.70	0.56
1:A:209:PHE:CZ	1:A:247:THR:HG21	2.41	0.56
1:A:424:ILE:HG12	1:A:450:TRP:CZ3	2.41	0.56
1:D:25:VAL:HG22	1:D:28:ARG:HH12	1.71	0.56
1:A:419:VAL:O	1:A:422:ALA:HB3	2.06	0.56
1:D:310:CYS:HB3	1:D:322:ILE:HD11	1.88	0.56
3:F:13:TRP:CZ3	3:F:27:GLN:HB3	2.41	0.56
1:D:438:PHE:O	1:D:442:LYS:HB2	2.05	0.55
1:D:499:MET:HB3	1:D:503:PHE:CE2	2.41	0.55
1:D:502:LEU:HD13	1:D:539:ASN:O	2.06	0.55
3:C:195:MET:O	3:C:199:LEU:HD13	2.06	0.55
1:A:29:LEU:HD22	1:A:64:GLU:HG2	1.87	0.55
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.88	0.55
1:D:442:LYS:HB2	1:D:443:LEU:HD12	1.89	0.55
1:A:22:ASN:O	1:A:28:ARG:HD3	2.06	0.55
1:D:331:LYS:HD3	1:D:368:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PHE:CE2	1:A:170:PHE:HB2	2.41	0.55
1:A:99:VAL:HG12	1:A:101:GLU:H	1.70	0.55
1:D:398:ARG:HG3	1:D:399:GLN:N	2.22	0.55
2:B:8:ASN:ND2	2:B:375:ARG:NH2	2.54	0.55
1:D:564:LEU:HB3	1:D:583:LEU:HD21	1.88	0.55
2:B:378:THR:O	2:B:379:LEU:HD23	2.07	0.55
2:E:170:ARG:HG3	2:E:208:THR:HG22	1.88	0.55
3:F:29:LYS:O	3:F:33:GLU:HG2	2.05	0.55
2:B:42:LEU:CD1	2:B:109:GLN:HG2	2.37	0.55
1:D:369:PHE:CE1	1:D:384:ILE:HG23	2.42	0.55
1:A:45:GLU:OE1	1:A:46:ARG:N	2.38	0.55
1:A:287:PHE:CZ	1:A:306:VAL:HG22	2.41	0.55
3:F:172:PRO:HA	3:F:209:TRP:CZ2	2.42	0.55
2:E:403:ARG:O	2:E:404:LYS:HG3	2.07	0.55
2:B:11:GLN:CA	2:B:11:GLN:HE21	2.20	0.55
1:D:331:LYS:HA	1:D:368:LEU:HD21	1.88	0.55
2:B:332:LYS:NZ	2:B:410:VAL:HG11	2.22	0.55
1:A:522:LEU:N	1:A:523:PRO:CD	2.69	0.55
2:E:136:LEU:N	2:E:136:LEU:CD1	2.69	0.55
1:A:434:LEU:O	1:A:438:PHE:HB3	2.07	0.55
1:D:522:LEU:N	1:D:523:PRO:CD	2.69	0.55
1:A:287:PHE:HZ	1:A:306:VAL:HG22	1.72	0.55
2:E:85:ASP:CG	2:E:88:LYS:HB2	2.27	0.55
2:E:85:ASP:OD2	2:E:88:LYS:HD2	2.07	0.55
1:D:548:GLY:HA3	1:D:586:LEU:HD21	1.88	0.55
2:E:339:ASN:O	2:E:340:ASP:HB2	2.07	0.55
1:D:334:VAL:HG13	1:D:372:GLN:HG2	1.88	0.55
1:A:404:LEU:HD23	1:A:404:LEU:H	1.72	0.55
1:D:516:ILE:HA	1:D:519:LYS:HB2	1.88	0.55
3:F:176:THR:O	3:F:179:HIS:HB2	2.06	0.55
2:B:358:MET:CE	2:B:366:PHE:CD2	2.89	0.55
1:D:353:SER:C	1:D:355:ILE:H	2.10	0.55
1:D:427:MET:HE1	1:D:443:LEU:HD23	1.88	0.55
2:E:136:LEU:N	2:E:136:LEU:HD12	2.22	0.55
1:D:375:ASP:O	1:D:381:ARG:NH1	2.40	0.54
1:A:545:GLN:HG3	1:A:585:VAL:HB	1.89	0.54
1:D:288:GLN:NE2	1:D:325:GLN:O	2.38	0.54
2:B:241:THR:HG23	2:B:253:LEU:HD21	1.88	0.54
3:F:212:SER:C	3:F:214:ARG:H	2.09	0.54
1:A:469:LEU:HD22	1:A:477:TRP:CZ3	2.42	0.54
1:A:162:VAL:O	1:A:165:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:PRO:HD2	2:E:222:MET:HE1	1.88	0.54
2:E:12:TRP:CZ2	2:E:368:MET:HE1	2.42	0.54
3:F:70:ARG:HG3	3:F:70:ARG:HH11	1.70	0.54
1:D:57:ASP:HB2	2:E:157:PHE:CD2	2.42	0.54
1:A:472:LYS:HG3	1:A:472:LYS:O	2.07	0.54
3:F:65:LEU:HD21	3:F:100:LEU:HD21	1.90	0.54
2:B:134:TYR:HB3	2:B:137:LYS:HA	1.89	0.54
1:D:307:LYS:HE2	1:D:311:GLU:OE2	2.07	0.54
1:A:181:VAL:O	1:A:184:ALA:HB3	2.07	0.54
1:D:218:ASP:O	1:D:222:LEU:HD22	2.08	0.54
2:E:370:ASP:HB3	2:E:373:THR:CG2	2.25	0.54
1:A:388:LEU:HD11	1:A:430:LEU:CD2	2.37	0.54
1:D:248:LEU:HD22	1:D:270:LEU:HD22	1.89	0.54
2:B:377:ILE:HG22	2:B:378:THR:H	1.72	0.54
1:D:353:SER:N	1:D:354:PRO:HD2	2.22	0.54
1:D:492:ASP:O	1:D:498:ARG:HD3	2.07	0.54
3:F:121:ARG:HG2	3:F:147:THR:CB	2.38	0.54
1:D:545:GLN:HG3	1:D:585:VAL:HB	1.88	0.54
1:A:274:VAL:HG11	1:A:283:LEU:HD11	1.89	0.54
2:B:14:PHE:HD1	2:B:14:PHE:C	2.10	0.54
2:E:47:ASP:HB3	2:E:49:GLY:H	1.72	0.54
3:C:171:SER:HB2	3:C:197:ASP:HB2	1.89	0.54
1:D:392:ASN:OD1	1:D:397:ILE:HG12	2.08	0.54
1:D:48:ARG:HG3	1:D:80:VAL:HG22	1.89	0.54
1:A:240:LEU:O	1:A:242:ALA:N	2.41	0.54
1:D:391:VAL:O	1:D:391:VAL:HG12	2.08	0.54
3:C:222:GLN:HG3	3:C:252:HIS:HB3	1.90	0.54
3:F:134:LEU:C	3:F:136:LYS:H	2.11	0.54
2:E:170:ARG:HG3	2:E:208:THR:CG2	2.38	0.54
2:E:291:VAL:C	2:E:292:LYS:HG2	2.28	0.54
3:C:160:ASP:O	3:C:162:GLN:HG3	2.07	0.54
1:A:483:ILE:HD13	1:A:521:MET:HG3	1.90	0.54
3:F:265:TYR:O	3:F:266:CYS:HB2	2.08	0.54
2:E:272:PRO:HG2	2:E:318:ARG:HH21	1.73	0.54
1:A:162:VAL:HA	1:A:165:GLU:OE2	2.08	0.54
1:D:38:ILE:O	1:D:42:LEU:HD23	2.07	0.54
1:A:32:ILE:O	1:A:72:GLN:NE2	2.40	0.54
1:D:350:MET:HB3	1:D:391:VAL:HG21	1.89	0.53
1:D:561:LYS:HE2	1:D:565:GLU:OE2	2.08	0.53
2:B:17:VAL:HG13	2:B:440:TYR:CE2	2.43	0.53
1:A:331:LYS:HG2	1:A:368:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:HG3	2:E:106:ASN:ND2	2.09	0.53
2:E:209:ASP:O	2:E:210:ARG:HG3	2.08	0.53
1:D:271:GLN:C	1:D:273:ALA:H	2.12	0.53
3:F:94:VAL:HG23	3:F:132:GLU:OE2	2.08	0.53
2:E:334:CYS:O	2:E:338:GLU:HG2	2.08	0.53
1:A:141:PHE:CE1	1:A:180:MET:SD	2.96	0.53
1:D:392:ASN:HD21	1:D:397:ILE:CD1	2.22	0.53
1:D:46:ARG:HD2	1:D:50:GLU:OE2	2.08	0.53
2:B:435:THR:CG2	2:B:436:THR:N	2.71	0.53
1:A:397:ILE:HG22	1:A:434:LEU:HD23	1.90	0.53
2:B:285:ILE:HD13	2:B:333:LEU:HD11	1.89	0.53
1:D:405:LEU:CB	1:D:406:PRO:HD3	2.27	0.53
1:A:274:VAL:O	1:A:278:ILE:HD12	2.08	0.53
3:C:164:PHE:HB2	3:C:234:LEU:HD13	1.90	0.53
1:A:282:ASP:C	1:A:285:PRO:HD2	2.28	0.53
3:F:159:VAL:HG11	3:F:278:LEU:HD13	1.90	0.53
3:F:93:SER:O	3:F:97:VAL:HG12	2.07	0.53
3:C:30:SER:O	3:C:33:GLU:HB2	2.08	0.53
1:D:498:ARG:HH21	1:D:536:VAL:HG21	1.74	0.53
1:A:58:THR:HG23	1:A:59:ILE:H	1.73	0.53
3:F:283:LYS:HA	3:F:283:LYS:HE2	1.91	0.53
3:C:174:ILE:HD11	3:C:183:LEU:HD11	1.91	0.53
1:A:323:MET:CE	1:A:356:LEU:HD22	2.39	0.53
2:E:65:SER:HA	2:E:428:GLU:OE2	2.08	0.53
2:B:79:SER:HA	2:B:122:TRP:CZ2	2.44	0.53
1:D:473:PHE:HB3	1:D:477:TRP:CE3	2.44	0.53
2:B:84:PHE:CE1	2:B:91:GLU:HB2	2.44	0.53
1:D:346:ALA:HA	1:D:349:ILE:CG2	2.39	0.53
1:A:561:LYS:N	1:A:562:PRO:CD	2.72	0.53
1:D:58:THR:HG23	1:D:59:ILE:N	2.19	0.52
1:A:60:TYR:CG	1:A:60:TYR:O	2.61	0.52
1:D:32:ILE:CA	1:D:35:LEU:HD22	2.39	0.52
2:B:47:ASP:HB3	2:B:49:GLY:N	2.24	0.52
1:A:391:VAL:O	1:A:395:ILE:HG12	2.08	0.52
3:C:7:THR:HG22	3:C:11:ASP:OD1	2.10	0.52
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.09	0.52
2:B:68:ARG:HG2	2:B:68:ARG:HH11	1.74	0.52
1:D:59:ILE:HG12	1:D:96:LEU:CD2	2.40	0.52
1:D:443:LEU:CD1	1:D:443:LEU:H	2.19	0.52
2:B:377:ILE:HG22	2:B:378:THR:N	2.24	0.52
2:E:27:GLU:OE1	2:E:48:LYS:NZ	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:CD2	1:A:202:LYS:HD3	2.39	0.52
1:A:434:LEU:HB3	1:A:438:PHE:HD2	1.75	0.52
3:C:214:ARG:HH21	3:C:242:GLN:HG2	1.73	0.52
1:D:58:THR:OG1	1:D:59:ILE:N	2.39	0.52
1:D:538:PHE:C	1:D:538:PHE:CD1	2.83	0.52
2:B:358:MET:HE2	2:B:366:PHE:CD2	2.44	0.52
1:D:61:ASP:HB3	1:D:62:GLU:OE1	2.10	0.52
1:A:59:ILE:HG13	1:A:96:LEU:HG	1.92	0.52
1:A:198:LEU:HD21	1:A:202:LYS:HD3	1.92	0.52
1:D:330:ILE:O	1:D:334:VAL:HG23	2.10	0.52
3:F:134:LEU:O	3:F:136:LYS:N	2.43	0.52
3:F:143:TRP:O	3:F:147:THR:OG1	2.28	0.52
1:A:46:ARG:O	1:A:50:GLU:N	2.42	0.52
1:A:567:LEU:O	1:A:570:ASP:HB2	2.10	0.52
1:A:165:GLU:O	1:A:169:TYR:HD1	1.92	0.52
3:C:39:LEU:O	3:C:185:ARG:NH2	2.42	0.52
3:C:135:ARG:HG2	3:C:135:ARG:NH1	2.25	0.52
1:A:57:ASP:O	1:A:58:THR:C	2.48	0.52
3:F:89:ARG:HG3	3:F:265:TYR:OH	2.10	0.52
1:A:571:GLN:OE1	1:A:571:GLN:N	2.43	0.52
1:D:331:LYS:CD	1:D:368:LEU:HD21	2.39	0.52
1:A:48:ARG:HD3	1:A:88:CYS:SG	2.50	0.52
1:A:353:SER:OG	1:A:361:THR:HG21	2.10	0.52
2:E:11:GLN:HG3	2:E:391:VAL:HG11	1.92	0.52
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.92	0.52
2:E:148:THR:O	2:E:148:THR:HG22	2.10	0.52
1:A:8:MET:O	1:A:8:MET:SD	2.68	0.51
3:C:103:LEU:HB3	3:C:111:ILE:HD12	1.91	0.51
1:D:332:GLU:C	1:D:334:VAL:H	2.13	0.51
1:A:584:THR:HG22	1:A:584:THR:O	2.10	0.51
1:A:477:TRP:CE3	1:A:482:ILE:HD11	2.44	0.51
1:D:564:LEU:O	1:D:568:THR:HG23	2.10	0.51
1:D:579:ALA:O	1:D:583:LEU:HG	2.10	0.51
3:F:32:CYS:O	3:F:36:LYS:HG3	2.11	0.51
1:A:370:LEU:HG	1:A:403:SER:OG	2.10	0.51
1:A:61:ASP:HB3	1:A:62:GLU:OE1	2.10	0.51
1:A:94:GLU:HG3	1:A:131:LEU:CD1	2.40	0.51
3:F:290:ASP:HB3	3:F:291:PRO:HD2	1.93	0.51
2:E:12:TRP:CH2	2:E:431:ILE:HD12	2.46	0.51
2:E:358:MET:HE3	2:E:431:ILE:HD13	1.93	0.51
2:B:333:LEU:N	2:B:333:LEU:HD23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLN:O	1:D:273:ALA:N	2.44	0.51
2:B:102:LEU:HD23	2:B:185:ILE:HG21	1.91	0.51
1:D:100:GLU:HG2	2:E:110:PHE:HZ	1.75	0.51
3:F:99:LEU:HG	3:F:103:LEU:HD11	1.93	0.51
1:A:21:ARG:HG3	2:B:131:PRO:CG	2.40	0.51
3:C:199:LEU:HD12	3:C:199:LEU:N	2.26	0.51
2:E:325:VAL:HG22	2:E:326:HIS:CD2	2.45	0.51
3:C:62:PHE:C	3:C:62:PHE:CD1	2.84	0.51
2:E:221:ASN:ND2	2:E:224:GLU:HG3	2.22	0.51
2:B:386:ASN:O	2:B:387:LYS:HE2	2.10	0.51
3:F:200:TRP:CE3	3:F:216:ALA:HB3	2.45	0.51
1:D:336:ASP:O	1:D:342:LYS:HD3	2.10	0.51
1:D:256:SER:HB3	1:D:259:VAL:HG23	1.92	0.51
1:A:56:THR:O	1:A:59:ILE:HD13	2.10	0.51
1:D:32:ILE:O	1:D:35:LEU:HD22	2.11	0.51
3:C:266:CYS:SG	4:G:2:LEU:CD1	2.99	0.51
1:A:161:ALA:O	1:A:165:GLU:HG3	2.11	0.51
1:A:29:LEU:O	1:A:33:LYS:HG3	2.10	0.51
3:F:100:LEU:CA	3:F:103:LEU:HD12	2.35	0.51
1:A:196:LEU:HD12	1:A:205:ILE:CG1	2.40	0.51
1:D:32:ILE:HA	1:D:35:LEU:CD2	2.39	0.51
1:A:583:LEU:C	1:A:585:VAL:H	2.14	0.51
1:D:9:SER:O	1:D:12:PRO:HD2	2.10	0.51
1:A:327:LEU:HB3	1:A:328:PRO:HD3	1.92	0.51
2:B:68:ARG:HD3	2:B:443:GLN:OE1	2.10	0.51
1:D:478:ALA:O	1:D:483:ILE:HG13	2.11	0.51
1:A:541:ALA:HB1	1:A:578:PHE:O	2.11	0.51
3:F:97:VAL:O	3:F:101:VAL:HG23	2.11	0.51
2:B:243:VAL:HG13	2:B:293:PHE:CZ	2.46	0.51
3:C:152:TYR:HA	3:C:186:LEU:CD2	2.41	0.51
2:B:356:VAL:HG12	2:B:357:VAL:N	2.25	0.51
2:E:425:HIS:HB2	2:E:430:ILE:HB	1.92	0.51
1:D:310:CYS:HB3	1:D:322:ILE:CD1	2.40	0.50
1:D:267:PHE:O	1:D:270:LEU:HB2	2.10	0.50
1:A:330:ILE:HG23	1:A:345:LEU:HD21	1.94	0.50
1:D:419:VAL:O	1:D:422:ALA:HB3	2.11	0.50
1:D:409:VAL:O	1:D:412:ALA:HB3	2.10	0.50
2:B:351:ASN:O	2:B:351:ASN:ND2	2.41	0.50
1:A:211:ASN:OD1	1:D:8:MET:SD	2.69	0.50
2:B:373:THR:HG22	2:B:375:ARG:H	1.76	0.50
3:F:236:LEU:HD12	3:F:250:TRP:CZ3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ASP:HB3	2:B:228:VAL:CG2	2.40	0.50
1:A:432:GLY:HA3	1:A:472:LYS:CE	2.35	0.50
3:C:100:LEU:HA	3:C:103:LEU:HD12	1.93	0.50
1:A:291:MET:HE1	1:A:329:CYS:HB2	1.93	0.50
1:D:291:MET:O	1:D:333:LEU:HD21	2.10	0.50
1:A:334:VAL:HG13	1:A:372:GLN:HG2	1.93	0.50
3:C:263:PRO:HB2	3:C:291:PRO:HD3	1.93	0.50
1:A:124:LEU:HD11	1:A:154:CYS:HB2	1.94	0.50
1:A:197:GLU:OE2	1:A:200:ASN:ND2	2.38	0.50
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.94	0.50
1:A:62:GLU:N	1:A:62:GLU:OE1	2.45	0.50
1:A:570:ASP:OD1	1:A:571:GLN:OE1	2.30	0.50
2:E:11:GLN:HG3	2:E:391:VAL:CG1	2.41	0.50
3:C:176:THR:HA	3:C:232:ASN:OD1	2.11	0.50
1:A:443:LEU:N	1:A:443:LEU:HD12	2.26	0.50
2:B:330:ARG:HG3	2:B:330:ARG:NH1	2.14	0.50
1:D:392:ASN:CG	1:D:397:ILE:HG12	2.32	0.50
1:A:406:PRO:O	1:A:410:GLU:N	2.41	0.50
2:B:13:CYS:SG	2:B:391:VAL:HA	2.52	0.50
3:F:121:ARG:HG2	3:F:147:THR:HG21	1.94	0.50
1:D:205:ILE:HA	1:D:208:MET:HE2	1.93	0.50
1:D:58:THR:CG2	1:D:59:ILE:H	2.12	0.49
1:D:427:MET:HG2	1:D:447:CYS:SG	2.51	0.49
1:A:401:SER:OG	1:A:438:PHE:CZ	2.65	0.49
1:D:215:ASP:O	1:D:221:ARG:HD3	2.12	0.49
1:A:477:TRP:CZ3	1:A:482:ILE:HD11	2.47	0.49
1:A:349:ILE:HG23	1:A:350:MET:CE	2.42	0.49
1:A:349:ILE:HG23	1:A:350:MET:HE2	1.94	0.49
1:D:583:LEU:C	1:D:585:VAL:H	2.16	0.49
3:C:17:LEU:CD1	3:C:98:THR:HG22	2.41	0.49
1:D:448:MET:HE1	1:D:466:LEU:HD21	1.93	0.49
3:F:67:GLU:OE1	3:F:70:ARG:NH2	2.45	0.49
2:B:13:CYS:SG	2:B:391:VAL:HG22	2.51	0.49
3:F:199:LEU:N	3:F:199:LEU:CD1	2.76	0.49
2:E:271:GLU:CG	2:E:318:ARG:HG2	2.42	0.49
1:A:217:GLN:OE1	2:B:239:CYS:CB	2.58	0.49
1:A:587:SER:C	1:A:589:ALA:H	2.15	0.49
2:B:221:ASN:ND2	2:B:224:GLU:HG3	2.26	0.49
2:E:151:THR:HG22	2:E:152:LEU:N	2.27	0.49
1:A:21:ARG:HH12	2:B:133:GLY:N	2.10	0.49
1:D:394:VAL:HG12	1:D:394:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ILE:O	1:D:352:LEU:HD12	2.12	0.49
1:A:198:LEU:HA	1:A:201:VAL:HB	1.95	0.49
3:F:265:TYR:HB3	3:F:269:CYS:HB2	1.95	0.49
3:F:163:ILE:HG23	3:F:236:LEU:CD2	2.41	0.49
1:A:287:PHE:CE1	1:A:291:MET:SD	3.04	0.49
1:A:271:GLN:CG	1:A:272:LYS:N	2.75	0.49
2:B:33:THR:HG21	2:B:99:ILE:HG13	1.93	0.49
2:B:147:THR:O	2:B:147:THR:HG22	2.13	0.49
1:A:470:VAL:C	1:A:472:LYS:H	2.15	0.49
1:A:21:ARG:HH12	2:B:133:GLY:H	1.60	0.49
1:A:46:ARG:NH1	2:B:153:ARG:NH1	2.56	0.49
3:C:134:LEU:C	3:C:136:LYS:H	2.15	0.49
1:A:86:VAL:HG21	1:A:118:GLU:HB2	1.95	0.49
1:D:552:ASP:OD1	1:D:554:SER:HB3	2.11	0.49
1:A:196:LEU:HD12	1:A:205:ILE:HG12	1.95	0.49
1:D:334:VAL:CG1	1:D:372:GLN:HG2	2.43	0.49
3:C:25:GLU:HG3	3:C:142:VAL:HG23	1.94	0.49
1:D:313:LEU:HD13	1:D:321:VAL:CG2	2.42	0.49
1:A:236:PRO:O	1:A:239:ASP:OD2	2.31	0.49
3:C:71:ILE:HG22	3:C:275:ILE:HD11	1.95	0.49
1:D:564:LEU:HD13	1:D:583:LEU:HD23	1.95	0.49
1:D:527:ARG:HB3	1:D:527:ARG:CZ	2.42	0.49
1:D:404:LEU:HD23	1:D:404:LEU:H	1.77	0.49
1:D:465:ASN:OD1	1:D:469:LEU:HD12	2.13	0.49
3:C:265:TYR:O	3:C:266:CYS:HB2	2.13	0.49
3:C:264:ASN:ND2	3:C:267:TYR:HA	2.27	0.49
1:A:479:HIS:ND1	1:A:516:ILE:HG23	2.28	0.49
1:D:449:ALA:O	1:D:452:VAL:HG12	2.12	0.49
1:A:483:ILE:N	1:A:484:PRO:CD	2.76	0.49
3:F:7:THR:HG22	3:F:11:ASP:OD2	2.13	0.49
3:F:215:GLY:HA3	4:H:5:1ZN:H14	1.95	0.49
2:E:114:THR:HG22	2:E:183:ILE:HD13	1.95	0.49
1:D:411:LEU:HB2	1:D:423:ILE:HG13	1.95	0.48
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.26	0.48
1:D:102:THR:CG2	1:D:105:ARG:HH22	2.20	0.48
1:A:544:LEU:HD23	1:A:547:ILE:HD11	1.95	0.48
1:A:443:LEU:CD1	1:A:443:LEU:N	2.75	0.48
1:D:58:THR:HA	1:D:60:TYR:CD1	2.47	0.48
1:A:187:SER:HB3	1:A:223:LEU:HD22	1.93	0.48
3:C:55:CYS:SG	3:C:275:ILE:HG22	2.53	0.48
1:A:292:LYS:HE2	1:A:329:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:THR:O	1:D:584:THR:HG22	2.13	0.48
3:F:76:PRO:HB2	3:F:110:ARG:CG	2.42	0.48
1:A:267:PHE:CD2	1:A:287:PHE:HD2	2.32	0.48
1:A:578:PHE:O	1:A:582:ALA:HB2	2.12	0.48
2:E:14:PHE:HZ	2:E:17:VAL:CG2	2.26	0.48
1:A:353:SER:C	1:A:355:ILE:H	2.16	0.48
3:F:49:ARG:HG3	3:F:49:ARG:O	2.12	0.48
3:C:63:HIS:O	3:C:66:MET:HB2	2.13	0.48
1:D:140:TRP:CG	2:E:106:ASN:HA	2.48	0.48
1:D:62:GLU:N	1:D:62:GLU:OE1	2.45	0.48
1:D:478:ALA:O	1:D:482:ILE:HB	2.13	0.48
1:A:236:PRO:CG	1:A:239:ASP:OD2	2.59	0.48
3:F:266:CYS:C	3:F:267:TYR:HD1	2.15	0.48
1:A:398:ARG:HA	1:A:401:SER:HB3	1.96	0.48
1:A:164:ALA:HA	1:A:167:ARG:NH2	2.29	0.48
1:A:452:VAL:O	1:A:452:VAL:HG22	2.13	0.48
1:A:215:ASP:OD1	1:A:216:GLU:N	2.47	0.48
1:A:54:PHE:CE1	2:B:155:PRO:HB2	2.48	0.48
1:D:178:THR:HG23	2:E:189:TYR:CE2	2.48	0.48
2:B:387:LYS:HB3	2:B:388:PRO:CD	2.43	0.48
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.49	0.48
2:E:228:VAL:HG12	2:E:247:SER:HB3	1.94	0.48
2:B:358:MET:HE2	2:B:366:PHE:HD2	1.77	0.48
2:B:387:LYS:HD3	2:B:388:PRO:HD3	1.95	0.48
1:A:267:PHE:CE2	1:A:287:PHE:HD2	2.31	0.48
2:E:87:LEU:HD12	2:E:87:LEU:N	2.27	0.48
1:D:267:PHE:O	1:D:270:LEU:N	2.45	0.48
2:B:14:PHE:HZ	2:B:17:VAL:HG22	1.79	0.48
2:B:33:THR:HG22	2:B:46:GLY:HA3	1.96	0.48
2:E:382:SER:OG	2:E:385:ASN:HB2	2.14	0.48
1:A:360:ASN:O	1:A:364:HIS:HB2	2.14	0.48
1:A:95:SER:O	1:A:98:THR:HB	2.14	0.48
1:D:427:MET:HA	1:D:427:MET:CE	2.44	0.48
1:A:28:ARG:HH22	1:A:62:GLU:CD	2.17	0.48
3:F:170:LEU:HD12	3:F:224:ILE:HG22	1.96	0.48
2:E:373:THR:HG23	2:E:375:ARG:CG	2.43	0.48
2:E:373:THR:CG2	2:E:375:ARG:HG3	2.44	0.48
1:D:402:GLN:C	1:D:405:LEU:HD11	2.34	0.48
1:A:291:MET:CE	1:A:329:CYS:HB2	2.43	0.48
1:A:406:PRO:HG2	1:A:407:ALA:H	1.78	0.48
1:A:507:VAL:HA	1:A:510:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:O	1:A:587:SER:HB2	2.13	0.48
1:A:157:ARG:HB3	1:A:157:ARG:HH11	1.78	0.48
1:A:525:VAL:HG13	1:A:540:VAL:HG13	1.96	0.48
1:D:10:LEU:HB2	2:E:149:VAL:HG11	1.96	0.48
1:D:99:VAL:HG12	1:D:101:GLU:H	1.79	0.48
1:A:211:ASN:OD1	1:D:8:MET:HE1	2.12	0.48
2:B:373:THR:CG2	2:B:375:ARG:HG3	2.44	0.48
3:C:202:ASP:O	3:C:219:THR:HA	2.13	0.48
1:D:456:TYR:CD2	3:F:73:GLY:HA2	2.49	0.48
2:B:230:THR:HG22	2:B:245:SER:OG	2.14	0.48
1:A:490:SER:HB2	1:A:528:MET:CE	2.44	0.48
2:B:425:HIS:ND1	2:B:426:PRO:HD2	2.29	0.48
3:F:243:LEU:HD23	3:F:243:LEU:C	2.34	0.48
2:B:148:THR:O	2:B:148:THR:HG22	2.14	0.48
2:E:102:LEU:HD23	2:E:185:ILE:HG21	1.95	0.48
1:D:483:ILE:N	1:D:484:PRO:CD	2.77	0.48
1:A:470:VAL:C	1:A:472:LYS:N	2.68	0.48
2:E:404:LYS:HD2	2:E:407:GLU:OE1	2.14	0.48
1:D:541:ALA:HB1	1:D:578:PHE:O	2.14	0.48
1:A:486:VAL:O	1:A:501:THR:HG23	2.14	0.48
1:D:59:ILE:HG12	1:D:96:LEU:HD21	1.95	0.47
3:F:179:HIS:O	3:F:183:LEU:HG	2.13	0.47
1:D:219:SER:O	1:D:222:LEU:CD2	2.62	0.47
2:B:414:ASP:OD2	2:B:417:LYS:HE3	2.14	0.47
1:D:495:TYR:CE1	1:D:496:LEU:HG	2.49	0.47
3:F:25:GLU:OE1	3:F:139:ASN:ND2	2.41	0.47
1:D:424:ILE:HG12	1:D:450:TRP:CZ3	2.48	0.47
3:F:185:ARG:O	3:F:187:GLN:N	2.46	0.47
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.94	0.47
2:B:301:MET:HE2	2:B:350:TRP:CE2	2.49	0.47
3:F:17:LEU:HD21	3:F:23:LEU:HG	1.96	0.47
1:D:19:GLU:HG3	1:D:27:LEU:HB3	1.96	0.47
1:D:57:ASP:O	1:D:58:THR:C	2.50	0.47
1:A:8:MET:C	1:A:8:MET:SD	2.93	0.47
3:F:29:LYS:HD2	3:F:145:TYR:CZ	2.48	0.47
3:F:267:TYR:N	3:F:267:TYR:CD1	2.82	0.47
3:F:125:GLN:HG2	3:F:130:TYR:CD2	2.50	0.47
3:C:244:VAL:HG11	3:C:249:ASN:HB3	1.95	0.47
1:A:207:PRO:O	1:A:211:ASN:ND2	2.37	0.47
1:D:303:SER:OG	1:D:333:LEU:HD13	2.15	0.47
3:F:132:GLU:HG3	3:F:135:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LEU:HD12	3:C:149:LEU:O	2.14	0.47
2:E:9:ASP:CG	2:E:375:ARG:HH21	2.17	0.47
1:A:93:LEU:CB	1:A:112:LEU:HD21	2.45	0.47
1:A:26:GLN:N	1:A:26:GLN:OE1	2.47	0.47
1:D:456:TYR:C	1:D:456:TYR:CD1	2.88	0.47
2:E:377:ILE:HG22	2:E:378:THR:H	1.79	0.47
1:D:186:ALA:HA	1:D:212:LEU:HD13	1.97	0.47
1:A:280:LYS:HD2	1:A:317:CYS:SG	2.54	0.47
1:D:60:TYR:O	1:D:61:ASP:OD1	2.32	0.47
1:D:520:HIS:C	1:D:523:PRO:HD2	2.35	0.47
2:E:231:ALA:HB3	2:E:291:VAL:HG23	1.95	0.47
1:A:395:ILE:CD1	1:A:400:LEU:HD11	2.45	0.47
2:B:176:HIS:ND1	2:B:196:ASP:OD1	2.48	0.47
2:E:435:THR:O	2:E:436:THR:C	2.50	0.47
1:A:202:LYS:HG2	1:A:243:LEU:CD1	2.45	0.47
2:E:251:ILE:CD1	2:E:251:ILE:H	2.27	0.47
3:F:118:HIS:C	3:F:120:SER:H	2.16	0.47
3:C:212:SER:HA	3:C:219:THR:HG23	1.95	0.47
1:D:129:VAL:N	1:D:130:PRO:CD	2.78	0.47
3:F:158:LEU:CD2	3:F:161:GLY:HA2	2.43	0.47
1:D:486:VAL:O	1:D:501:THR:HG23	2.15	0.47
1:A:194:LYS:HG3	1:A:194:LYS:O	2.15	0.47
3:C:203:PRO:HB3	3:C:220:PHE:CE2	2.50	0.47
1:D:409:VAL:HA	1:D:446:LEU:HD21	1.97	0.47
1:D:434:LEU:O	1:D:438:PHE:HB3	2.15	0.47
1:A:63:ASP:OD1	1:A:101:GLU:HG3	2.15	0.47
3:F:40:THR:HG23	3:F:152:TYR:CD2	2.50	0.47
1:A:509:SER:O	1:A:550:ILE:HD13	2.14	0.47
1:A:45:GLU:CD	1:A:45:GLU:N	2.63	0.47
2:B:387:LYS:HD3	2:B:388:PRO:CD	2.45	0.47
1:A:151:PHE:HE2	1:A:170:PHE:HB2	1.80	0.47
3:F:202:ASP:O	3:F:219:THR:HA	2.14	0.47
1:D:42:LEU:O	1:D:43:GLY:O	2.33	0.47
1:D:511:VAL:HG23	1:D:511:VAL:O	2.15	0.47
1:A:451:LEU:O	1:A:500:THR:HG21	2.14	0.47
1:D:280:LYS:HA	1:D:284:VAL:HG23	1.97	0.47
1:D:503:PHE:O	1:D:507:VAL:HG23	2.15	0.47
3:C:134:LEU:O	3:C:136:LYS:N	2.47	0.47
3:F:274:ALA:HA	3:F:287:LEU:O	2.15	0.47
1:D:398:ARG:HH21	1:D:402:GLN:HE22	1.63	0.46
2:B:327:GLU:O	2:B:330:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:251:ILE:N	2:E:251:ILE:CD1	2.72	0.46
3:F:174:ILE:HD12	3:F:194:PRO:HB2	1.95	0.46
2:E:202:LEU:HB2	2:E:214:ILE:HD13	1.97	0.46
2:B:424:TRP:O	2:B:425:HIS:C	2.54	0.46
3:C:236:LEU:HD12	3:C:237:VAL:H	1.80	0.46
2:B:82:PRO:O	2:B:83:GLU:HG2	2.14	0.46
1:D:427:MET:N	1:D:428:PRO:CD	2.77	0.46
1:A:504:CYS:O	1:A:508:LEU:HG	2.16	0.46
2:B:244:TYR:CZ	2:B:252:ARG:HD2	2.51	0.46
1:D:24:ASP:OD1	1:D:26:GLN:OE1	2.33	0.46
1:D:57:ASP:O	1:D:58:THR:O	2.33	0.46
3:C:25:GLU:HG3	3:C:142:VAL:CG2	2.44	0.46
3:C:121:ARG:O	3:C:125:GLN:HG2	2.15	0.46
1:A:58:THR:OG1	1:A:59:ILE:N	2.47	0.46
1:D:321:VAL:HG23	1:D:322:ILE:N	2.29	0.46
4:G:6:FGA:HG3	4:G:7:DAM:HM1	1.72	0.46
1:A:140:TRP:CZ2	2:B:107:ALA:HB2	2.50	0.46
1:A:490:SER:HB2	1:A:528:MET:HE3	1.96	0.46
2:B:182:SER:O	2:B:194:SER:HA	2.16	0.46
1:D:60:TYR:O	1:D:60:TYR:CG	2.68	0.46
1:D:141:PHE:C	1:D:141:PHE:CD1	2.89	0.46
1:A:50:GLU:O	1:A:53:PRO:HD2	2.15	0.46
2:B:221:ASN:O	2:B:223:GLU:N	2.47	0.46
1:D:189:LEU:CD1	1:D:208:MET:HE3	2.44	0.46
1:D:46:ARG:O	1:D:50:GLU:N	2.49	0.46
2:E:68:ARG:HH11	2:E:68:ARG:HG2	1.80	0.46
1:D:98:THR:HG21	1:D:140:TRP:CE3	2.51	0.46
1:D:404:LEU:HD12	1:D:408:ILE:HD11	1.97	0.46
2:E:188:ASP:O	2:E:189:TYR:HB2	2.14	0.46
3:F:153:LEU:O	3:F:185:ARG:HD2	2.16	0.46
2:E:222:MET:HE2	2:E:222:MET:HA	1.97	0.46
1:D:330:ILE:HG22	1:D:330:ILE:O	2.14	0.46
2:E:97:ASN:ND2	2:E:116:ASP:OD1	2.46	0.46
2:B:172:PHE:HB3	2:B:203:TRP:CZ3	2.51	0.46
1:A:439:PHE:CE2	1:A:469:LEU:HD21	2.51	0.46
1:D:310:CYS:C	1:D:312:ASN:H	2.19	0.46
2:E:196:ASP:HB2	2:E:199:ARG:H	1.81	0.46
2:B:243:VAL:HG13	2:B:293:PHE:HZ	1.79	0.46
2:B:380:GLU:OE1	2:B:395:ARG:NH2	2.49	0.46
1:D:514:GLN:HA	1:D:517:THR:HB	1.96	0.46
1:A:178:THR:CG2	1:A:180:MET:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:HG2	1:A:199:ASP:OD1	2.15	0.46
2:E:321:GLU:HB3	2:E:323:TYR:CE1	2.50	0.46
1:A:469:LEU:HD22	1:A:477:TRP:HZ3	1.81	0.46
2:B:373:THR:HG22	2:B:375:ARG:HG3	1.97	0.46
1:D:200:ASN:HA	1:D:203:SER:OG	2.15	0.46
3:C:165:CYS:HA	3:C:238:SER:O	2.15	0.46
3:F:25:GLU:HG3	3:F:142:VAL:HG23	1.97	0.46
1:D:331:LYS:HA	1:D:368:LEU:CD2	2.45	0.46
1:A:427:MET:HE3	1:A:427:MET:HA	1.97	0.46
2:E:312:ASP:OD1	2:E:314:ASN:HB2	2.15	0.46
1:A:373:LEU:HD13	1:A:384:ILE:HG21	1.96	0.46
2:B:251:ILE:CD1	2:B:251:ILE:H	2.18	0.46
3:C:115:ARG:HH21	3:C:189:VAL:HG23	1.81	0.46
1:A:102:THR:HG23	2:B:206:GLU:OE2	2.15	0.46
1:D:302:ALA:O	1:D:305:LYS:N	2.47	0.46
1:A:511:VAL:O	1:A:511:VAL:HG23	2.15	0.46
1:A:138:GLY:O	1:A:144:ARG:HD3	2.15	0.46
2:B:327:GLU:OE2	2:B:330:ARG:NH1	2.48	0.45
1:D:124:LEU:HD22	1:D:128:PHE:HB3	1.98	0.45
2:E:396:LYS:HD3	2:E:407:GLU:CD	2.37	0.45
1:A:224:ALA:O	1:A:226:GLU:N	2.49	0.45
2:E:358:MET:SD	2:E:422:THR:OG1	2.74	0.45
2:E:65:SER:O	2:E:66:HIS:HB2	2.16	0.45
2:E:23:ASP:HB3	2:E:24:ASP:H	1.64	0.45
1:D:452:VAL:O	1:D:452:VAL:HG13	2.14	0.45
1:D:427:MET:HB3	1:D:465:ASN:HD21	1.81	0.45
1:D:568:THR:HB	1:D:580:GLN:OE1	2.17	0.45
3:F:155:LEU:HD21	3:F:195:MET:HE2	1.98	0.45
3:F:6:PHE:O	3:F:7:THR:C	2.54	0.45
3:C:113:ILE:HD12	3:C:153:LEU:HD21	1.98	0.45
3:F:279:ASP:OD1	3:F:279:ASP:C	2.54	0.45
1:D:157:ARG:HH11	1:D:157:ARG:CG	2.29	0.45
3:F:20:CYS:SG	3:F:92:TYR:CE2	3.10	0.45
1:A:409:VAL:O	1:A:412:ALA:N	2.49	0.45
1:D:57:ASP:HB3	2:E:129:LYS:CE	2.46	0.45
1:A:141:PHE:CD1	1:A:141:PHE:C	2.89	0.45
1:D:318:ARG:CG	1:D:319:GLU:N	2.64	0.45
3:C:188:GLU:O	3:C:190:PRO:HD3	2.16	0.45
1:A:267:PHE:CZ	1:A:287:PHE:HB2	2.51	0.45
1:A:427:MET:N	1:A:428:PRO:CD	2.79	0.45
2:E:389:ARG:CG	2:E:389:ARG:HH11	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:291:VAL:O	2:E:292:LYS:HG2	2.16	0.45
1:D:171:ARG:HH12	1:D:204:GLU:HG3	1.82	0.45
1:D:454:HIS:HB3	3:F:287:LEU:HD21	1.97	0.45
4:H:2:LEU:H	4:H:7:DAM:C	2.30	0.45
2:E:119:ILE:HD12	2:E:119:ILE:N	2.31	0.45
1:D:57:ASP:HB3	2:E:129:LYS:HE3	1.98	0.45
2:E:396:LYS:HD3	2:E:407:GLU:OE2	2.16	0.45
1:A:198:LEU:HD11	1:A:236:PRO:HD2	1.98	0.45
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.94	0.45
1:D:561:LYS:N	1:D:562:PRO:CD	2.78	0.45
1:A:559:GLU:HA	1:A:562:PRO:HG2	1.98	0.45
1:D:267:PHE:CE2	1:D:287:PHE:CD2	3.02	0.45
2:B:47:ASP:HB2	2:B:51:ARG:N	2.31	0.45
1:A:495:TYR:O	1:A:499:MET:HG3	2.16	0.45
3:C:132:GLU:O	3:C:136:LYS:HG3	2.17	0.45
2:E:172:PHE:HD2	2:E:203:TRP:CE3	2.35	0.45
2:B:263:ASP:OD1	2:B:263:ASP:N	2.50	0.45
2:E:130:ARG:HB2	2:E:131:PRO:HD2	1.99	0.45
1:D:406:PRO:O	1:D:407:ALA:C	2.55	0.45
2:B:382:SER:OG	2:B:385:ASN:HB2	2.17	0.45
3:C:76:PRO:HD3	3:C:107:TYR:CE2	2.51	0.45
1:A:39:ALA:HB1	1:A:79:LEU:HD22	1.99	0.45
1:D:352:LEU:C	1:D:354:PRO:HD2	2.37	0.45
1:D:539:ASN:HA	1:D:539:ASN:HD22	1.63	0.45
1:D:522:LEU:N	1:D:523:PRO:HD3	2.32	0.45
1:A:119:HIS:HB3	1:A:124:LEU:HB2	1.99	0.45
3:F:76:PRO:HG3	3:F:107:TYR:CE1	2.52	0.45
2:B:351:ASN:C	2:B:351:ASN:HD22	2.18	0.45
1:D:334:VAL:HG13	1:D:372:GLN:OE1	2.17	0.45
2:E:306:LEU:O	2:E:325:VAL:HG13	2.16	0.45
1:A:502:LEU:O	1:A:506:ASN:OD1	2.34	0.45
2:B:281:PHE:O	2:B:282:SER:C	2.55	0.45
1:D:516:ILE:CA	1:D:519:LYS:HB2	2.47	0.45
3:F:155:LEU:HD11	3:F:195:MET:HE3	1.99	0.45
2:B:305:TYR:HE1	2:B:341:CYS:O	1.99	0.45
3:C:250:TRP:CZ2	3:C:286:PHE:HE2	2.35	0.45
2:B:92:ILE:N	2:B:92:ILE:HD12	2.31	0.45
1:A:16:LEU:HB3	1:A:38:ILE:HD11	1.99	0.45
1:A:197:GLU:CD	1:A:197:GLU:N	2.65	0.45
1:A:564:LEU:HB3	1:A:583:LEU:HD21	1.99	0.45
3:C:200:TRP:CE3	3:C:216:ALA:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:TYR:HB3	2:B:369:PHE:CE2	2.52	0.45
3:C:68:LEU:HD23	3:C:68:LEU:O	2.17	0.45
1:A:350:MET:HB3	1:A:391:VAL:HG21	1.95	0.45
1:D:350:MET:SD	1:D:369:PHE:CD1	3.10	0.45
1:A:432:GLY:CA	1:A:472:LYS:HE3	2.36	0.45
1:A:226:GLU:CD	1:A:227:ALA:N	2.70	0.45
1:D:366:LEU:O	1:D:370:LEU:HB2	2.17	0.45
1:A:522:LEU:HD22	1:A:551:LEU:HD11	1.99	0.45
2:B:199:ARG:HG2	2:B:216:ASP:HA	1.99	0.44
2:B:325:VAL:HG13	2:B:326:HIS:CD2	2.52	0.44
2:B:435:THR:O	2:B:436:THR:C	2.56	0.44
3:C:266:CYS:C	3:C:267:TYR:CD1	2.86	0.44
1:D:549:PRO:HD3	1:D:586:LEU:CD2	2.47	0.44
1:D:334:VAL:HG22	1:D:372:GLN:OE1	2.17	0.44
1:D:440:ASP:HA	1:D:444:ASN:HB2	1.99	0.44
2:E:263:ASP:N	2:E:263:ASP:OD1	2.49	0.44
1:D:326:ILE:HD12	1:D:326:ILE:N	2.32	0.44
2:E:197:ASP:HB3	2:E:228:VAL:CG2	2.45	0.44
1:A:254:ASP:O	1:A:260:ARG:HD3	2.17	0.44
2:E:162:LEU:C	2:E:162:LEU:HD23	2.38	0.44
2:E:120:LYS:HG2	2:E:171:ILE:HG12	1.99	0.44
1:D:400:LEU:O	1:D:404:LEU:HD23	2.17	0.44
1:D:412:ALA:HA	1:D:450:TRP:HZ2	1.82	0.44
3:F:65:LEU:O	3:F:69:PHE:CD2	2.70	0.44
3:F:79:ASN:HA	3:F:79:ASN:HD22	1.57	0.44
3:F:39:LEU:HD13	3:F:153:LEU:HD23	1.99	0.44
1:A:427:MET:CE	1:A:427:MET:HA	2.47	0.44
1:A:539:ASN:HD22	1:A:539:ASN:HA	1.65	0.44
1:A:40:LEU:HD22	1:A:79:LEU:HD21	1.99	0.44
2:E:327:GLU:OE2	2:E:330:ARG:HD2	2.17	0.44
1:D:44:VAL:HG12	1:D:45:GLU:OE2	2.17	0.44
3:F:107:TYR:HB3	3:F:110:ARG:HB2	1.99	0.44
1:A:50:GLU:C	1:A:53:PRO:HD2	2.37	0.44
2:E:388:PRO:O	2:E:389:ARG:HG2	2.17	0.44
2:B:28:ALA:HB1	2:B:51:ARG:NH2	2.32	0.44
2:B:47:ASP:OD2	2:B:51:ARG:CZ	2.65	0.44
1:A:502:LEU:HD11	1:A:540:VAL:HG23	1.99	0.44
1:A:257:TRP:CE2	1:A:258:ARG:HG2	2.53	0.44
2:E:193:LEU:HD12	2:E:193:LEU:C	2.37	0.44
3:F:139:ASN:OD1	3:F:141:ASN:HB2	2.18	0.44
1:D:291:MET:HE1	1:D:329:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ASN:HD22	1:A:542:LYS:HD2	1.83	0.44
1:A:358:LYS:HG2	1:A:359:ASP:N	2.33	0.44
1:A:339:GLN:NE2	1:A:377:CYS:HB2	2.32	0.44
1:A:339:GLN:CD	1:A:377:CYS:HB2	2.37	0.44
1:D:475:LYS:HB2	1:D:512:CYS:HA	1.98	0.44
1:A:245:MET:O	1:A:249:ARG:HB2	2.17	0.44
2:E:47:ASP:HB3	2:E:49:GLY:N	2.33	0.44
1:A:502:LEU:HD21	1:A:528:MET:SD	2.58	0.44
2:B:302:THR:HG22	2:B:309:LYS:HG2	1.99	0.44
3:C:129:PHE:HZ	3:C:146:PHE:CD2	2.36	0.44
1:A:348:VAL:O	1:A:350:MET:N	2.51	0.44
3:C:81:LEU:HD13	3:C:112:THR:CB	2.34	0.44
1:D:502:LEU:HD11	1:D:540:VAL:CG2	2.48	0.44
1:A:155:TYR:CE2	1:A:196:LEU:HD23	2.52	0.44
1:D:155:TYR:CE2	1:D:163:LYS:HD3	2.52	0.44
1:A:271:GLN:OE1	1:A:309:PHE:CD1	2.71	0.44
1:D:336:ASP:HB3	1:D:342:LYS:CG	2.47	0.44
2:E:320:VAL:HG12	2:E:321:GLU:HG3	2.00	0.44
3:C:158:LEU:HG	3:C:161:GLY:HA2	2.00	0.44
2:E:252:ARG:CZ	2:E:268:LEU:HD13	2.48	0.44
1:D:553:ASN:O	1:D:557:GLN:HG2	2.18	0.44
2:B:351:ASN:C	2:B:351:ASN:ND2	2.71	0.44
3:C:188:GLU:HG3	3:C:189:VAL:N	2.33	0.44
1:A:287:PHE:HZ	1:A:306:VAL:CG2	2.29	0.44
1:D:587:SER:C	1:D:589:ALA:H	2.21	0.44
1:A:483:ILE:HD13	1:A:521:MET:SD	2.57	0.44
3:C:76:PRO:HB2	3:C:110:ARG:HG2	1.98	0.44
3:C:8:LYS:HG3	3:C:8:LYS:H	1.48	0.44
1:A:219:SER:HA	1:A:222:LEU:HD21	2.00	0.44
1:D:470:VAL:C	1:D:472:LYS:H	2.20	0.44
1:D:483:ILE:HG22	1:D:487:LEU:HD11	1.99	0.44
1:A:382:LEU:CD1	1:A:411:LEU:HD13	2.47	0.44
1:D:267:PHE:CZ	1:D:287:PHE:HB2	2.53	0.44
1:A:323:MET:CE	1:A:356:LEU:HD13	2.47	0.44
3:F:91:TYR:CE1	3:F:135:ARG:NH2	2.85	0.44
1:D:204:GLU:O	1:D:207:PRO:HD2	2.18	0.44
2:E:127:ARG:CZ	2:E:163:MET:CE	2.96	0.44
2:E:248:LYS:HA	2:E:248:LYS:HD3	1.85	0.44
1:A:439:PHE:CZ	1:A:469:LEU:HD11	2.53	0.43
1:D:462:ALA:O	1:D:465:ASN:HB3	2.18	0.43
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HA	1:A:547:ILE:HG12	2.00	0.43
2:B:303:ARG:NH1	2:B:359:THR:OG1	2.47	0.43
3:F:40:THR:HG23	3:F:152:TYR:HD2	1.81	0.43
2:E:323:TYR:HB3	2:E:369:PHE:CE2	2.53	0.43
2:B:222:MET:CE	2:B:225:LEU:HD13	2.48	0.43
2:E:244:TYR:OH	2:E:252:ARG:HD2	2.19	0.43
1:D:350:MET:C	1:D:352:LEU:H	2.20	0.43
1:D:141:PHE:CE1	1:D:180:MET:CG	3.01	0.43
1:D:155:TYR:CZ	1:D:163:LYS:HD3	2.54	0.43
1:A:267:PHE:HE2	1:A:287:PHE:HB2	1.81	0.43
1:A:561:LYS:HD2	1:A:588:LEU:HB3	2.00	0.43
1:A:133:LYS:HD3	1:A:169:TYR:OH	2.18	0.43
3:F:134:LEU:C	3:F:136:LYS:N	2.71	0.43
1:D:165:GLU:O	1:D:169:TYR:HD1	2.00	0.43
3:F:169:GLY:O	3:F:198:LEU:HA	2.18	0.43
2:E:399:ALA:HB3	2:E:402:LYS:CE	2.35	0.43
1:D:321:VAL:CG2	1:D:322:ILE:N	2.81	0.43
1:D:519:LYS:HB3	1:D:520:HIS:H	1.67	0.43
3:F:175:ASP:HB2	3:F:179:HIS:HE1	1.83	0.43
1:A:133:LYS:NZ	1:A:165:GLU:OE1	2.46	0.43
1:A:449:ALA:O	1:A:452:VAL:HG12	2.19	0.43
3:C:180:ILE:O	3:C:183:LEU:HB2	2.19	0.43
2:B:28:ALA:HB1	2:B:51:ARG:HH21	1.82	0.43
2:B:410:VAL:C	2:B:412:SER:H	2.22	0.43
3:C:228:PHE:O	3:C:232:ASN:ND2	2.43	0.43
1:D:113:ARG:HG2	1:D:153:VAL:HG11	1.99	0.43
2:E:362:TYR:O	2:E:365:PHE:HB2	2.17	0.43
2:E:110:PHE:CZ	2:E:123:LYS:HG3	2.52	0.43
2:B:21:VAL:HG22	2:B:21:VAL:O	2.18	0.43
3:F:24:SER:OG	3:F:27:GLN:HG3	2.19	0.43
2:B:241:THR:CG2	2:B:253:LEU:HD21	2.48	0.43
2:B:368:MET:HE3	2:B:424:TRP:CZ3	2.53	0.43
2:B:247:SER:HA	2:B:287:SER:OG	2.18	0.43
3:F:244:VAL:HG23	3:F:247:GLY:H	1.83	0.43
2:E:374:LYS:HA	2:E:374:LYS:HD3	1.75	0.43
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.18	0.43
1:A:332:GLU:C	1:A:334:VAL:H	2.22	0.43
2:B:298:ARG:HH21	2:B:314:ASN:ND2	2.12	0.43
1:D:233:GLN:HG3	1:D:273:ALA:HB1	2.01	0.43
3:C:106:ARG:HG3	3:C:106:ARG:HH11	1.83	0.43
3:F:110:ARG:C	3:F:111:ILE:HG13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:CYS:O	1:A:333:LEU:HG	2.18	0.43
1:D:368:LEU:C	1:D:370:LEU:N	2.71	0.43
2:B:68:ARG:HG2	2:B:68:ARG:NH1	2.33	0.43
2:E:252:ARG:NH2	2:E:268:LEU:HD13	2.34	0.43
1:D:518:THR:O	1:D:518:THR:HG22	2.19	0.43
1:D:398:ARG:C	1:D:400:LEU:H	2.22	0.43
1:A:201:VAL:O	1:A:206:ILE:HG12	2.19	0.43
3:F:118:HIS:HA	3:F:123:ILE:HG21	2.01	0.43
3:F:155:LEU:HD21	3:F:195:MET:CE	2.49	0.43
3:F:88:ASP:O	3:F:90:GLY:N	2.47	0.43
1:D:127:HIS:O	1:D:130:PRO:HD2	2.19	0.43
1:A:125:GLU:HG3	1:A:158:VAL:HG12	2.00	0.43
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.53	0.43
1:D:307:LYS:O	1:D:311:GLU:HG3	2.18	0.43
1:D:38:ILE:O	1:D:42:LEU:CD2	2.67	0.43
2:B:26:ALA:HB3	2:B:29:ASP:OD2	2.19	0.43
1:A:348:VAL:C	1:A:350:MET:N	2.72	0.43
3:F:209:TRP:CD2	3:F:224:ILE:CD1	3.02	0.43
2:E:387:LYS:HB3	2:E:388:PRO:CD	2.45	0.43
2:B:339:ASN:O	2:B:340:ASP:HB2	2.19	0.43
3:F:263:PRO:HB2	3:F:291:PRO:HD3	2.00	0.43
2:B:219:PRO:HD2	2:B:222:MET:HE1	2.00	0.43
1:D:60:TYR:O	1:D:61:ASP:CG	2.57	0.43
1:A:201:VAL:HG12	1:A:201:VAL:O	2.18	0.43
1:A:28:ARG:NH2	1:A:62:GLU:OE1	2.51	0.43
1:A:46:ARG:NH1	1:A:50:GLU:OE2	2.52	0.43
2:E:87:LEU:CD1	2:E:87:LEU:H	2.28	0.43
1:A:271:GLN:C	1:A:273:ALA:H	2.22	0.43
2:E:219:PRO:HG2	2:E:222:MET:HE2	2.01	0.43
3:C:56:GLY:HA3	3:C:259:ILE:O	2.18	0.43
2:E:111:LEU:HD12	2:E:111:LEU:C	2.39	0.43
1:A:439:PHE:CE1	1:A:444:ASN:HA	2.54	0.42
3:F:130:TYR:O	3:F:133:CYS:HB2	2.19	0.42
1:A:227:ALA:O	1:A:228:CYS:C	2.57	0.42
2:E:36:PHE:CE1	2:E:43:LEU:HD13	2.53	0.42
1:A:499:MET:SD	1:A:539:ASN:OD1	2.78	0.42
2:B:134:TYR:CB	2:B:137:LYS:HA	2.48	0.42
3:C:68:LEU:HD23	3:C:68:LEU:C	2.39	0.42
3:F:68:LEU:C	3:F:68:LEU:HD23	2.39	0.42
1:D:437:GLU:HG2	1:D:438:PHE:N	2.34	0.42
1:D:322:ILE:HG22	1:D:322:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ALA:CB	2:B:51:ARG:NH2	2.82	0.42
3:C:17:LEU:HD11	3:C:98:THR:CG2	2.49	0.42
2:B:332:LYS:HA	2:B:332:LYS:HD3	1.88	0.42
1:D:330:ILE:HG23	1:D:345:LEU:HD21	2.00	0.42
2:B:309:LYS:HD3	2:B:319:PRO:HG3	2.01	0.42
1:A:336:ASP:O	1:A:342:LYS:HD3	2.19	0.42
1:A:437:GLU:OE1	1:A:437:GLU:N	2.52	0.42
1:A:208:MET:HB2	1:A:208:MET:HE2	1.99	0.42
3:C:121:ARG:HG2	3:C:147:THR:CB	2.49	0.42
2:E:253:LEU:HD23	2:E:253:LEU:C	2.39	0.42
2:B:14:PHE:HA	2:B:442:PHE:HD1	1.83	0.42
3:F:212:SER:C	3:F:214:ARG:N	2.72	0.42
3:F:277:GLU:O	3:F:284:TYR:HA	2.20	0.42
1:D:58:THR:O	1:D:59:ILE:C	2.57	0.42
1:D:62:GLU:O	1:D:63:ASP:C	2.57	0.42
2:B:21:VAL:CA	2:B:383:ARG:NH1	2.68	0.42
1:A:204:GLU:C	1:A:207:PRO:HD2	2.40	0.42
2:B:8:ASN:CG	2:B:375:ARG:HH21	2.22	0.42
1:D:505:ILE:C	1:D:507:VAL:H	2.23	0.42
3:F:214:ARG:HH21	3:F:242:GLN:HG2	1.85	0.42
1:A:39:ALA:CB	1:A:79:LEU:HD22	2.49	0.42
3:F:42:GLU:HB3	3:F:46:GLN:OE1	2.20	0.42
3:F:160:ASP:HB3	3:F:162:GLN:OE1	2.18	0.42
1:A:43:GLY:O	1:A:44:VAL:HG23	2.19	0.42
2:B:153:ARG:HD2	2:B:153:ARG:HA	1.83	0.42
3:F:172:PRO:HG3	3:F:209:TRP:CE3	2.55	0.42
1:A:75:THR:O	1:A:76:PHE:CD1	2.66	0.42
3:C:117:ASN:HB3	3:C:199:LEU:O	2.19	0.42
1:D:489:MET:HB2	1:D:501:THR:OG1	2.19	0.42
1:D:470:VAL:C	1:D:472:LYS:N	2.72	0.42
2:E:281:PHE:O	2:E:282:SER:C	2.56	0.42
1:A:465:ASN:O	1:A:469:LEU:HB2	2.19	0.42
1:A:10:LEU:O	1:A:11:TYR:C	2.56	0.42
1:D:398:ARG:C	1:D:400:LEU:N	2.72	0.42
1:D:401:SER:HA	1:D:404:LEU:HD21	2.01	0.42
1:A:21:ARG:NH1	2:B:133:GLY:N	2.68	0.42
2:B:358:MET:CG	2:B:359:THR:N	2.82	0.42
1:D:186:ALA:CA	1:D:212:LEU:HD13	2.49	0.42
1:D:517:THR:O	1:D:521:MET:HB3	2.20	0.42
1:A:439:PHE:C	1:A:439:PHE:CD1	2.93	0.42
2:B:178:TYR:HB2	2:B:196:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:LEU:HB3	1:D:360:ASN:HB2	2.00	0.42
3:F:129:PHE:O	3:F:133:CYS:SG	2.71	0.42
3:F:188:GLU:O	3:F:190:PRO:HD3	2.20	0.42
2:E:272:PRO:CD	2:E:318:ARG:HE	2.32	0.42
2:E:199:ARG:NH2	2:E:218:LYS:HD3	2.34	0.42
1:A:120:SER:C	1:A:122:SER:N	2.70	0.42
3:F:51:PRO:HA	3:F:278:LEU:O	2.19	0.42
1:D:418:ARG:NH2	3:F:70:ARG:NH2	2.67	0.42
1:A:170:PHE:CE2	1:A:189:LEU:HD12	2.54	0.42
3:C:165:CYS:SG	3:C:238:SER:HB3	2.60	0.42
3:C:88:ASP:OD1	3:C:129:PHE:HB2	2.19	0.42
1:A:218:ASP:O	1:A:222:LEU:HD22	2.19	0.42
2:E:402:LYS:H	2:E:402:LYS:HG3	1.41	0.42
1:A:553:ASN:OD1	1:A:557:GLN:NE2	2.53	0.42
3:C:212:SER:C	3:C:214:ARG:H	2.23	0.42
3:F:81:LEU:CD1	3:F:112:THR:HB	2.50	0.42
3:F:70:ARG:HG3	3:F:70:ARG:NH1	2.35	0.42
3:F:91:TYR:HE1	3:F:135:ARG:NH2	2.18	0.42
2:E:383:ARG:HB3	2:E:383:ARG:HH11	1.85	0.42
1:D:40:LEU:HD23	1:D:79:LEU:HD21	2.01	0.42
2:B:196:ASP:HB3	2:B:197:ASP:H	1.53	0.42
1:A:178:THR:HG21	1:A:180:MET:HB3	2.01	0.42
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.54	0.42
1:A:237:GLN:O	1:A:240:LEU:HG	2.19	0.42
1:A:353:SER:O	1:A:355:ILE:N	2.47	0.42
2:E:425:HIS:CG	2:E:426:PRO:HD2	2.55	0.42
3:C:134:LEU:C	3:C:136:LYS:N	2.73	0.42
1:D:524:THR:HG23	1:D:527:ARG:HH22	1.84	0.42
2:B:393:LYS:O	2:B:394:PRO:C	2.58	0.42
2:B:255:ASP:OD1	2:B:257:ARG:HB2	2.20	0.42
3:F:142:VAL:HA	3:F:145:TYR:CD2	2.54	0.42
1:D:437:GLU:CG	1:D:438:PHE:N	2.82	0.42
3:F:117:ASN:H	3:F:167:HIS:CD2	2.38	0.42
3:C:202:ASP:HB3	3:C:242:GLN:NE2	2.34	0.42
1:A:406:PRO:O	1:A:407:ALA:C	2.59	0.42
2:E:278:ARG:CG	2:E:279:SER:H	2.32	0.42
1:D:268:THR:HG21	1:D:308:GLU:OE1	2.19	0.42
3:C:133:CYS:SG	3:C:143:TRP:HB2	2.60	0.42
1:A:468:LYS:HD3	1:A:471:GLU:OE1	2.20	0.42
3:F:208:GLY:H	3:F:223:ASP:CG	2.23	0.42
1:D:455:VAL:HG13	3:F:71:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HB3	1:A:404:LEU:HD21	2.01	0.41
1:D:433:GLN:O	1:D:434:LEU:HG	2.20	0.41
1:D:317:CYS:O	1:D:318:ARG:C	2.58	0.41
1:D:105:ARG:O	1:D:109:VAL:HG23	2.20	0.41
4:G:2:LEU:H	4:G:7:DAM:C	2.33	0.41
3:F:44:ASN:ND2	3:F:183:LEU:O	2.53	0.41
1:D:248:LEU:O	1:D:248:LEU:HD12	2.20	0.41
2:E:85:ASP:OD1	2:E:88:LYS:HB2	2.20	0.41
2:B:17:VAL:HG13	2:B:440:TYR:CD2	2.55	0.41
1:D:338:ASN:OD1	1:D:340:HIS:HB3	2.19	0.41
2:B:332:LYS:HZ2	2:B:410:VAL:HG11	1.84	0.41
2:B:42:LEU:HD12	2:B:109:GLN:HG2	2.02	0.41
2:E:136:LEU:O	2:E:137:LYS:C	2.58	0.41
2:B:22:ASP:CG	2:B:23:ASP:N	2.74	0.41
1:D:346:ALA:HB1	1:D:384:ILE:CD1	2.50	0.41
3:C:265:TYR:HB3	3:C:269:CYS:HB2	2.01	0.41
2:E:272:PRO:HD2	2:E:318:ARG:HE	1.85	0.41
1:A:352:LEU:O	1:A:355:ILE:HB	2.20	0.41
2:E:172:PHE:HB3	2:E:203:TRP:CZ3	2.55	0.41
3:C:107:TYR:HB3	3:C:110:ARG:HB2	2.01	0.41
3:F:63:HIS:O	3:F:66:MET:HB2	2.21	0.41
1:A:100:GLU:H	1:A:100:GLU:HG3	1.38	0.41
1:A:211:ASN:CA	1:D:8:MET:HE3	2.49	0.41
2:B:370:ASP:HB3	2:B:373:THR:HB	2.03	0.41
1:D:35:LEU:HB2	1:D:72:GLN:HG2	2.02	0.41
3:C:67:GLU:O	3:C:71:ILE:HG12	2.20	0.41
1:D:467:LYS:HE2	1:D:471:GLU:OE2	2.19	0.41
2:B:230:THR:CG2	2:B:288:ILE:O	2.67	0.41
2:B:393:LYS:O	2:B:395:ARG:HD3	2.21	0.41
3:C:86:TYR:CD2	3:C:119:GLU:OE2	2.73	0.41
1:A:348:VAL:C	1:A:350:MET:H	2.23	0.41
1:D:439:PHE:CE1	1:D:477:TRP:HH2	2.38	0.41
3:F:176:THR:HA	3:F:232:ASN:OD1	2.19	0.41
2:B:271:GLU:HG3	2:B:318:ARG:HG2	2.03	0.41
1:D:332:GLU:O	1:D:334:VAL:N	2.53	0.41
3:C:66:MET:HA	3:C:66:MET:HE2	2.02	0.41
2:B:425:HIS:HB2	2:B:430:ILE:HB	2.02	0.41
1:D:514:GLN:O	1:D:514:GLN:HG2	2.20	0.41
3:F:282:LEU:HA	3:F:282:LEU:HD23	1.84	0.41
1:A:439:PHE:HE1	1:A:444:ASN:HA	1.86	0.41
1:D:58:THR:HA	1:D:60:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ASP:C	1:D:285:PRO:HD2	2.40	0.41
1:A:121:PRO:O	1:A:125:GLU:HB2	2.20	0.41
1:A:36:SER:O	1:A:40:LEU:HB2	2.21	0.41
2:E:389:ARG:NH1	2:E:389:ARG:CG	2.82	0.41
2:E:388:PRO:CB	2:E:389:ARG:HE	2.33	0.41
1:A:170:PHE:HE2	1:A:189:LEU:HD12	1.84	0.41
2:B:175:ALA:HB3	2:B:203:TRP:HZ2	1.85	0.41
2:B:23:ASP:HB3	2:B:24:ASP:H	1.71	0.41
2:E:33:THR:HG22	2:E:46:GLY:HA3	2.03	0.41
3:F:245:MET:HA	3:F:271:ASN:HB2	2.03	0.41
2:B:193:LEU:C	2:B:193:LEU:HD12	2.40	0.41
1:A:310:CYS:C	1:A:312:ASN:H	2.23	0.41
2:B:176:HIS:HD1	2:B:196:ASP:CG	2.23	0.41
1:D:291:MET:HB3	1:D:333:LEU:HD11	2.02	0.41
2:E:388:PRO:HB2	2:E:389:ARG:HE	1.85	0.41
2:E:197:ASP:O	2:E:229:ILE:N	2.37	0.41
2:B:339:ASN:OD1	2:B:341:CYS:SG	2.74	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
3:C:199:LEU:N	3:C:199:LEU:CD1	2.84	0.41
3:C:222:GLN:HG3	3:C:252:HIS:CB	2.50	0.41
1:A:77:THR:HG21	1:A:118:GLU:OE1	2.21	0.41
1:D:504:CYS:O	1:D:508:LEU:HG	2.20	0.41
1:D:197:GLU:CD	1:D:197:GLU:H	2.24	0.41
1:D:423:ILE:HG22	1:D:424:ILE:N	2.36	0.41
1:A:552:ASP:O	1:A:556:LEU:HG	2.21	0.41
2:E:272:PRO:HG2	2:E:318:ARG:NH2	2.35	0.41
3:F:159:VAL:HG11	3:F:278:LEU:CD1	2.51	0.41
3:C:117:ASN:HB2	3:C:200:TRP:CE2	2.56	0.41
3:F:202:ASP:OD2	3:F:214:ARG:HG3	2.21	0.41
1:D:256:SER:HB3	1:D:259:VAL:CG2	2.50	0.41
1:D:257:TRP:HD1	2:E:257:ARG:O	2.04	0.41
3:F:229:ASN:ND2	3:F:255:ASN:HB3	2.35	0.41
3:C:10:LEU:HD23	3:C:10:LEU:N	2.34	0.41
1:A:391:VAL:O	1:A:391:VAL:CG1	2.67	0.41
1:D:412:ALA:HB1	1:D:450:TRP:CZ2	2.56	0.41
1:A:197:GLU:CG	1:A:199:ASP:OD1	2.69	0.41
1:D:32:ILE:O	1:D:35:LEU:CD2	2.69	0.41
2:E:315:MET:CE	2:E:318:ARG:HB2	2.51	0.41
2:E:272:PRO:CG	2:E:318:ARG:HE	2.31	0.41
3:F:154:PRO:HA	3:F:185:ARG:HH11	1.83	0.41
3:F:113:ILE:O	3:F:153:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HA	1:A:134:ARG:NH2	2.35	0.41
2:B:333:LEU:N	2:B:333:LEU:CD2	2.83	0.41
2:B:332:LYS:O	2:B:333:LEU:C	2.59	0.41
2:E:231:ALA:HB3	2:E:245:SER:OG	2.21	0.41
1:A:322:ILE:CD1	1:A:355:ILE:HG21	2.51	0.41
2:E:149:VAL:HG12	2:E:149:VAL:O	2.20	0.41
3:C:153:LEU:HA	3:C:154:PRO:HD3	1.88	0.41
3:C:76:PRO:HG3	3:C:107:TYR:CE1	2.56	0.41
2:B:222:MET:HA	2:B:222:MET:HE3	2.02	0.41
1:D:387:ASN:O	1:D:390:CYS:HB3	2.21	0.41
1:A:85:TYR:N	1:A:85:TYR:CD1	2.89	0.41
2:E:301:MET:SD	2:E:357:VAL:CG2	3.09	0.41
1:A:369:PHE:CE1	1:A:384:ILE:HG23	2.56	0.41
2:B:250:THR:HB	2:B:268:LEU:CD1	2.41	0.41
2:E:222:MET:HE3	2:E:222:MET:HA	2.00	0.41
1:A:354:PRO:C	1:A:355:ILE:HG13	2.41	0.41
2:B:244:TYR:OH	2:B:252:ARG:HD2	2.21	0.41
1:A:256:SER:OG	1:A:259:VAL:HG23	2.21	0.41
1:A:8:MET:CE	1:A:10:LEU:HD23	2.51	0.40
1:A:180:MET:CE	1:A:183:ARG:HH21	2.34	0.40
3:C:115:ARG:NH2	3:C:189:VAL:HG23	2.37	0.40
1:D:192:PHE:O	1:D:195:VAL:HG22	2.22	0.40
1:D:586:LEU:O	1:D:587:SER:HB2	2.21	0.40
3:F:204:ASP:OD2	3:F:219:THR:HB	2.21	0.40
3:F:10:LEU:O	3:F:11:ASP:C	2.59	0.40
1:A:221:ARG:O	1:A:222:LEU:C	2.59	0.40
2:E:301:MET:HG2	2:E:348:CYS:SG	2.61	0.40
1:A:388:LEU:O	1:A:389:ASP:C	2.58	0.40
2:B:197:ASP:O	2:B:229:ILE:N	2.44	0.40
1:D:248:LEU:CD2	1:D:270:LEU:HD22	2.52	0.40
2:B:309:LYS:HG3	2:B:309:LYS:O	2.20	0.40
3:C:16:GLN:HG2	3:C:21:LYS:HB2	2.03	0.40
1:D:93:LEU:HA	1:D:93:LEU:HD23	1.98	0.40
1:D:353:SER:C	1:D:355:ILE:N	2.75	0.40
2:B:325:VAL:O	2:B:367:ARG:NE	2.51	0.40
1:D:284:VAL:HB	1:D:285:PRO:HD3	2.04	0.40
1:A:571:GLN:CD	1:A:571:GLN:N	2.64	0.40
3:F:209:TRP:CE2	3:F:224:ILE:HD13	2.56	0.40
1:A:120:SER:O	1:A:121:PRO:C	2.59	0.40
3:F:212:SER:HA	3:F:219:THR:CG2	2.51	0.40
2:E:68:ARG:HB3	2:E:443:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:ND2	1:A:481:THR:HG22	2.37	0.40
1:A:10:LEU:HB2	2:B:149:VAL:HG12	2.03	0.40
1:A:505:ILE:C	1:A:507:VAL:N	2.74	0.40
2:B:47:ASP:OD2	2:B:51:ARG:NH2	2.54	0.40
2:B:221:ASN:HD21	2:B:224:GLU:CG	2.31	0.40
1:D:332:GLU:C	1:D:334:VAL:N	2.75	0.40
1:D:336:ASP:OD2	1:D:341:VAL:HG11	2.22	0.40
2:B:368:MET:CE	2:B:424:TRP:CZ3	3.05	0.40
2:B:261:LEU:HB2	2:B:263:ASP:OD1	2.21	0.40
2:B:111:LEU:C	2:B:111:LEU:HD12	2.42	0.40
3:C:246:GLU:HA	3:C:246:GLU:OE1	2.21	0.40
1:D:25:VAL:HA	1:D:28:ARG:NH1	2.36	0.40
1:D:570:ASP:O	1:D:576:LYS:CE	2.65	0.40
3:F:209:TRP:CD2	3:F:224:ILE:HD13	2.57	0.40
1:A:467:LYS:HB2	1:A:507:VAL:HG12	2.01	0.40
1:D:499:MET:HE1	3:F:77:ASP:O	2.21	0.40
1:D:451:LEU:O	1:D:500:THR:HG21	2.22	0.40
2:B:247:SER:O	2:B:287:SER:HA	2.21	0.40
2:B:186:ASN:HB3	2:B:188:ASP:OD1	2.22	0.40
1:D:361:THR:O	1:D:361:THR:HG22	2.22	0.40
1:A:73:LEU:CD1	1:A:92:PRO:HB2	2.51	0.40
1:A:73:LEU:HD11	1:A:92:PRO:HB2	2.02	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	580/582 (100%)	441 (76%)	110 (19%)	29 (5%)	3	8
1	D	580/582 (100%)	465 (80%)	88 (15%)	27 (5%)	3	9
2	B	413/447 (92%)	368 (89%)	38 (9%)	7 (2%)	11	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	413/447 (92%)	364 (88%)	41 (10%)	8 (2%)	10	32
3	C	286/309 (93%)	246 (86%)	35 (12%)	5 (2%)	11	35
3	F	286/309 (93%)	234 (82%)	40 (14%)	12 (4%)	3	11
4	G	1/7 (14%)	1 (100%)	0	0	100	100
4	H	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2560/2690 (95%)	2120 (83%)	352 (14%)	88 (3%)	5	16

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	157	ARG
1	A	241	GLU
1	A	318	ARG
1	A	558	SER
3	C	207	GLY
1	D	58	THR
1	D	272	LYS
1	D	318	ARG
1	D	558	SER
2	E	66	HIS
2	E	385	ASN
3	F	207	GLY
1	A	44	VAL
1	A	57	ASP
1	A	198	LEU
1	A	237	GLN
1	A	240	LEU
1	A	333	LEU
2	B	66	HIS
2	B	222	MET
2	B	364	ASN
2	B	385	ASN
3	C	135	ARG
3	C	270	GLY
1	D	43	GLY
1	D	44	VAL
1	D	61	ASP
1	D	237	GLN
1	D	333	LEU

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Mol	Chain	Res	Type
2	E	400	SER
3	F	8	LYS
3	F	135	ARG
1	A	61	ASP
1	A	63	ASP
1	A	358	LYS
2	B	67	SER
2	B	411	ASP
1	D	63	ASP
1	D	480	ALA
2	E	389	ARG
3	F	28	VAL
1	A	43	GLY
1	A	121	PRO
1	A	225	VAL
3	C	22	GLN
3	C	280	ASP
1	D	358	LYS
1	D	442	LYS
1	D	473	PHE
1	D	584	THR
2	E	222	MET
3	F	62	PHE
3	F	89	ARG
3	F	186	LEU
1	A	272	LYS
1	A	273	ALA
1	A	473	PHE
1	A	512	CYS
1	D	306	VAL
1	D	401	SER
1	A	355	ILE
1	A	511	VAL
1	A	584	THR
1	D	64	GLU
1	D	233	GLN
1	D	241	GLU
1	D	279	THR
1	D	355	ILE
3	F	29	LYS
3	F	270	GLY
1	D	99	VAL

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Mol	Chain	Res	Type
1	D	482	ILE
3	F	168	GLY
1	A	306	VAL
1	A	349	ILE
1	A	513	GLY
1	D	354	PRO
2	E	149	VAL
2	E	388	PRO
3	F	203	PRO
1	D	511	VAL
1	D	513	GLY
3	F	208	GLY
1	A	482	ILE
1	A	585	VAL
2	B	401	GLY
2	E	401	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	509/509 (100%)	469 (92%)	40 (8%)	15	38
1	D	509/509 (100%)	475 (93%)	34 (7%)	20	47
2	B	386/408 (95%)	357 (92%)	29 (8%)	17	41
2	E	386/408 (95%)	359 (93%)	27 (7%)	19	44
3	C	254/274 (93%)	239 (94%)	15 (6%)	24	54
3	F	254/274 (93%)	242 (95%)	12 (5%)	32	66
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2302/2386 (96%)	2145 (93%)	157 (7%)	20	46

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	19	GLU
1	A	34	LYS
1	A	37	THR
1	A	40	LEU
1	A	45	GLU
1	A	48	ARG
1	A	57	ASP
1	A	58	THR
1	A	63	ASP
1	A	76	PHE
1	A	87	HIS
1	A	100	GLU
1	A	102	THR
1	A	103	VAL
1	A	121	PRO
1	A	141	PHE
1	A	145	THR
1	A	153	VAL
1	A	157	ARG
1	A	177	ASP
1	A	180	MET
1	A	199	ASP
1	A	204	GLU
1	A	209	PHE
1	A	219	SER
1	A	222	LEU
1	A	226	GLU
1	A	238	GLU
1	A	239	ASP
1	A	267	PHE
1	A	404	LEU
1	A	405	LEU
1	A	437	GLU
1	A	439	PHE
1	A	447	CYS
1	A	469	LEU
1	A	495	TYR
1	A	512	CYS
1	A	571	GLN
2	B	8	ASN
2	B	9	ASP
2	B	11	GLN

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Mol	Chain	Res	Type
2	B	14	PHE
2	B	17	VAL
2	B	23	ASP
2	B	47	ASP
2	B	151	THR
2	B	153	ARG
2	B	156	VAL
2	B	161	ASP
2	B	169	ARG
2	B	228	VAL
2	B	230	THR
2	B	234	PHE
2	B	302	THR
2	B	326	HIS
2	B	330	ARG
2	B	333	LEU
2	B	351	ASN
2	B	385	ASN
2	B	386	ASN
2	B	388	PRO
2	B	389	ARG
2	B	403	ARG
2	B	422	THR
2	B	431	ILE
2	B	435	THR
2	B	443	GLN
3	C	12	GLN
3	C	18	ASN
3	C	30	SER
3	C	34	LYS
3	C	40	THR
3	C	49	ARG
3	C	52	VAL
3	C	57	ASP
3	C	110	ARG
3	C	125	GLN
3	C	160	ASP
3	C	173	SER
3	C	239	ARG
3	C	244	VAL
3	C	267	TYR
1	D	9	SER

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Mol	Chain	Res	Type
1	D	16	LEU
1	D	19	GLU
1	D	26	GLN
1	D	28	ARG
1	D	35	LEU
1	D	37	THR
1	D	40	LEU
1	D	58	THR
1	D	76	PHE
1	D	78	THR
1	D	100	GLU
1	D	131	LEU
1	D	141	PHE
1	D	157	ARG
1	D	180	MET
1	D	196	LEU
1	D	204	GLU
1	D	222	LEU
1	D	250	GLN
1	D	267	PHE
1	D	282	ASP
1	D	405	LEU
1	D	423	ILE
1	D	427	MET
1	D	437	GLU
1	D	443	LEU
1	D	444	ASN
1	D	476	GLU
1	D	481	THR
1	D	495	TYR
1	D	539	ASN
1	D	559	GLU
1	D	581	GLU
2	E	8	ASN
2	E	17	VAL
2	E	23	ASP
2	E	81	GLU
2	E	160	MET
2	E	169	ARG
2	E	222	MET
2	E	228	VAL
2	E	272	PRO

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Mol	Chain	Res	Type
2	E	298	ARG
2	E	302	THR
2	E	303	ARG
2	E	316	GLU
2	E	325	VAL
2	E	326	HIS
2	E	357	VAL
2	E	373	THR
2	E	384	GLU
2	E	385	ASN
2	E	387	LYS
2	E	388	PRO
2	E	389	ARG
2	E	390	THR
2	E	395	ARG
2	E	402	LYS
2	E	431	ILE
2	E	435	THR
3	F	34	LYS
3	F	40	THR
3	F	49	ARG
3	F	79	ASN
3	F	110	ARG
3	F	147	THR
3	F	160	ASP
3	F	196	CYS
3	F	236	LEU
3	F	239	ARG
3	F	267	TYR
3	F	282	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	289	ASN
1	A	339	GLN
1	A	514	GLN
1	A	539	ASN
1	A	557	GLN
2	B	11	GLN
2	B	351	ASN

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Mol	Chain	Res	Type
2	B	438	ASN
3	C	16	GLN
3	C	122	GLN
3	C	242	GLN
1	D	230	ASN
1	D	271	GLN
1	D	392	ASN
1	D	402	GLN
1	D	479	HIS
1	D	539	ASN
2	E	11	GLN
2	E	443	GLN
3	F	79	ASN
3	F	125	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	G	1	4	3,4,5	0.56	0	0,4,6	0.00	-
4	ACB	G	3	4	3,8,9	1.11	0	2,10,12	0.68	0
4	1ZN	G	5	4	19,23,24	1.31	2 (10%)	19,29,31	0.94	1 (5%)
4	FGA	G	6	4	5,8,9	1.27	0	2,9,11	0.70	0
4	DAM	G	7	3,4	5,5,6	2.65	2 (40%)	3,5,7	3.09	2 (66%)
4	DAL	H	1	4	3,4,5	0.62	0	0,4,6	0.00	-
4	ACB	H	3	4	3,8,9	1.13	0	2,10,12	0.75	0
4	1ZN	H	5	4	19,23,24	1.39	2 (10%)	19,29,31	0.92	0
4	FGA	H	6	4	5,8,9	1.32	1 (20%)	2,9,11	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DAM	H	7	3,4	5,5,6	3.12	2 (40%)	3,5,7	3.10	2 (66%)

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	G	1	4	-	0/0/2/4	0/0/0/0
4	ACB	G	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	G	5	4	-	0/22/25/27	0/1/1/1
4	FGA	G	6	4	-	0/3/8/9	0/0/0/0
4	DAM	G	7	3,4	-	0/0/4/6	0/0/0/0
4	DAL	H	1	4	-	0/0/2/4	0/0/0/0
4	ACB	H	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	H	5	4	-	0/22/25/27	0/1/1/1
4	FGA	H	6	4	-	0/3/8/9	0/0/0/0
4	DAM	H	7	3,4	-	0/0/4/6	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	CG-CD	2.13	1.55	1.49
4	H	5	1ZN	C9-C4	2.61	1.44	1.38
4	G	5	1ZN	C3-C2	2.82	1.56	1.52
4	G	5	1ZN	C9-C4	2.86	1.44	1.38
4	H	5	1ZN	C3-C2	3.75	1.57	1.52
4	G	7	DAM	C-CA	3.91	1.50	1.45
4	G	7	DAM	CA-N	3.96	1.44	1.34
4	H	7	DAM	CA-N	4.34	1.45	1.34
4	H	7	DAM	C-CA	5.02	1.52	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	DAM	O-C-CA	-4.72	119.84	125.27
4	G	7	DAM	O-C-CA	-4.65	119.92	125.27
4	G	7	DAM	CB-CA-N	-2.62	120.28	126.25
4	H	7	DAM	CB-CA-N	-2.52	120.49	126.25
4	G	5	1ZN	C17-C16-C15	-2.17	120.05	123.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	6	FGA	1	0
4	G	7	DAM	2	0
4	H	5	1ZN	1	0
4	H	7	DAM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	582/582 (100%)	0.62	78 (13%) 4 2	53, 104, 164, 173	0
1	D	582/582 (100%)	0.82	91 (15%) 3 1	48, 100, 173, 188	0
2	B	421/447 (94%)	0.20	15 (3%) 46 39	38, 67, 115, 131	0
2	E	421/447 (94%)	0.08	7 (1%) 73 70	34, 60, 111, 133	0
3	C	288/309 (93%)	0.20	4 (1%) 78 75	60, 88, 119, 154	0
3	F	288/309 (93%)	0.48	21 (7%) 18 12	75, 99, 129, 157	0
4	G	2/7 (28%)	0.84	0 100 100	95, 95, 95, 117	0
4	H	2/7 (28%)	0.21	0 100 100	108, 108, 108, 117	0
All	All	2586/2690 (96%)	0.45	216 (8%) 14 9	34, 88, 161, 188	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	551	LEU	6.9
1	A	511	VAL	6.9
1	D	348	VAL	6.9
1	D	548	GLY	6.5
1	D	556	LEU	6.3
1	A	588	LEU	6.1
1	A	589	ALA	6.0
1	D	549	PRO	5.4
1	D	567	LEU	5.3
1	D	512	CYS	5.3
1	D	515	ASP	5.3
2	B	446	VAL	5.1
1	A	587	SER	4.9
1	D	547	ILE	4.8
1	D	580	GLN	4.8
1	A	395	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	368	LEU	4.7
1	A	481	THR	4.7
2	E	148	THR	4.7
1	A	512	CYS	4.6
1	A	388	LEU	4.6
1	D	553	ASN	4.6
1	D	345	LEU	4.5
1	D	518	THR	4.5
1	D	429	LEU	4.5
1	D	560	VAL	4.5
1	A	586	LEU	4.4
1	D	526	LEU	4.4
1	A	473	PHE	4.4
1	A	352	LEU	4.4
3	F	170	LEU	4.4
1	D	517	THR	4.3
1	D	541	ALA	4.2
1	A	477	TRP	4.1
1	A	466	LEU	4.1
1	D	390	CYS	4.1
3	F	39	LEU	4.0
1	D	550	ILE	4.0
1	A	544	LEU	4.0
1	D	400	LEU	4.0
1	A	349	ILE	4.0
1	D	525	VAL	3.8
1	D	352	LEU	3.7
1	A	508	LEU	3.7
3	F	45	VAL	3.7
1	D	505	ILE	3.6
1	A	431	ALA	3.6
1	A	556	LEU	3.6
1	A	564	LEU	3.6
1	D	516	ILE	3.6
3	F	152	TYR	3.6
1	D	509	SER	3.6
2	B	265	HIS	3.6
1	A	355	ILE	3.6
1	A	480	ALA	3.5
1	D	387	ASN	3.5
1	D	331	LYS	3.5
1	D	554	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	562	PRO	3.5
1	A	505	ILE	3.5
1	D	344	ALA	3.5
3	F	238	SER	3.5
1	D	347	SER	3.4
3	F	158	LEU	3.4
3	F	157	ALA	3.4
1	A	482	ILE	3.4
1	D	365	LEU	3.4
1	A	560	VAL	3.4
3	F	28	VAL	3.4
1	A	469	LEU	3.4
1	D	441	GLU	3.4
1	D	445	SER	3.4
1	D	583	LEU	3.3
3	F	180	ILE	3.3
1	D	394	VAL	3.3
1	D	395	ILE	3.3
3	F	146	PHE	3.3
1	D	544	LEU	3.3
1	D	327	LEU	3.2
1	D	586	LEU	3.2
1	D	589	ALA	3.2
1	A	549	PRO	3.1
1	A	440	ASP	3.1
1	A	443	LEU	3.1
2	B	134	TYR	3.1
1	D	349	ILE	3.1
3	F	225	SER	3.1
1	A	550	ILE	3.1
1	A	479	HIS	3.1
1	A	369	PHE	3.0
2	B	264	ARG	3.0
1	D	399	GLN	3.0
1	D	529	ALA	3.0
1	D	306	VAL	3.0
3	C	91	TYR	2.9
2	B	155	PRO	2.9
1	D	302	ALA	2.9
2	B	131	PRO	2.9
2	B	65	SER	2.9
1	A	551	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	568	THR	2.9
1	D	522	LEU	2.8
1	D	584	THR	2.8
1	A	516	ILE	2.8
1	A	470	VAL	2.8
1	D	563	ILE	2.8
1	D	304	HIS	2.8
1	D	402	GLN	2.8
3	F	229	ASN	2.7
1	A	402	GLN	2.7
2	E	149	VAL	2.7
1	A	270	LEU	2.7
2	E	65	SER	2.7
1	A	439	PHE	2.7
1	D	454	HIS	2.7
1	D	511	VAL	2.7
3	F	198	LEU	2.7
1	A	356	LEU	2.7
1	A	520	HIS	2.7
1	D	447	CYS	2.6
3	F	278	LEU	2.6
2	B	389	ARG	2.6
1	A	274	VAL	2.6
1	D	557	GLN	2.6
1	D	528	MET	2.6
1	A	389	ASP	2.6
1	A	401	SER	2.6
1	D	362	ILE	2.6
1	A	444	ASN	2.6
1	A	358	LYS	2.6
1	A	561	LYS	2.6
1	D	588	LEU	2.6
1	D	545	GLN	2.6
2	E	150	THR	2.6
2	B	386	ASN	2.6
1	A	313	LEU	2.5
1	A	521	MET	2.5
1	A	264	ALA	2.5
1	A	385	ILE	2.5
1	D	356	LEU	2.5
1	A	513	GLY	2.5
1	A	504	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	151	THR	2.5
1	A	433	GLN	2.5
1	D	372	GLN	2.5
1	A	525	VAL	2.4
1	A	373	LEU	2.4
2	B	136	LEU	2.4
1	A	478	ALA	2.4
1	D	540	VAL	2.4
1	A	547	ILE	2.4
2	E	147	THR	2.4
1	A	540	VAL	2.4
1	D	521	MET	2.4
1	A	438	PHE	2.4
1	D	569	GLN	2.4
1	D	565	GLU	2.4
1	D	364	HIS	2.4
1	A	346	ALA	2.4
1	D	538	PHE	2.4
1	D	489	MET	2.4
2	B	443	GLN	2.4
3	C	216	ALA	2.4
1	A	396	GLY	2.4
1	D	343	SER	2.4
3	F	34	LYS	2.4
1	D	404	LEU	2.3
2	B	267	LYS	2.3
1	A	447	CYS	2.3
1	A	240	LEU	2.3
1	A	405	LEU	2.3
3	F	177	LEU	2.3
1	D	350	MET	2.3
1	D	431	ALA	2.3
1	D	305	LYS	2.3
1	D	334	VAL	2.3
1	D	527	ARG	2.3
1	D	346	ALA	2.3
1	A	472	LYS	2.3
1	A	548	GLY	2.3
2	B	59	GLN	2.3
1	A	559	GLU	2.2
3	F	136	LYS	2.2
1	D	432	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	578	PHE	2.2
2	E	265	HIS	2.2
1	A	517	THR	2.2
1	D	274	VAL	2.2
3	F	140	ALA	2.2
1	D	578	PHE	2.2
1	D	564	LEU	2.2
1	A	292	LYS	2.2
1	D	449	ALA	2.2
2	B	149	VAL	2.2
1	D	444	ASN	2.1
1	A	484	PRO	2.1
1	A	579	ALA	2.1
2	B	127	ARG	2.1
1	A	268	THR	2.1
1	D	367	PRO	2.1
1	A	263	VAL	2.1
3	C	58	VAL	2.1
3	F	164	PHE	2.1
1	D	375	ASP	2.1
3	C	8	LYS	2.1
1	D	388	LEU	2.1
1	D	558	SER	2.1
1	A	487	LEU	2.1
1	A	583	LEU	2.1
1	A	322	ILE	2.0
1	A	345	LEU	2.0
3	F	23	LEU	2.0
1	D	496	LEU	2.0
3	F	260	PHE	2.0
1	A	450	TRP	2.0
1	D	514	GLN	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( $\text{\AA}^2$ )	Q<0.9
4	DAL	H	1	5/6	0.94	0.17	-	108,108,110,112	0
4	ACB	H	3	9/10	0.90	0.21	-	108,111,113,113	0
4	DAM	G	7	6/7	0.95	0.09	-	99,101,102,104	0
4	FGA	G	6	9/10	0.85	0.35	-	100,101,106,107	0
4	DAM	H	7	6/7	0.94	0.12	-	112,113,116,116	0
4	DAL	G	1	5/6	0.97	0.17	-	92,94,96,98	0
4	1ZN	G	5	23/24	0.92	0.33	-	99,102,106,107	0
4	ACB	G	3	9/10	0.97	0.23	-	93,95,102,104	0
4	1ZN	H	5	23/24	0.90	0.28	-	106,109,113,115	0
4	FGA	H	6	9/10	0.84	0.24	-	102,111,118,118	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( $\text{\AA}^2$ )	Q<0.9
5	MN	C	501	1/1	0.99	0.19	0.86	69,69,69,69	0
5	MN	F	511	1/1	0.96	0.19	0.58	82,82,82,82	0
5	MN	C	502	1/1	0.98	0.12	-1.15	69,69,69,69	0
5	MN	F	512	1/1	0.98	0.10	-1.18	91,91,91,91	0

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

There are no such residues in this entry.