



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TT5  
Title : Structure of APPBP1-UBA3-Ubc12N26: a unique E1-E2 interaction required for optimal conjugation of the ubiquitin-like protein NEDD8  
Authors : Huang, D.T.; Miller, D.W.; Mathew, R.; Cassell, R.; Holton, J.M.; Roussel, M.F.; Schulman, B.A.  
Deposited on : 2004-06-21  
Resolution : 2.60 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

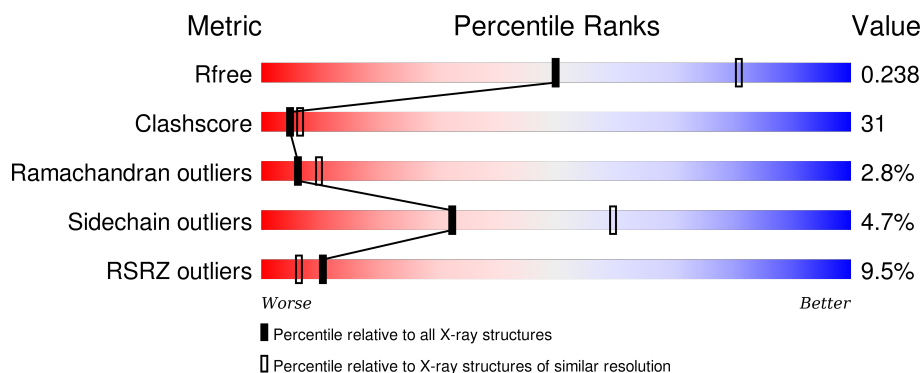
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



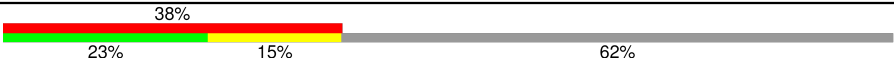
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	531	<div> <div>5%</div> <div>56% 38% . . .</div> </div>
1	C	531	<div> <div>8%</div> <div>50% 41% 5% . .</div> </div>
2	B	434	<div> <div>4%</div> <div>59% 33% . 5%</div> </div>
2	D	434	<div> <div>18%</div> <div>48% 39% . 9%</div> </div>
3	E	26	<div> <div>8%</div> <div>42% 8% 50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	26	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (23%), red (38%), and yellow (15%). A grey bar extends to the right, labeled 62%.

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14637 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 amyloid protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	4	0	0
			4108	2600	701	792	15			
1	C	512	Total	C	N	O	S	4	0	0
			4020	2546	684	775	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	GB 4502169
A	0	SER	-	CLONING ARTIFACT	GB 4502169
A	?	-	ASN	DELETION	GB 4502169
A	?	-	GLU	DELETION	GB 4502169
A	?	-	ASN	DELETION	GB 4502169
A	?	-	GLY	DELETION	GB 4502169
A	?	-	ALA	DELETION	GB 4502169
C	-1	GLY	-	CLONING ARTIFACT	GB 4502169
C	0	SER	-	CLONING ARTIFACT	GB 4502169
C	?	-	ASN	DELETION	GB 4502169
C	?	-	GLU	DELETION	GB 4502169
C	?	-	ASN	DELETION	GB 4502169
C	?	-	GLY	DELETION	GB 4502169
C	?	-	ALA	DELETION	GB 4502169

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	0	0
			3152	2010	540	584	18			
2	D	395	Total	C	N	O	S	12	0	0
			2866	1806	503	540	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	CLONING ARTIFACT	GB 38045942
B	10	LYS	-	CLONING ARTIFACT	GB 38045942
B	11	LEU	-	CLONING ARTIFACT	GB 38045942
D	9	MET	-	CLONING ARTIFACT	GB 38045942
D	10	LYS	-	CLONING ARTIFACT	GB 38045942
D	11	LEU	-	CLONING ARTIFACT	GB 38045942

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total 108	C 72	N 19	O 16	S 1	2	0	0
3	F	10	Total 83	C 55	N 15	O 13		9	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

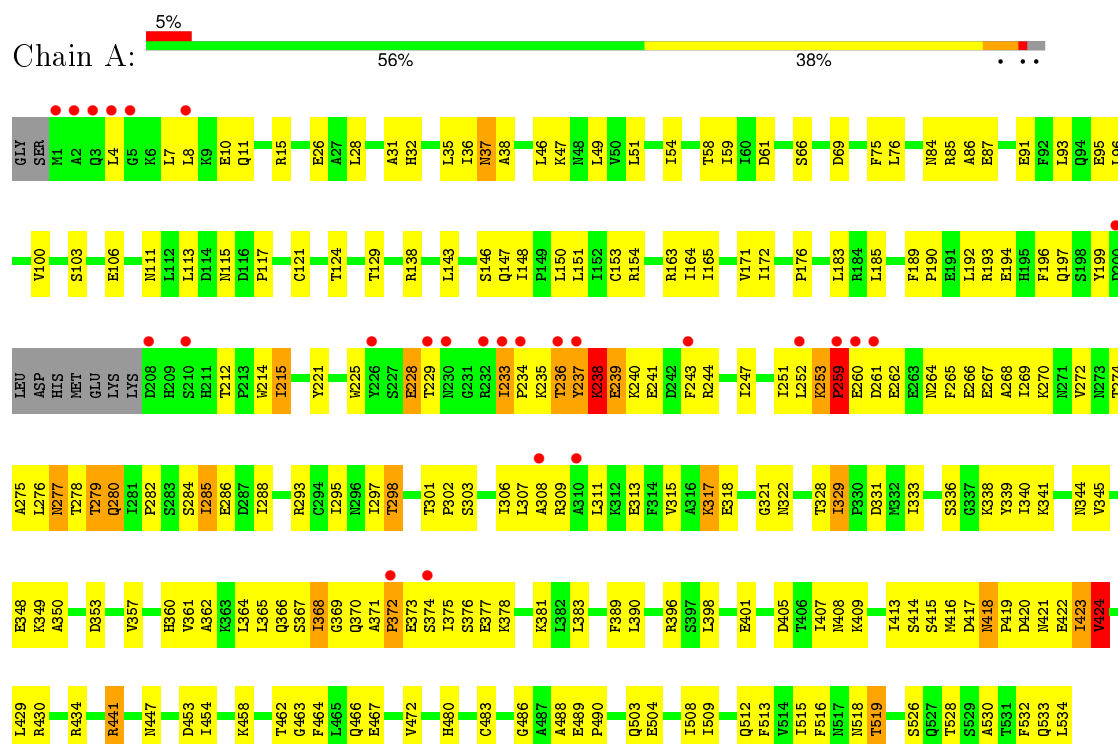
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	114	Total	O	0	0
			114	114		
5	C	45	Total	O	0	0
			45	45		
5	D	29	Total	O	0	0
			29	29		
5	E	5	Total	O	0	0
			5	5		

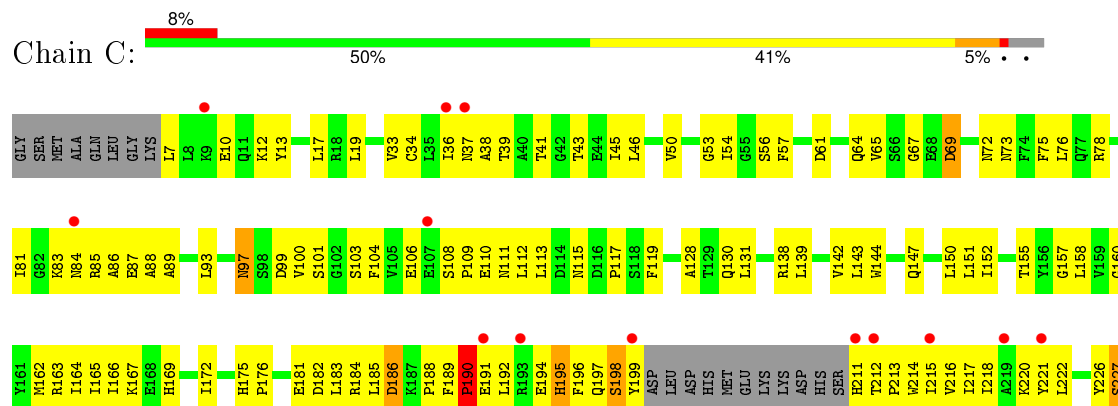
### 3 Residue-property plots

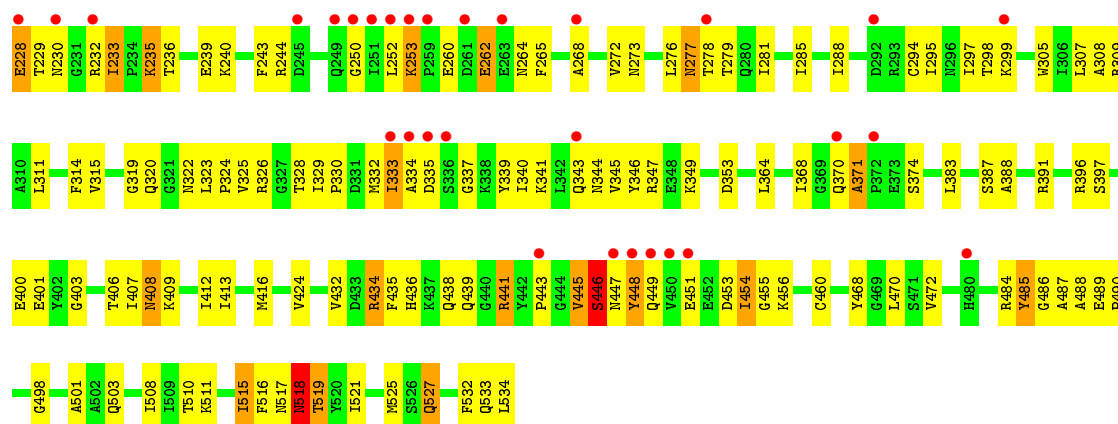
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: amyloid protein-binding protein 1

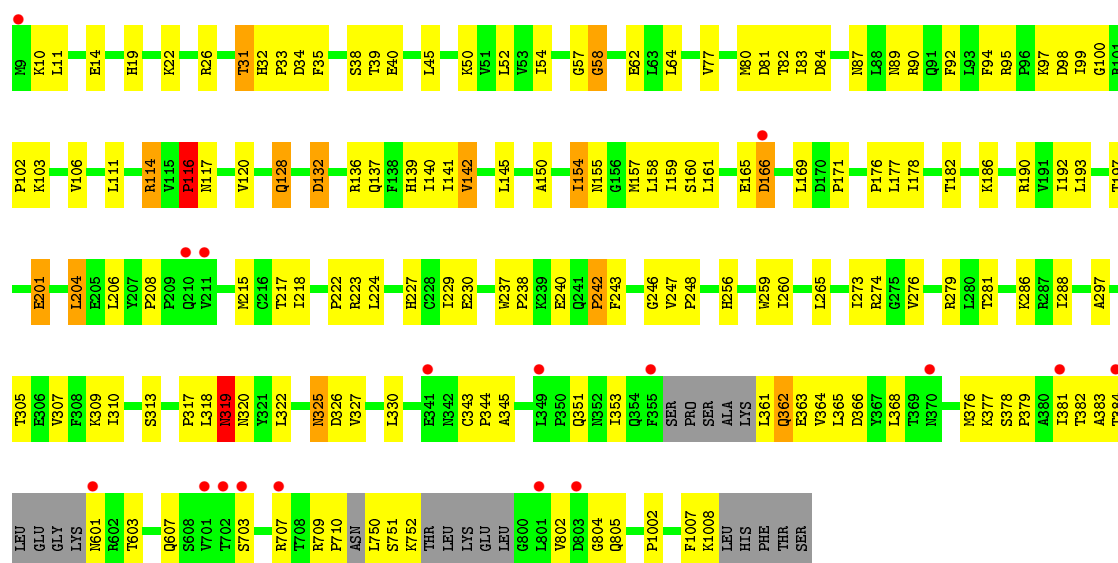


- Molecule 1: amyloid protein-binding protein 1

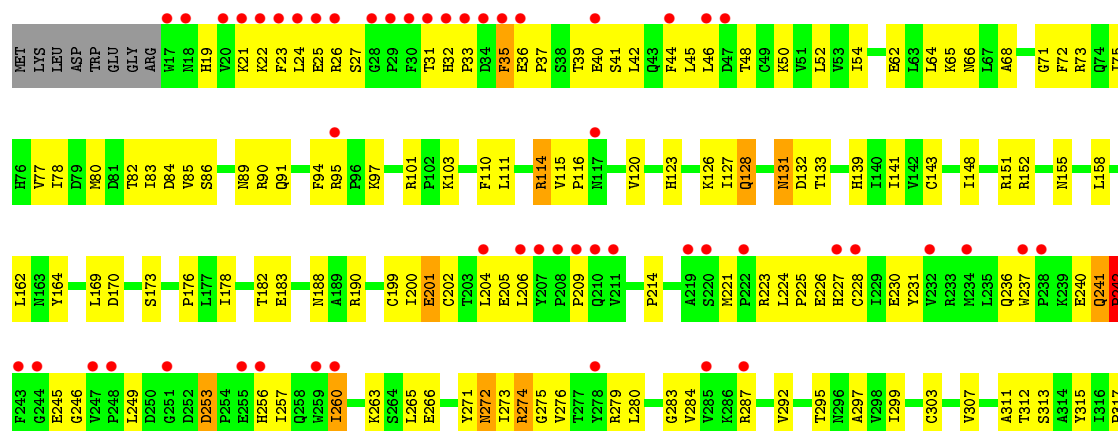


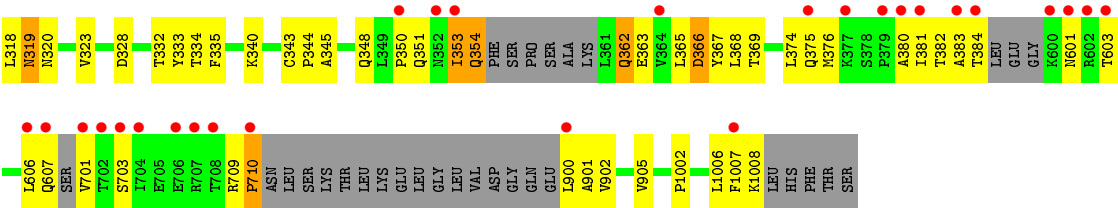


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1

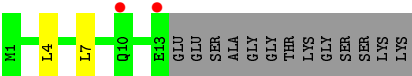
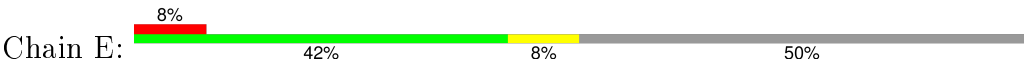


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1

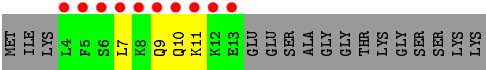




● Molecule 3: Ubiquitin-conjugating enzyme E2 M



● Molecule 3: Ubiquitin-conjugating enzyme E2 M





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.41Å 122.77Å 195.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60 18.10 – 2.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.00-2.60) 98.9 (18.10-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.237 , 0.279 0.238 , 0.238	Depositor DCC
$R_{free}$ test set	3377 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 67222 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.44	1/4187 (0.0%)	0.69	9/5664 (0.2%)
1	C	0.34	0/4099	0.59	0/5547
2	B	0.42	0/3219	0.69	3/4380 (0.1%)
2	D	0.41	0/2923	0.74	4/3962 (0.1%)
3	E	0.37	0/108	0.50	0/139
3	F	0.63	0/83	0.83	0/107
All	All	0.40	1/14619 (0.0%)	0.67	16/19799 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TYR	CB-CG	-5.14	1.44	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ASP	CB-CG-OD2	-11.96	107.54	118.30
1	A	233	ILE	N-CA-C	8.36	133.57	111.00
1	A	279	THR	N-CA-C	-7.06	91.94	111.00
2	D	710	PRO	N-CA-CB	6.54	111.15	103.30
1	A	239	GLU	N-CA-C	-6.06	94.63	111.00
1	A	260	GLU	N-CA-C	-5.93	94.98	111.00
2	B	710	PRO	N-CA-CB	5.57	109.99	103.30
1	A	260	GLU	CB-CA-C	5.56	121.52	110.40
1	A	519	THR	N-CA-C	5.52	125.89	111.00
2	D	1002	PRO	N-CA-CB	5.51	109.91	103.30
2	D	253	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	238	LYS	N-CA-C	5.28	125.27	111.00
2	B	319	ASN	N-CA-C	-5.12	97.18	111.00
1	A	259	PRO	CA-N-CD	-5.10	104.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	VAL	CB-CA-C	-5.05	101.80	111.40
2	B	1002	PRO	N-CA-CB	5.01	109.31	103.30

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	4108	0	4038	288	0
1	C	4020	0	3937	264	0
2	B	3152	0	2998	165	0
2	D	2866	0	2608	212	0
3	E	108	0	128	3	0
3	F	83	0	92	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	105	0	0	12	0
5	B	114	0	0	9	0
5	C	45	0	0	4	0
5	D	29	0	0	3	0
5	E	5	0	0	0	0
All	All	14637	0	13801	882	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 31.

All (882) 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:518:ASN:ND2	1:A:534:LEU:H	1.07	1.41
1:A:518:ASN:ND2	1:A:534:LEU:N	1.76	1.31
1:A:225:TRP:NE1	1:A:233:ILE:HD11	1.58	1.19
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.19	1.18
1:A:235:LYS:HB2	1:A:239:GLU:HG3	1.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:ILE:HG12	2:D:1008:LYS:HA	1.38	1.06
2:B:111:LEU:HD23	2:B:120:VAL:HG21	1.36	1.05
2:D:249:LEU:HD11	2:D:256:HIS:HB3	1.40	1.03
1:A:434:ARG:HH12	1:A:463:GLY:HA3	1.21	1.02
1:C:214:TRP:HA	1:C:217:ILE:HD13	1.38	1.02
1:A:396:ARG:NH1	1:A:408:ASN:HD21	1.57	1.01
1:A:489:GLU:H	2:B:19:HIS:CD2	1.79	1.00
1:A:518:ASN:HD21	1:A:534:LEU:N	1.48	0.99
2:D:155:ASN:HB2	2:D:200:ILE:HD12	1.42	0.99
1:A:236:THR:O	1:A:240:LYS:HB2	1.60	0.99
2:D:83:ILE:HD13	2:D:103:LYS:HG2	1.44	0.98
1:A:396:ARG:HH12	1:A:408:ASN:HD21	0.98	0.98
1:A:396:ARG:HH12	1:A:408:ASN:ND2	1.61	0.97
1:A:259:PRO:HB3	1:A:261:ASP:CG	1.84	0.97
2:B:128:GLN:H	2:B:128:GLN:HE21	0.97	0.97
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.45	0.96
1:A:278:THR:HG22	1:A:279:THR:O	1.67	0.95
1:A:172:ILE:HD13	1:A:390:LEU:HD22	1.46	0.94
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.13	0.94
1:C:244:ARG:HH21	1:C:273:ASN:HB2	1.31	0.94
1:C:143:LEU:HD12	1:C:150:LEU:HD22	1.48	0.94
1:A:233:ILE:HG23	1:A:239:GLU:HB2	1.48	0.94
1:C:489:GLU:H	2:D:19:HIS:CD2	1.85	0.94
2:D:249:LEU:HD11	2:D:256:HIS:CB	1.99	0.93
2:D:353:ILE:CG1	2:D:1008:LYS:HA	1.97	0.93
1:A:235:LYS:CB	1:A:239:GLU:HG3	1.98	0.92
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.51	0.92
1:A:244:ARG:HG2	1:A:272:VAL:HG11	1.52	0.92
1:A:489:GLU:H	2:B:19:HIS:HD2	0.94	0.91
2:D:27:SER:HA	2:D:35:PHE:HZ	1.35	0.90
1:A:251:ILE:CG2	1:A:259:PRO:HB2	2.00	0.90
2:D:95:ARG:HD2	2:D:97:LYS:HE2	1.54	0.90
1:A:251:ILE:O	1:A:259:PRO:HG2	1.72	0.90
1:C:489:GLU:H	2:D:19:HIS:HD2	1.18	0.90
1:A:46:LEU:CD2	1:A:59:ILE:HD11	2.00	0.90
2:D:31:THR:HG21	2:D:35:PHE:CG	2.08	0.89
2:D:50:LYS:H	2:D:139:HIS:HD2	1.17	0.89
2:D:249:LEU:CD1	2:D:256:HIS:HB3	2.02	0.89
1:A:225:TRP:HE1	1:A:233:ILE:HD11	1.35	0.88
2:B:84:ASP:H	2:B:87:ASN:ND2	1.69	0.88
1:A:243:PHE:O	1:A:247:ILE:HD13	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:HD22	1:A:534:LEU:N	1.57	0.88
2:D:253:ASP:CG	2:D:256:HIS:HB2	1.93	0.88
1:A:251:ILE:O	1:A:259:PRO:HD2	1.73	0.87
1:A:35:LEU:HD23	1:A:59:ILE:HD12	1.55	0.87
1:A:447:ASN:ND2	2:B:26:ARG:HH21	1.72	0.87
2:D:295:THR:O	2:D:299:ILE:HD12	1.75	0.87
2:B:223:ARG:H	2:B:227:HIS:HD2	1.23	0.87
1:A:518:ASN:HD22	1:A:533:GLN:CA	1.87	0.86
1:A:233:ILE:HG22	1:A:233:ILE:O	1.73	0.86
1:A:236:THR:CA	1:A:240:LYS:HD2	2.04	0.86
1:C:311:LEU:HD21	1:C:387:SER:HB2	1.55	0.85
2:B:128:GLN:H	2:B:128:GLN:NE2	1.72	0.85
1:C:41:THR:O	1:C:45:ILE:HD13	1.75	0.85
1:C:307:LEU:HD22	1:C:383:LEU:HD22	1.57	0.85
2:D:368:LEU:O	2:D:376:MET:HG2	1.75	0.85
2:D:83:ILE:CD1	2:D:103:LYS:HG2	2.07	0.85
1:C:515:ILE:H	1:C:515:ILE:HD13	1.40	0.84
1:A:518:ASN:HD22	1:A:533:GLN:HA	1.41	0.84
1:A:434:ARG:NH1	1:A:463:GLY:HA3	1.92	0.84
1:C:130:GLN:HE22	1:C:155:THR:H	1.24	0.84
2:D:353:ILE:HG12	2:D:1008:LYS:CA	2.08	0.84
1:A:266:GLU:OE1	1:A:269:ILE:HD12	1.78	0.84
1:A:183:LEU:HD13	1:A:215:ILE:HD11	1.60	0.84
2:D:353:ILE:HG22	2:D:354:GLN:H	1.42	0.83
1:A:518:ASN:HD21	1:A:534:LEU:H	0.84	0.83
2:D:27:SER:HA	2:D:35:PHE:CZ	2.13	0.83
2:B:128:GLN:HE21	2:B:128:GLN:N	1.77	0.83
1:A:228:GLU:HG2	1:A:229:THR:H	1.43	0.83
2:D:84:ASP:OD2	2:D:86:SER:OG	1.96	0.82
1:A:454:ILE:HD12	1:A:480:HIS:HA	1.60	0.82
1:C:438:GLN:HG2	1:C:439:GLN:HE22	1.45	0.82
2:D:83:ILE:HD11	2:D:103:LYS:HA	1.61	0.81
1:C:484:ARG:HA	2:D:26:ARG:NH1	1.96	0.81
1:C:438:GLN:HG2	1:C:439:GLN:NE2	1.96	0.81
2:D:353:ILE:H	2:D:353:ILE:HD12	1.45	0.81
1:C:489:GLU:N	2:D:19:HIS:HD2	1.79	0.80
1:A:225:TRP:CE2	1:A:233:ILE:HD11	2.17	0.80
2:D:32:HIS:O	2:D:35:PHE:HB3	1.80	0.80
1:C:449:GLN:HB3	1:C:453:ASP:OD2	1.81	0.80
1:A:251:ILE:O	1:A:259:PRO:CG	2.30	0.80
2:B:32:HIS:HD2	2:B:34:ASP:H	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:THR:HG21	2:D:35:PHE:CD2	2.17	0.80
1:A:274:THR:O	1:A:277:ASN:ND2	2.15	0.79
1:A:454:ILE:CD1	1:A:480:HIS:HA	2.12	0.79
1:A:251:ILE:HG22	1:A:259:PRO:HB2	1.63	0.78
1:C:484:ARG:HA	2:D:26:ARG:HH11	1.48	0.78
1:A:251:ILE:O	1:A:259:PRO:CD	2.31	0.78
2:D:253:ASP:OD2	2:D:256:HIS:CD2	2.36	0.78
2:D:46:LEU:HA	2:D:71:GLY:O	1.83	0.78
2:D:31:THR:HG22	2:D:32:HIS:N	1.99	0.77
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.49	0.77
1:A:241:GLU:HA	1:A:244:ARG:HH11	1.50	0.77
1:A:447:ASN:HD22	2:B:26:ARG:NH2	1.82	0.77
2:D:249:LEU:CD2	2:D:260:ILE:HD11	2.15	0.77
2:B:318:LEU:O	2:B:319:ASN:O	2.01	0.77
1:A:251:ILE:HG23	1:A:259:PRO:HB2	1.67	0.77
2:B:31:THR:HG23	2:B:35:PHE:HB3	1.67	0.77
2:B:703:SER:O	2:B:707:ARG:N	2.18	0.76
1:A:454:ILE:HD13	1:A:483:CYS:SG	2.26	0.76
1:A:252:LEU:C	1:A:259:PRO:HD2	2.06	0.76
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.66	0.76
1:A:113:LEU:O	1:A:117:PRO:HG3	1.85	0.75
1:A:237:TYR:O	1:A:241:GLU:HB3	1.86	0.75
2:D:260:ILE:N	2:D:260:ILE:HD13	2.01	0.75
1:A:233:ILE:HD13	1:A:233:ILE:N	2.02	0.75
1:A:518:ASN:HD22	1:A:533:GLN:C	1.89	0.75
2:D:42:LEU:HG	2:D:46:LEU:HD11	1.67	0.75
2:B:243:PHE:O	2:B:247:VAL:HG21	1.88	0.74
2:D:362:GLN:O	2:D:366:ASP:HB2	1.85	0.74
2:D:363:GLU:O	2:D:367:TYR:HB3	1.86	0.74
1:A:518:ASN:HD22	1:A:534:LEU:H	1.18	0.74
1:A:240:LYS:O	1:A:244:ARG:HG3	1.87	0.74
1:C:298:THR:HG22	1:C:299:LYS:H	1.51	0.74
1:C:454:ILE:HG23	1:C:455:GLY:H	1.51	0.74
1:A:4:LEU:O	1:A:8:LEU:HB2	1.88	0.74
1:A:423:ILE:O	1:A:423:ILE:HD13	1.87	0.74
1:A:518:ASN:HB3	1:A:532:PHE:O	1.86	0.74
1:C:45:ILE:HD12	1:C:498:GLY:HA2	1.69	0.73
2:D:170:ASP:O	2:D:173:SER:HB3	1.87	0.73
1:A:409:LYS:O	1:A:413:ILE:HG12	1.88	0.73
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.18	0.73
1:A:518:ASN:CG	1:A:519:THR:H	1.90	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:GLY:N	5:B:1015:HOH:O	2.22	0.73
1:A:172:ILE:HD13	1:A:390:LEU:CD2	2.19	0.72
2:D:295:THR:HG22	2:D:299:ILE:HD11	1.72	0.72
1:A:163:ARG:NH1	1:A:401:GLU:OE2	2.22	0.72
1:A:282:PRO:HB2	1:A:285:ILE:CD1	2.11	0.72
1:C:339:TYR:HE2	2:D:224:LEU:HD21	1.53	0.72
2:D:380:ALA:O	2:D:902:VAL:HA	1.89	0.72
1:A:84:ASN:ND2	1:A:87:GLU:H	1.87	0.72
1:A:489:GLU:N	2:B:19:HIS:HD2	1.80	0.72
1:A:253:LYS:N	1:A:259:PRO:CD	2.53	0.71
1:C:412:ILE:HD11	1:C:534:LEU:HD22	1.70	0.71
1:C:515:ILE:N	1:C:515:ILE:HD13	2.06	0.71
1:A:235:LYS:HG2	1:A:239:GLU:OE2	1.90	0.71
1:A:236:THR:O	1:A:240:LYS:CB	2.35	0.71
1:A:306:ILE:HD11	1:A:370:GLN:HE22	1.55	0.70
5:A:573:HOH:O	2:B:186:LYS:HE3	1.91	0.70
1:C:434:ARG:HH11	1:C:434:ARG:HG2	1.56	0.70
2:D:295:THR:HG22	2:D:299:ILE:CD1	2.21	0.70
1:A:518:ASN:HD21	1:A:534:LEU:CA	2.05	0.69
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.74	0.69
1:C:281:ILE:HD12	1:C:323:LEU:HG	1.73	0.69
1:A:340:ILE:HD11	2:B:273:ILE:CD1	2.22	0.69
1:C:262:GLU:HB2	1:C:264:ASN:OD1	1.92	0.69
1:C:222:LEU:HG	1:C:226:TYR:CE2	2.27	0.69
2:B:32:HIS:CD2	2:B:34:ASP:H	2.11	0.69
1:A:253:LYS:N	1:A:259:PRO:HD2	2.08	0.69
2:D:78:ILE:HD13	2:D:123:HIS:HB2	1.75	0.68
1:C:217:ILE:H	1:C:217:ILE:HD12	1.56	0.68
1:A:285:ILE:N	1:A:285:ILE:HD12	2.08	0.68
1:A:233:ILE:HG23	1:A:239:GLU:CB	2.21	0.68
1:C:518:ASN:O	1:C:532:PHE:O	2.11	0.68
1:C:46:LEU:HD23	1:C:93:LEU:HD13	1.76	0.68
2:B:237:TRP:O	2:B:240:GLU:O	2.11	0.68
2:D:65:LYS:HE3	2:D:66:ASN:OD1	1.93	0.68
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.29	0.68
2:D:353:ILE:HG13	2:D:1007:PHE:O	1.94	0.67
1:A:228:GLU:HG2	1:A:229:THR:N	2.08	0.67
1:A:344:ASN:O	1:A:348:GLU:HG2	1.94	0.67
2:D:201:GLU:HG2	2:D:345:ALA:HB2	1.75	0.67
1:C:253:LYS:HE3	1:C:260:GLU:OE2	1.94	0.67
2:D:237:TRP:CH2	2:D:249:LEU:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:HB2	5:A:605:HOH:O	1.94	0.67
1:A:297:ILE:HG22	1:A:298:THR:N	2.10	0.67
1:A:279:THR:HG22	1:A:322:ASN:ND2	2.09	0.67
1:C:10:GLU:HG3	2:D:279:ARG:HH12	1.60	0.67
1:C:13:TYR:O	1:C:17:LEU:HG	1.93	0.67
2:B:256:HIS:O	2:B:260:ILE:HG12	1.95	0.66
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.77	0.66
1:A:462:THR:O	1:A:466:GLN:HG3	1.95	0.66
2:D:83:ILE:HD12	2:D:94:PHE:CE1	2.30	0.66
1:C:328:THR:C	1:C:329:ILE:HD12	2.15	0.66
2:D:353:ILE:HG22	2:D:354:GLN:N	2.10	0.66
1:A:46:LEU:HD22	1:A:59:ILE:HD11	1.77	0.66
2:D:201:GLU:O	2:D:204:LEU:HG	1.96	0.66
2:D:50:LYS:H	2:D:139:HIS:CD2	2.08	0.66
1:A:7:LEU:O	1:A:11:GLN:HG3	1.96	0.66
1:C:244:ARG:NH2	1:C:273:ASN:HB2	2.06	0.66
1:C:164:ILE:HD11	1:C:508:ILE:HD11	1.76	0.66
1:A:240:LYS:HG2	1:A:276:LEU:HD12	1.78	0.65
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.78	0.65
2:D:45:LEU:HD11	2:D:72:PHE:CZ	2.30	0.65
1:C:515:ILE:H	1:C:515:ILE:CD1	2.08	0.65
2:D:201:GLU:HA	2:D:204:LEU:CD2	2.26	0.65
2:B:318:LEU:O	2:B:319:ASN:C	2.34	0.65
1:C:297:ILE:HD12	1:C:297:ILE:O	1.97	0.65
1:C:486:GLY:HA3	2:D:22:LYS:NZ	2.11	0.65
1:C:400:GLU:O	1:C:406:THR:HG23	1.97	0.65
1:C:37:ASN:C	1:C:39:THR:H	1.99	0.65
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.78	0.65
1:A:269:ILE:O	1:A:272:VAL:HG12	1.96	0.65
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.79	0.65
1:A:518:ASN:OD1	1:A:519:THR:N	2.30	0.65
1:C:341:LYS:O	1:C:345:VAL:HG23	1.97	0.65
2:D:201:GLU:HA	2:D:204:LEU:HD21	1.77	0.65
1:A:267:GLU:HA	1:A:270:LYS:HE2	1.79	0.64
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.78	0.64
1:A:235:LYS:CG	1:A:239:GLU:OE2	2.45	0.64
1:C:297:ILE:HD13	1:C:368:ILE:HD11	1.79	0.64
2:B:57:GLY:C	5:B:1015:HOH:O	2.35	0.64
2:D:249:LEU:HD22	2:D:260:ILE:HD11	1.79	0.64
1:C:232:ARG:C	1:C:233:ILE:HD13	2.18	0.64
1:A:278:THR:HG22	1:A:279:THR:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HD3	1:A:238:LYS:O	1.98	0.64
1:A:447:ASN:ND2	2:B:26:ARG:HE	1.95	0.64
2:D:31:THR:CG2	2:D:35:PHE:CG	2.78	0.64
2:D:42:LEU:O	2:D:46:LEU:HG	1.98	0.64
1:C:281:ILE:CD1	1:C:323:LEU:HG	2.28	0.64
1:A:251:ILE:HG23	1:A:261:ASP:HB2	1.80	0.63
2:D:381:ILE:HA	2:D:901:ALA:O	1.98	0.63
1:A:228:GLU:CG	1:A:229:THR:N	2.61	0.63
1:C:347:ARG:NH1	2:D:274:ARG:HG3	2.13	0.63
1:C:7:LEU:HD23	5:C:560:HOH:O	1.97	0.63
2:D:46:LEU:O	2:D:73:ARG:HB2	1.98	0.63
1:C:184:ARG:CZ	1:C:325:VAL:HG12	2.28	0.63
1:C:215:ILE:HG13	1:C:332:MET:CE	2.28	0.63
1:C:163:ARG:NH1	1:C:401:GLU:OE2	2.32	0.63
3:F:10:GLN:HG2	3:F:11:LYS:H	1.64	0.63
2:B:54:ILE:HD12	2:B:54:ILE:N	2.13	0.63
1:C:236:THR:HG22	1:C:239:GLU:H	1.64	0.63
1:A:49:LEU:HB3	1:A:54:ILE:HD12	1.78	0.63
1:C:138:ARG:O	1:C:142:VAL:HG23	1.98	0.63
1:A:259:PRO:HB3	1:A:261:ASP:OD2	1.99	0.62
2:D:182:THR:OG1	2:D:299:ILE:HD13	1.98	0.62
2:D:42:LEU:HG	2:D:46:LEU:CD1	2.30	0.62
2:B:155:ASN:O	2:B:159:ILE:HG12	1.99	0.62
2:B:32:HIS:HD2	2:B:34:ASP:N	1.98	0.62
2:D:318:LEU:HD11	2:D:334:THR:HG23	1.81	0.62
2:D:353:ILE:HG12	2:D:1008:LYS:CB	2.29	0.62
1:A:357:VAL:O	1:A:361:VAL:HG23	2.00	0.61
1:C:525:MET:HG3	2:D:315:TYR:CE2	2.34	0.61
1:A:284:SER:O	1:A:288:ILE:HG12	1.98	0.61
1:A:46:LEU:HD21	1:A:59:ILE:HD11	1.79	0.61
1:A:121:CYS:HA	1:A:148:ILE:HD11	1.81	0.61
2:D:253:ASP:OD2	2:D:256:HIS:HB2	2.00	0.61
2:B:242:PRO:HG3	2:B:259:TRP:CZ2	2.35	0.61
1:C:294:CYS:O	1:C:309:ARG:HD2	1.99	0.61
1:A:235:LYS:CG	1:A:239:GLU:HG3	2.29	0.61
1:A:336:SER:O	1:A:340:ILE:HG12	1.99	0.61
2:B:274:ARG:HG3	5:B:1104:HOH:O	2.00	0.61
1:A:236:THR:C	1:A:240:LYS:HB2	2.20	0.61
1:A:193:ARG:O	1:A:197:GLN:HG3	2.00	0.61
2:B:223:ARG:O	2:B:273:ILE:HD12	2.00	0.61
1:A:458:LYS:O	1:A:458:LYS:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:THR:HG23	2:B:39:THR:O	1.99	0.61
1:A:516:PHE:CD1	1:A:518:ASN:O	2.53	0.61
1:A:84:ASN:HD21	1:A:86:ALA:HB3	1.66	0.61
1:C:340:ILE:O	1:C:344:ASN:ND2	2.34	0.61
1:C:451:GLU:HG3	1:C:451:GLU:O	2.00	0.61
1:C:213:PRO:HB2	1:C:216:VAL:HG23	1.83	0.60
1:C:199:TYR:HB2	1:C:220:LYS:HE2	1.83	0.60
1:C:486:GLY:HA3	2:D:22:LYS:HZ3	1.67	0.60
1:C:37:ASN:HB3	1:C:39:THR:HG23	1.84	0.60
1:A:418:ASN:ND2	1:A:420:ASP:H	2.00	0.60
1:A:259:PRO:HB3	1:A:261:ASP:CB	2.31	0.60
1:C:525:MET:HG3	2:D:315:TYR:CD2	2.35	0.60
1:C:78:ARG:HD2	1:C:81:ILE:HD11	1.82	0.60
1:C:54:ILE:O	1:C:54:ILE:HD12	2.02	0.60
2:D:350:PRO:HB3	2:D:1006:LEU:O	2.02	0.60
1:A:259:PRO:O	1:A:261:ASP:N	2.34	0.60
1:C:347:ARG:HH12	2:D:274:ARG:HG3	1.67	0.60
2:D:318:LEU:O	2:D:319:ASN:C	2.39	0.60
1:A:333:ILE:HD13	2:B:223:ARG:NH2	2.16	0.60
2:D:226:GLU:H	2:D:226:GLU:CD	2.05	0.60
2:D:237:TRP:CZ2	2:D:249:LEU:HB2	2.37	0.60
1:C:226:TYR:CE1	1:C:233:ILE:HG23	2.36	0.60
2:D:182:THR:CG2	2:D:183:GLU:N	2.65	0.60
1:C:298:THR:HG22	1:C:299:LYS:N	2.14	0.60
1:C:186:ASP:OD2	1:C:279:THR:HB	2.01	0.60
2:B:361:LEU:C	2:B:363:GLU:H	2.06	0.60
2:D:362:GLN:HE22	2:D:365:LEU:HD23	1.67	0.59
2:D:318:LEU:O	2:D:319:ASN:O	2.19	0.59
2:D:85:VAL:HG23	5:D:1028:HOH:O	2.02	0.59
1:C:371:ALA:HB3	1:C:374:SER:OG	2.02	0.59
1:A:516:PHE:CE1	1:A:518:ASN:O	2.55	0.59
2:B:246:GLY:O	2:B:248:PRO:HD3	2.02	0.59
1:A:272:VAL:O	1:A:276:LEU:HG	2.02	0.59
1:A:259:PRO:C	1:A:261:ASP:N	2.55	0.59
1:C:409:LYS:O	1:C:413:ILE:HG12	2.01	0.59
2:B:361:LEU:HB3	2:B:750:LEU:HA	1.84	0.59
2:D:260:ILE:HD13	2:D:260:ILE:H	1.66	0.59
1:C:162:MET:O	1:C:519:THR:HA	2.03	0.59
1:A:235:LYS:HB2	1:A:239:GLU:CG	2.15	0.59
1:A:214:TRP:HB2	1:A:268:ALA:HA	1.84	0.59
1:A:434:ARG:HH12	1:A:463:GLY:CA	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:NH1	1:A:408:ASN:ND2	2.34	0.59
1:A:303:SER:HA	1:A:306:ILE:HD12	1.84	0.59
1:A:396:ARG:NH1	1:A:396:ARG:HG3	2.13	0.59
1:A:421:ASN:O	1:A:424:VAL:HG22	2.02	0.59
2:D:249:LEU:HD11	2:D:256:HIS:HB2	1.84	0.59
2:B:111:LEU:HD23	2:B:120:VAL:CG2	2.23	0.58
1:C:518:ASN:ND2	1:C:534:LEU:H	2.00	0.58
2:D:127:ILE:HG12	2:D:128:GLN:OE1	2.03	0.58
2:D:271:TYR:O	2:D:272:ASN:HB2	2.03	0.58
1:A:518:ASN:HD21	1:A:534:LEU:CB	2.16	0.58
1:A:233:ILE:HD13	1:A:233:ILE:H	1.65	0.58
2:D:369:THR:HA	2:D:376:MET:O	2.04	0.58
1:C:84:ASN:HB3	1:C:87:GLU:HG2	1.85	0.58
2:D:190:ARG:HB2	2:D:320:ASN:O	2.04	0.58
1:A:279:THR:O	1:A:280:GLN:HB2	2.04	0.58
2:D:381:ILE:HD12	2:D:381:ILE:N	2.19	0.58
2:B:139:HIS:CB	2:B:140:ILE:HD12	2.34	0.58
1:A:441:ARG:NH2	1:A:453:ASP:OD2	2.36	0.58
1:A:237:TYR:O	1:A:241:GLU:CB	2.51	0.58
1:C:222:LEU:HA	1:C:243:PHE:HE1	1.68	0.58
2:D:162:LEU:HA	2:D:173:SER:OG	2.03	0.58
2:D:44:PHE:CE1	3:F:9:GLN:HA	2.39	0.58
2:D:44:PHE:CD2	3:F:9:GLN:HG2	2.38	0.58
2:D:253:ASP:OD2	2:D:256:HIS:HD2	1.86	0.57
1:A:333:ILE:HD13	2:B:223:ARG:HH22	1.69	0.57
1:C:213:PRO:HG3	1:C:334:ALA:HB2	1.85	0.57
2:B:381:ILE:HD12	2:B:381:ILE:N	2.19	0.57
1:C:445:VAL:HG12	1:C:446:SER:N	2.19	0.57
1:C:297:ILE:HD13	1:C:368:ILE:CD1	2.34	0.57
1:C:115:ASN:O	1:C:117:PRO:HD3	2.03	0.57
1:C:295:ILE:O	1:C:309:ARG:NH1	2.37	0.57
2:B:132:ASP:HA	2:B:157:MET:CE	2.34	0.57
1:A:233:ILE:HD12	1:A:239:GLU:HB3	1.86	0.57
1:C:215:ILE:HG13	1:C:332:MET:HE3	1.84	0.57
1:C:329:ILE:HD11	1:C:346:TYR:CD1	2.38	0.57
1:C:337:GLY:O	1:C:341:LYS:HG3	2.05	0.57
1:C:325:VAL:HG21	1:C:349:LYS:HG2	1.85	0.57
2:B:142:VAL:HG13	2:B:178:ILE:HB	1.85	0.57
2:B:201:GLU:HG2	2:B:345:ALA:HB2	1.86	0.57
1:A:371:ALA:HB3	1:A:374:SER:HB3	1.86	0.57
1:A:143:LEU:HD12	1:A:150:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HD13	2:B:154:ILE:O	2.04	0.57
1:C:152:ILE:HD12	1:C:152:ILE:N	2.20	0.57
1:C:297:ILE:HD13	1:C:368:ILE:CG1	2.35	0.57
1:C:56:SER:HB3	1:C:101:SER:HB2	1.87	0.57
1:C:163:ARG:NH2	1:C:396:ARG:O	2.37	0.57
2:B:222:PRO:HB3	5:B:1041:HOH:O	2.05	0.57
2:D:31:THR:HG21	2:D:35:PHE:CD1	2.40	0.56
1:C:158:LEU:HG	2:D:23:PHE:CE2	2.40	0.56
2:B:83:ILE:HG22	2:B:99:ILE:HD13	1.88	0.56
1:A:407:ILE:HD12	5:A:592:HOH:O	2.05	0.56
2:D:284:VAL:O	2:D:287:ARG:HG2	2.05	0.56
1:A:285:ILE:N	1:A:285:ILE:CD1	2.68	0.56
1:C:333:ILE:HD13	2:D:223:ARG:NH2	2.20	0.56
2:B:265:LEU:HD23	2:B:276:VAL:HB	1.87	0.56
2:D:265:LEU:HD23	2:D:276:VAL:HB	1.87	0.56
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.87	0.56
1:C:340:ILE:HG22	1:C:344:ASN:HD21	1.70	0.56
1:C:439:GLN:HB3	1:C:441:ARG:HG2	1.87	0.56
1:C:279:THR:HG22	1:C:322:ASN:ND2	2.20	0.56
1:A:295:ILE:HA	5:A:595:HOH:O	2.05	0.56
1:C:232:ARG:O	1:C:233:ILE:HD13	2.05	0.56
1:A:35:LEU:HB3	1:A:59:ILE:CD1	2.35	0.56
1:C:438:GLN:HE21	1:C:439:GLN:HE22	1.52	0.56
2:B:31:THR:CG2	2:B:35:PHE:HB3	2.33	0.56
1:C:45:ILE:CD1	1:C:498:GLY:HA2	2.36	0.56
2:B:80:MET:HG3	2:B:80:MET:O	2.05	0.56
1:C:112:LEU:HD13	1:C:119:PHE:HD2	1.71	0.56
2:D:42:LEU:HD11	2:D:46:LEU:HD21	1.88	0.56
1:C:329:ILE:HD11	1:C:346:TYR:CG	2.40	0.56
2:D:114:ARG:O	2:D:116:PRO:HD3	2.05	0.56
2:B:136:ARG:HG3	2:B:161:LEU:HD22	1.86	0.56
1:C:84:ASN:ND2	1:C:86:ALA:HB3	2.21	0.56
1:A:366:GLN:C	1:A:368:ILE:H	2.08	0.56
2:B:54:ILE:CG2	2:B:145:LEU:HD11	2.36	0.55
2:B:206:LEU:C	2:B:208:PRO:HD3	2.27	0.55
1:A:214:TRP:CD1	1:A:267:GLU:HG2	2.40	0.55
1:A:84:ASN:HD22	1:A:87:GLU:H	1.54	0.55
2:B:141:ILE:CD1	2:B:158:LEU:HD21	2.36	0.55
2:D:303:CYS:O	2:D:307:VAL:HG23	2.06	0.55
1:C:143:LEU:CD1	1:C:150:LEU:HD22	2.28	0.55
1:A:447:ASN:ND2	2:B:26:ARG:NH2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:TYR:CE2	2:D:169:LEU:HD13	2.41	0.55
1:C:87:GLU:HG3	1:C:88:ALA:N	2.22	0.55
1:C:403:GLY:HA3	1:C:406:THR:HG22	1.89	0.55
1:A:518:ASN:CG	1:A:519:THR:N	2.60	0.55
2:D:83:ILE:HD12	2:D:94:PHE:CD1	2.41	0.55
2:D:31:THR:CG2	2:D:32:HIS:N	2.67	0.55
2:B:169:LEU:O	2:B:171:PRO:HD3	2.06	0.55
1:C:211:HIS:HA	1:C:335:ASP:CG	2.28	0.54
2:B:286:LYS:HB2	2:B:288:ILE:HG13	1.88	0.54
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.87	0.54
1:C:213:PRO:O	1:C:217:ILE:HD12	2.07	0.54
2:D:182:THR:HB	5:D:1035:HOH:O	2.06	0.54
1:A:415:SER:HB3	1:A:421:ASN:ND2	2.22	0.54
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.90	0.54
2:D:382:THR:O	2:D:900:LEU:HA	2.08	0.54
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.37	0.54
1:C:112:LEU:HD13	1:C:119:PHE:CD2	2.42	0.54
1:C:527:GLN:HE21	1:C:527:GLN:HA	1.70	0.54
2:B:82:THR:HG23	2:B:100:GLY:C	2.28	0.54
1:C:186:ASP:C	1:C:188:PRO:HD3	2.27	0.54
1:A:503:GLN:HE21	1:A:503:GLN:HA	1.72	0.54
2:B:190:ARG:HG3	2:B:192:ILE:CD1	2.37	0.54
1:A:84:ASN:ND2	1:A:106:GLU:HG2	2.23	0.54
1:A:329:ILE:HD13	1:A:329:ILE:N	2.22	0.54
1:C:213:PRO:HG3	1:C:334:ALA:CB	2.38	0.54
1:C:184:ARG:NE	1:C:325:VAL:HG12	2.23	0.54
1:C:37:ASN:O	1:C:39:THR:N	2.33	0.54
2:B:362:GLN:HG2	2:B:366:ASP:OD1	2.08	0.54
1:C:130:GLN:HE22	1:C:155:THR:N	2.01	0.54
2:D:381:ILE:O	2:D:603:THR:HA	2.07	0.54
1:C:370:GLN:O	1:C:371:ALA:HB2	2.07	0.54
2:B:136:ARG:CG	2:B:161:LEU:HD22	2.38	0.54
1:A:503:GLN:NE2	1:A:503:GLN:HA	2.23	0.54
2:D:362:GLN:NE2	2:D:365:LEU:HB3	2.23	0.53
1:A:297:ILE:HD12	1:A:297:ILE:N	2.23	0.53
1:A:434:ARG:NH1	1:A:463:GLY:CA	2.67	0.53
2:D:209:PRO:HG3	2:D:375:GLN:OE1	2.08	0.53
1:A:36:ILE:O	1:A:37:ASN:HB2	2.08	0.53
2:B:54:ILE:HD11	2:B:141:ILE:HG23	1.89	0.53
1:C:43:THR:HG21	1:C:73:ASN:HD21	1.72	0.53
1:C:76:LEU:HD21	1:C:89:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ILE:HD13	1:C:368:ILE:HG12	1.90	0.53
2:D:68:ALA:HB1	2:D:115:VAL:HG11	1.90	0.53
1:C:157:GLY:HA3	1:C:485:TYR:CG	2.43	0.53
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.91	0.53
1:A:331:ASP:OD1	2:B:223:ARG:HD2	2.07	0.53
2:B:224:LEU:H	2:B:227:HIS:CD2	2.26	0.53
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.91	0.53
2:D:283:GLY:O	2:D:287:ARG:HA	2.09	0.53
2:D:182:THR:HG22	2:D:183:GLU:N	2.22	0.53
1:C:218:ILE:HD11	1:C:268:ALA:O	2.08	0.53
1:C:240:LYS:O	1:C:244:ARG:HG3	2.09	0.53
1:A:340:ILE:HD11	2:B:273:ILE:HD13	1.90	0.53
1:C:36:ILE:HG21	1:C:131:LEU:HD21	1.91	0.53
2:B:709:ARG:O	2:B:750:LEU:N	2.42	0.53
2:D:131:ASN:C	2:D:131:ASN:HD22	2.12	0.53
1:C:84:ASN:ND2	1:C:106:GLU:HG2	2.23	0.52
1:A:372:PRO:HG2	1:A:373:GLU:H	1.74	0.52
2:D:249:LEU:HD21	2:D:260:ILE:HD11	1.88	0.52
1:A:151:LEU:HD13	1:A:164:ILE:HD13	1.92	0.52
2:B:325:ASN:ND2	2:B:327:VAL:H	2.06	0.52
2:D:224:LEU:H	2:D:227:HIS:HD2	1.57	0.52
1:C:175:HIS:N	1:C:176:PRO:HD3	2.24	0.52
1:A:235:LYS:O	1:A:240:LYS:HG3	2.09	0.52
2:D:201:GLU:HB3	2:D:343:CYS:SG	2.50	0.52
1:C:110:GLU:H	1:C:110:GLU:CD	2.13	0.52
1:A:329:ILE:HD13	5:A:559:HOH:O	2.09	0.52
2:D:260:ILE:CD1	2:D:260:ILE:H	2.22	0.52
2:D:178:ILE:HD12	2:D:178:ILE:N	2.25	0.52
2:B:117:ASN:ND2	5:B:1058:HOH:O	2.41	0.52
1:A:297:ILE:CG2	1:A:298:THR:N	2.73	0.52
1:C:10:GLU:CG	2:D:279:ARG:HH12	2.23	0.52
1:C:460:CYS:HA	5:C:573:HOH:O	2.09	0.52
1:A:243:PHE:HD2	1:A:272:VAL:HG21	1.75	0.52
1:A:467:GLU:HB2	5:A:584:HOH:O	2.10	0.52
1:C:297:ILE:C	1:C:297:ILE:HD12	2.29	0.52
1:C:396:ARG:NH2	1:C:406:THR:O	2.38	0.52
2:D:199:CYS:H	2:D:202:CYS:HB2	1.75	0.52
1:A:51:LEU:HB3	2:B:89:ASN:O	2.10	0.52
2:D:24:LEU:HD21	2:D:312:THR:HG21	1.92	0.52
1:A:265:PHE:O	1:A:268:ALA:HB3	2.10	0.51
1:A:276:LEU:O	1:A:277:ASN:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:MET:HB3	2:B:379:PRO:HG3	1.92	0.51
1:A:31:ALA:CB	1:A:509:ILE:HD12	2.40	0.51
1:C:484:ARG:O	1:C:486:GLY:N	2.43	0.51
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.44	0.51
1:A:87:GLU:O	1:A:91:GLU:HG3	2.10	0.51
2:B:218:ILE:HD12	2:B:230:GLU:HB3	1.92	0.51
2:D:21:LYS:HD3	2:D:25:GLU:OE1	2.10	0.51
1:A:54:ILE:O	1:A:100:VAL:HG22	2.09	0.51
2:B:351:GLN:HB3	2:B:1007:PHE:CB	2.40	0.51
2:D:241:GLN:HE21	2:D:245:GLU:C	2.14	0.51
1:A:95:GLU:HB3	2:B:95:ARG:CZ	2.41	0.51
2:D:237:TRP:CE2	2:D:249:LEU:HB2	2.46	0.51
1:A:259:PRO:C	1:A:261:ASP:H	2.11	0.51
1:A:370:GLN:O	1:A:371:ALA:HB2	2.11	0.51
1:C:115:ASN:C	1:C:117:PRO:HD3	2.31	0.51
1:C:252:LEU:HD23	1:C:252:LEU:H	1.74	0.51
2:D:225:PRO:HG3	2:D:274:ARG:O	2.11	0.51
2:B:274:ARG:HD2	5:B:1107:HOH:O	2.10	0.51
2:B:165:GLU:O	2:B:166:ASP:HB2	2.10	0.51
2:D:380:ALA:O	2:D:901:ALA:O	2.29	0.51
2:D:52:LEU:HD11	2:D:78:ILE:HG12	1.92	0.51
1:C:41:THR:O	1:C:45:ILE:CD1	2.54	0.51
1:C:189:PHE:CE1	1:C:191:GLU:HB2	2.46	0.51
1:A:95:GLU:HB3	2:B:95:ARG:NH2	2.26	0.51
2:B:305:THR:HG22	2:B:309:LYS:HE3	1.92	0.51
2:D:249:LEU:CD1	2:D:256:HIS:CB	2.74	0.51
2:B:132:ASP:HA	2:B:157:MET:HE2	1.92	0.51
2:B:378:SER:N	2:B:379:PRO:HD3	2.25	0.51
1:A:284:SER:OG	1:A:285:ILE:HD12	2.12	0.50
2:D:44:PHE:CD1	2:D:48:THR:HB	2.47	0.50
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.46	0.50
1:A:333:ILE:CD1	2:B:223:ARG:HH22	2.24	0.50
2:D:44:PHE:CE2	3:F:9:GLN:HG2	2.46	0.50
2:D:164:TYR:CE2	2:D:348:GLN:NE2	2.79	0.50
2:B:325:ASN:HD22	2:B:327:VAL:H	1.60	0.50
1:C:227:SER:O	1:C:229:THR:N	2.44	0.50
2:D:253:ASP:CG	2:D:256:HIS:CD2	2.84	0.50
1:C:272:VAL:O	1:C:276:LEU:HG	2.11	0.50
1:C:408:ASN:O	1:C:412:ILE:HD13	2.12	0.50
2:D:132:ASP:OD1	2:D:133:THR:N	2.45	0.50
1:A:377:GLU:O	1:A:381:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:HD12	1:C:172:ILE:N	2.26	0.50
1:A:518:ASN:HD21	1:A:534:LEU:HB2	1.77	0.50
2:D:249:LEU:CD2	2:D:260:ILE:CD1	2.89	0.50
1:C:213:PRO:O	1:C:217:ILE:CD1	2.59	0.50
1:A:251:ILE:O	1:A:252:LEU:HB2	2.11	0.50
1:C:335:ASP:O	2:D:221:MET:HB3	2.11	0.50
1:A:317:LYS:HD2	1:A:360:HIS:CE1	2.46	0.50
1:A:199:TYR:OH	1:A:338:LYS:HD3	2.11	0.50
1:A:278:THR:HG22	1:A:279:THR:H	1.76	0.50
1:C:439:GLN:O	1:C:441:ARG:HG2	2.11	0.50
2:D:21:LYS:HE2	2:D:42:LEU:HD22	1.92	0.50
2:B:317:PRO:O	2:B:318:LEU:C	2.49	0.50
1:A:66:SER:O	1:A:69:ASP:HB2	2.11	0.50
2:D:35:PHE:C	2:D:35:PHE:CD2	2.86	0.50
2:D:257:ILE:O	2:D:260:ILE:HG12	2.12	0.49
1:A:374:SER:O	1:A:375:ILE:HD13	2.12	0.49
1:A:192:LEU:HG	1:A:196:PHE:CE1	2.47	0.49
1:C:215:ILE:H	1:C:332:MET:CE	2.25	0.49
1:A:329:ILE:HD13	1:A:329:ILE:H	1.77	0.49
1:A:243:PHE:HD2	1:A:272:VAL:CG2	2.25	0.49
2:B:54:ILE:CD1	2:B:141:ILE:HG23	2.42	0.49
2:D:21:LYS:HD3	2:D:25:GLU:CD	2.33	0.49
1:A:317:LYS:HD2	1:A:360:HIS:HE1	1.77	0.49
1:A:252:LEU:HB2	1:A:259:PRO:HD2	1.94	0.49
2:D:365:LEU:O	2:D:369:THR:HB	2.13	0.49
1:A:35:LEU:HD23	1:A:59:ILE:CD1	2.35	0.49
2:D:263:LYS:O	2:D:266:GLU:HB3	2.12	0.49
1:C:217:ILE:N	1:C:217:ILE:HD12	2.26	0.49
1:A:430:ARG:NH1	1:A:464:PHE:HE1	2.11	0.49
1:C:325:VAL:CG2	1:C:349:LYS:HG2	2.43	0.49
1:C:485:TYR:O	1:C:487:ALA:N	2.39	0.49
1:C:196:PHE:O	1:C:198:SER:N	2.44	0.49
2:D:606:LEU:O	2:D:607:GLN:C	2.51	0.49
2:B:377:LYS:HB2	5:B:1095:HOH:O	2.13	0.49
1:C:488:ALA:C	1:C:490:PRO:HD3	2.32	0.49
1:A:235:LYS:O	1:A:240:LYS:N	2.45	0.49
2:B:139:HIS:HB3	2:B:140:ILE:HD12	1.95	0.48
2:B:81:ASP:HB2	2:B:103:LYS:HD2	1.94	0.48
2:B:128:GLN:NE2	2:B:128:GLN:N	2.47	0.48
2:D:139:HIS:O	2:D:176:PRO:HD2	2.13	0.48
1:C:181:GLU:CD	1:C:330:PRO:HG3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:PHE:HZ	1:C:353:ASP:OD2	1.96	0.48
1:C:435:PHE:CG	1:C:443:PRO:HG3	2.47	0.48
2:D:709:ARG:O	2:D:710:PRO:CB	2.60	0.48
1:C:416:MET:SD	1:C:424:VAL:HG22	2.54	0.48
1:C:222:LEU:HA	1:C:243:PHE:CE1	2.48	0.48
1:A:238:LYS:CD	1:A:238:LYS:O	2.62	0.48
1:A:241:GLU:OE1	1:A:244:ARG:HD2	2.14	0.48
1:C:36:ILE:O	1:C:37:ASN:HB2	2.14	0.48
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.43	0.48
1:C:309:ARG:HB3	1:C:364:LEU:HD21	1.96	0.48
2:B:361:LEU:HB3	2:B:750:LEU:CA	2.43	0.48
1:C:446:SER:HB3	1:C:448:TYR:CE2	2.49	0.48
2:D:62:GLU:HG3	5:D:1020:HOH:O	2.14	0.48
1:C:510:THR:O	1:C:511:LYS:HB2	2.14	0.48
1:C:214:TRP:HB2	1:C:268:ALA:HA	1.96	0.48
1:C:343:GLN:HE22	2:D:224:LEU:CD2	2.27	0.48
1:A:189:PHE:CD1	1:A:192:LEU:HB2	2.49	0.48
2:B:378:SER:OG	2:B:378:SER:O	2.28	0.48
2:D:90:ARG:NH1	2:D:91:GLN:HE21	2.11	0.48
1:A:486:GLY:HA3	2:B:22:LYS:HZ3	1.79	0.48
2:D:148:ILE:O	2:D:152:ARG:HG3	2.14	0.47
2:B:38:SER:OG	2:B:40:GLU:HG3	2.14	0.47
1:C:235:LYS:O	1:C:240:LYS:HE2	2.14	0.47
1:C:391:ARG:NH2	2:D:328:ASP:OD1	2.47	0.47
1:C:447:ASN:O	1:C:449:GLN:N	2.47	0.47
1:C:434:ARG:HG2	1:C:434:ARG:NH1	2.23	0.47
1:C:281:ILE:HD11	1:C:322:ASN:HA	1.95	0.47
2:B:140:ILE:HD11	3:E:7:LEU:HD22	1.95	0.47
2:B:83:ILE:HD11	2:B:106:VAL:HG21	1.96	0.47
2:B:229:ILE:HD13	2:B:281:THR:HA	1.97	0.47
1:C:218:ILE:HD12	1:C:272:VAL:HG22	1.95	0.47
1:C:189:PHE:CD2	1:C:349:LYS:HD3	2.50	0.47
2:D:276:VAL:HA	2:D:280:LEU:HD23	1.95	0.47
1:A:518:ASN:ND2	1:A:533:GLN:HA	2.19	0.47
1:A:306:ILE:CD1	1:A:370:GLN:HE22	2.24	0.47
3:F:10:GLN:HG2	3:F:11:LYS:N	2.29	0.47
2:B:94:PHE:CZ	2:B:103:LYS:HB3	2.49	0.47
2:D:253:ASP:O	2:D:257:ILE:N	2.48	0.47
1:C:150:LEU:HG	1:C:152:ILE:HD11	1.97	0.47
1:C:236:THR:HB	1:C:239:GLU:HG3	1.96	0.47
1:C:447:ASN:O	1:C:448:TYR:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HD12	2:B:177:LEU:HB2	1.97	0.47
2:B:52:LEU:HG	2:B:54:ILE:CD1	2.45	0.47
2:B:383:ALA:O	2:B:601:ASN:N	2.48	0.47
1:A:434:ARG:NH2	5:A:584:HOH:O	2.48	0.47
1:C:115:ASN:HB2	5:C:576:HOH:O	2.15	0.47
1:A:376:SER:OG	1:A:378:LYS:HG2	2.15	0.47
2:D:26:ARG:O	2:D:35:PHE:CZ	2.68	0.47
1:C:113:LEU:O	1:C:117:PRO:HG3	2.14	0.47
2:B:751:SER:O	2:B:752:LYS:C	2.53	0.47
1:C:236:THR:HB	1:C:239:GLU:OE1	2.15	0.46
2:D:701:VAL:C	2:D:703:SER:N	2.67	0.46
1:C:311:LEU:O	1:C:315:VAL:HG23	2.16	0.46
1:C:109:PRO:HB2	1:C:110:GLU:OE2	2.15	0.46
1:C:33:VAL:HG22	1:C:34:CYS:N	2.30	0.46
1:C:152:ILE:HD12	1:C:152:ILE:H	1.80	0.46
2:D:343:CYS:HA	2:D:344:PRO:HD3	1.75	0.46
1:A:349:LYS:HE3	1:A:353:ASP:OD2	2.15	0.46
1:A:362:ALA:O	1:A:366:GLN:HG3	2.15	0.46
1:A:238:LYS:HD3	1:A:238:LYS:HA	1.35	0.46
2:D:900:LEU:N	2:D:1008:LYS:O	2.49	0.46
2:D:353:ILE:CG2	2:D:354:GLN:H	2.20	0.46
1:C:307:LEU:HB3	1:C:383:LEU:CD2	2.46	0.46
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.97	0.46
1:C:339:TYR:CE2	2:D:224:LEU:HD21	2.42	0.46
1:C:36:ILE:N	1:C:36:ILE:HD12	2.31	0.46
2:B:52:LEU:HG	2:B:54:ILE:HD12	1.98	0.46
1:A:293:ARG:HG3	5:A:611:HOH:O	2.15	0.46
2:D:353:ILE:H	2:D:353:ILE:CD1	2.06	0.46
1:C:329:ILE:HG22	1:C:330:PRO:N	2.31	0.46
1:A:75:PHE:CE2	1:A:96:LEU:HD11	2.50	0.46
2:B:319:ASN:O	2:B:320:ASN:HB3	2.16	0.46
1:C:190:PRO:O	1:C:194:GLU:HG2	2.15	0.46
1:A:235:LYS:HB3	1:A:238:LYS:HB3	1.98	0.46
2:D:362:GLN:HE22	2:D:365:LEU:HB3	1.80	0.46
2:D:224:LEU:N	2:D:227:HIS:HD2	2.14	0.46
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.98	0.46
1:C:347:ARG:HH12	2:D:274:ARG:CG	2.29	0.46
2:D:283:GLY:O	2:D:287:ARG:CA	2.63	0.46
2:B:376:MET:CB	2:B:379:PRO:HG3	2.45	0.46
1:A:430:ARG:NH1	1:A:464:PHE:CE1	2.84	0.46
2:B:382:THR:HG23	2:B:603:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.16	0.46
1:C:162:MET:HG2	1:C:516:PHE:CZ	2.51	0.46
1:C:319:GLY:O	1:C:320:GLN:HB2	2.16	0.46
1:A:58:THR:HA	1:A:103:SER:O	2.16	0.46
2:D:271:TYR:O	2:D:272:ASN:CB	2.64	0.46
1:A:236:THR:O	1:A:240:LYS:CA	2.64	0.46
2:B:223:ARG:H	2:B:227:HIS:CD2	2.16	0.46
1:C:396:ARG:NH1	1:C:534:LEU:OXT	2.49	0.46
1:C:189:PHE:HE1	1:C:191:GLU:HB2	1.81	0.46
1:C:485:TYR:C	1:C:487:ALA:H	2.19	0.46
1:C:12:LYS:NZ	1:C:97:ASN:HD21	2.14	0.46
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.98	0.46
1:C:218:ILE:O	1:C:222:LEU:HB2	2.16	0.45
1:C:329:ILE:N	1:C:329:ILE:HD12	2.30	0.45
2:B:62:GLU:HG3	5:B:1016:HOH:O	2.16	0.45
1:A:28:LEU:HA	1:A:509:ILE:HG21	1.98	0.45
1:A:313:GLU:HB3	1:A:360:HIS:CE1	2.51	0.45
1:C:470:LEU:C	1:C:472:VAL:H	2.20	0.45
1:C:221:TYR:OH	1:C:250:GLY:HA3	2.15	0.45
1:A:422:GLU:HG2	1:A:530:ALA:HB3	1.98	0.45
2:B:322:LEU:C	2:B:322:LEU:HD23	2.37	0.45
1:A:297:ILE:HG22	1:A:298:THR:H	1.79	0.45
2:B:54:ILE:CD1	2:B:54:ILE:N	2.79	0.45
1:A:124:THR:HG21	1:A:509:ILE:CD1	2.47	0.45
2:B:193:LEU:HB2	2:B:197:THR:HG23	1.98	0.45
1:C:144:TRP:CH2	1:C:167:LYS:HG3	2.52	0.45
1:C:169:HIS:CD2	1:C:515:ILE:HD12	2.51	0.45
1:A:113:LEU:HD13	1:A:138:ARG:HG2	1.99	0.45
1:A:8:LEU:HD23	1:A:8:LEU:O	2.17	0.45
1:C:67:GLY:HA2	1:C:78:ARG:HH12	1.82	0.45
1:C:75:PHE:O	1:C:76:LEU:HD23	2.16	0.45
2:B:353:ILE:N	2:B:1008:LYS:O	2.49	0.45
2:B:237:TRP:CE3	2:B:260:ILE:HD11	2.51	0.45
2:B:361:LEU:O	2:B:364:VAL:HG22	2.17	0.45
2:B:90:ARG:HG2	2:B:90:ARG:HH11	1.80	0.45
2:D:383:ALA:O	2:D:384:THR:C	2.55	0.45
2:B:242:PRO:HB2	2:B:243:PHE:HD1	1.81	0.45
1:C:229:THR:HG22	1:C:230:ASN:N	2.32	0.45
1:C:144:TRP:CZ2	1:C:167:LYS:HE2	2.51	0.45
2:B:343:CYS:HA	2:B:344:PRO:HD3	1.77	0.45
1:A:265:PHE:O	1:A:269:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ILE:HD13	2:D:223:ARG:HH22	1.81	0.45
2:B:102:PRO:O	2:B:106:VAL:HG23	2.16	0.45
2:D:257:ILE:C	2:D:260:ILE:HG12	2.37	0.45
1:C:151:LEU:HD13	1:C:164:ILE:HD13	1.98	0.45
1:A:454:ILE:HD11	1:A:480:HIS:HA	1.95	0.45
2:D:126:LYS:NZ	2:D:128:GLN:HG2	2.32	0.45
1:A:512:GLN:O	1:A:513:PHE:HB2	2.16	0.45
1:A:235:LYS:O	1:A:236:THR:O	2.35	0.45
2:B:32:HIS:HB3	2:B:313:SER:O	2.17	0.45
1:C:37:ASN:C	1:C:39:THR:N	2.68	0.45
1:A:313:GLU:HB3	1:A:360:HIS:ND1	2.32	0.45
1:C:182:ASP:C	1:C:183:LEU:O	2.53	0.45
1:C:445:VAL:N	1:C:449:GLN:OE1	2.49	0.44
1:A:61:ASP:OD2	1:A:85:ARG:HD2	2.17	0.44
1:C:407:ILE:HD12	1:C:468:TYR:CD2	2.53	0.44
2:D:202:CYS:O	2:D:340:LYS:HE3	2.17	0.44
1:A:278:THR:CG2	1:A:279:THR:N	2.79	0.44
2:D:209:PRO:CG	2:D:375:GLN:OE1	2.64	0.44
2:B:368:LEU:O	2:B:376:MET:HB2	2.17	0.44
1:A:146:SER:O	1:A:147:GLN:HB2	2.17	0.44
1:A:275:ALA:C	1:A:277:ASN:N	2.68	0.44
1:C:397:SER:OG	1:C:400:GLU:HG3	2.17	0.44
1:A:221:TYR:CD1	1:A:247:ILE:HG13	2.53	0.44
2:D:253:ASP:CG	2:D:256:HIS:HD2	2.21	0.44
1:C:139:LEU:O	1:C:143:LEU:HG	2.18	0.44
1:C:164:ILE:O	1:C:164:ILE:HG23	2.18	0.44
1:A:340:ILE:CD1	2:B:273:ILE:HD13	2.47	0.44
2:B:190:ARG:HG3	2:B:192:ILE:HD11	2.00	0.44
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.47	0.44
1:C:33:VAL:O	1:C:57:PHE:HA	2.18	0.44
2:D:83:ILE:CD1	2:D:94:PHE:CE1	3.00	0.44
1:C:166:ILE:HG21	1:C:169:HIS:HB2	1.99	0.44
1:C:113:LEU:HD22	1:C:142:VAL:HG21	1.98	0.44
1:C:78:ARG:HA	1:C:81:ILE:CD1	2.48	0.44
1:C:50:VAL:O	1:C:53:GLY:N	2.49	0.44
2:D:241:GLN:O	2:D:242:PRO:C	2.56	0.44
2:D:83:ILE:CD1	2:D:103:LYS:HA	2.39	0.44
2:D:369:THR:HG23	2:D:376:MET:O	2.18	0.44
1:A:317:LYS:HB2	1:A:318:GLU:OE2	2.18	0.44
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.47	0.44
1:A:341:LYS:O	1:A:345:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:O	1:A:298:THR:HG22	2.18	0.44
1:A:350:ALA:HB1	5:A:581:HOH:O	2.18	0.44
1:C:326:ARG:HH21	1:C:388:ALA:HB3	1.83	0.44
1:A:508:ILE:HD13	1:A:515:ILE:HG21	2.00	0.44
1:A:518:ASN:CB	1:A:533:GLN:HA	2.47	0.44
2:B:190:ARG:NE	2:B:192:ILE:HD11	2.32	0.44
1:A:486:GLY:O	2:B:22:LYS:NZ	2.51	0.43
1:A:236:THR:CA	1:A:240:LYS:CD	2.88	0.43
1:A:235:LYS:HG3	1:A:239:GLU:OE2	2.17	0.43
1:C:213:PRO:HB3	1:C:332:MET:CE	2.48	0.43
1:C:486:GLY:CA	2:D:22:LYS:HZ2	2.31	0.43
2:D:42:LEU:CG	2:D:46:LEU:HD11	2.43	0.43
2:B:54:ILE:HG22	2:B:145:LEU:HD11	2.00	0.43
2:B:201:GLU:OE1	2:B:204:LEU:HD11	2.18	0.43
1:C:12:LYS:O	2:D:89:ASN:HB3	2.18	0.43
1:C:517:ASN:HD22	1:C:533:GLN:HG2	1.83	0.43
1:C:305:TRP:HA	1:C:308:ALA:HB3	1.99	0.43
2:D:26:ARG:O	2:D:35:PHE:HZ	2.01	0.43
1:A:84:ASN:CG	1:A:106:GLU:HG2	2.38	0.43
1:A:297:ILE:CG2	1:A:298:THR:H	2.31	0.43
2:B:54:ILE:HG22	2:B:145:LEU:CG	2.48	0.43
1:C:194:GLU:O	1:C:196:PHE:N	2.51	0.43
1:A:488:ALA:C	1:A:490:PRO:HD3	2.38	0.43
1:A:35:LEU:HB3	1:A:59:ILE:HD13	2.00	0.43
1:C:109:PRO:O	1:C:113:LEU:HG	2.18	0.43
1:C:65:VAL:HB	1:C:81:ILE:HA	2.00	0.43
2:B:381:ILE:HD12	2:B:381:ILE:H	1.82	0.43
1:A:504:GLU:O	1:A:508:ILE:HG12	2.18	0.43
2:D:333:TYR:CE2	2:D:335:PHE:HB3	2.54	0.43
2:D:31:THR:HG22	2:D:32:HIS:H	1.82	0.43
1:C:181:GLU:HG3	1:C:330:PRO:HG2	1.99	0.43
2:D:607:GLN:O	2:D:701:VAL:CB	2.67	0.43
1:A:309:ARG:HG3	1:A:364:LEU:HD11	2.01	0.43
1:C:152:ILE:HD11	1:C:165:ILE:HD12	2.00	0.43
1:C:436:HIS:HA	1:C:441:ARG:O	2.19	0.43
1:C:396:ARG:HD3	1:C:534:LEU:O	2.19	0.43
2:B:11:LEU:HD22	2:B:117:ASN:OD1	2.19	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.92	0.43
1:A:308:ALA:O	1:A:311:LEU:HB2	2.19	0.43
1:A:212:THR:H	1:A:264:ASN:HD21	1.66	0.43
1:A:378:LYS:HA	1:A:381:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HG3	1:A:389:PHE:CD1	2.54	0.43
1:A:259:PRO:CB	1:A:261:ASP:OD2	2.67	0.43
2:B:217:THR:OG1	2:B:223:ARG:NH2	2.49	0.43
1:C:454:ILE:HG13	1:C:455:GLY:N	2.33	0.43
2:D:317:PRO:O	2:D:318:LEU:C	2.57	0.43
1:A:353:ASP:O	1:A:357:VAL:HG23	2.18	0.43
1:A:365:LEU:O	1:A:369:GLY:N	2.51	0.43
1:A:414:SER:O	1:A:417:ASP:HB2	2.18	0.43
2:D:82:THR:HA	2:D:101:ARG:O	2.19	0.43
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.49	0.42
1:C:65:VAL:HG13	1:C:69:ASP:CB	2.49	0.42
1:A:75:PHE:O	1:A:76:LEU:HD23	2.18	0.42
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.50	0.42
1:A:518:ASN:ND2	1:A:533:GLN:CA	2.70	0.42
2:B:259:TRP:HE3	2:B:260:ILE:HD13	1.85	0.42
2:B:58:GLY:HA3	5:B:1063:HOH:O	2.18	0.42
1:C:407:ILE:HG12	1:C:408:ASN:N	2.34	0.42
1:C:186:ASP:OD2	1:C:279:THR:CB	2.68	0.42
1:A:341:LYS:HB2	5:A:587:HOH:O	2.18	0.42
1:A:225:TRP:CE2	1:A:233:ILE:CD1	2.98	0.42
1:C:69:ASP:OD2	1:C:85:ARG:NE	2.52	0.42
2:B:218:ILE:HD13	2:B:218:ILE:HA	1.89	0.42
1:A:129:THR:HA	1:A:153:CYS:O	2.20	0.42
2:B:31:THR:HG21	2:B:35:PHE:HD2	1.84	0.42
2:D:201:GLU:HA	2:D:204:LEU:HD23	1.99	0.42
1:C:344:ASN:HA	1:C:347:ARG:HD2	2.00	0.42
2:B:10:LYS:CD	2:B:11:LEU:H	2.33	0.42
1:A:176:PRO:HG3	1:A:389:PHE:CG	2.54	0.42
2:B:365:LEU:C	2:B:365:LEU:HD23	2.40	0.42
1:A:398:LEU:HD12	1:A:398:LEU:HA	1.90	0.42
1:A:185:LEU:HD11	1:A:215:ILE:CD1	2.49	0.42
2:B:145:LEU:CD1	2:B:150:ALA:HB1	2.50	0.42
1:C:435:PHE:CD1	1:C:443:PRO:HG3	2.55	0.42
1:C:212:THR:HA	1:C:213:PRO:HD3	1.87	0.42
1:C:448:TYR:CD2	1:C:448:TYR:N	2.88	0.42
2:D:201:GLU:OE1	2:D:204:LEU:CD2	2.68	0.42
2:D:201:GLU:OE1	2:D:204:LEU:HD21	2.19	0.42
2:D:284:VAL:HG12	2:D:287:ARG:HH12	1.85	0.42
1:A:328:THR:HA	5:A:559:HOH:O	2.20	0.42
1:A:165:ILE:HG21	5:A:544:HOH:O	2.20	0.42
1:A:10:GLU:OE2	2:B:279:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:O	1:A:240:LYS:N	2.52	0.42
1:A:261:ASP:O	1:A:264:ASN:N	2.47	0.42
1:C:87:GLU:HB3	1:C:104:PHE:CD1	2.54	0.42
2:B:190:ARG:HB2	2:B:320:ASN:O	2.20	0.42
2:D:45:LEU:HA	2:D:45:LEU:HD12	1.79	0.42
2:B:325:ASN:C	2:B:325:ASN:HD22	2.23	0.42
2:B:81:ASP:O	2:B:103:LYS:HG3	2.19	0.42
1:A:190:PRO:O	1:A:194:GLU:HG3	2.20	0.42
1:A:276:LEU:O	1:A:277:ASN:O	2.37	0.42
1:C:332:MET:C	2:D:223:ARG:NH1	2.73	0.42
2:D:365:LEU:O	2:D:369:THR:CB	2.67	0.42
2:D:228:CYS:SG	2:D:273:ILE:HD12	2.60	0.42
2:D:230:GLU:O	2:D:231:TYR:C	2.58	0.42
1:A:526:SER:O	1:A:528:THR:HG23	2.20	0.42
1:C:285:ILE:HA	1:C:288:ILE:HD12	2.01	0.42
2:D:36:GLU:HA	2:D:37:PRO:HD3	1.66	0.42
2:D:151:ARG:HB3	2:D:200:ILE:HD13	2.01	0.41
1:C:45:ILE:HG13	1:C:501:ALA:HB3	2.02	0.41
1:A:115:ASN:C	1:A:117:PRO:HD3	2.40	0.41
2:B:361:LEU:C	2:B:363:GLU:N	2.72	0.41
2:B:165:GLU:O	2:B:166:ASP:CB	2.67	0.41
1:C:12:LYS:HZ3	1:C:97:ASN:HD21	1.67	0.41
1:C:64:GLN:HA	1:C:83:LYS:O	2.19	0.41
2:B:33:PRO:HD2	3:E:4:LEU:HD21	2.02	0.41
1:C:150:LEU:HD12	1:C:151:LEU:H	1.84	0.41
1:C:453:ASP:HA	1:C:456:LYS:HB3	2.02	0.41
1:A:418:ASN:C	1:A:418:ASN:HD22	2.23	0.41
2:B:83:ILE:CD1	2:B:106:VAL:HG21	2.50	0.41
2:B:141:ILE:HD12	2:B:158:LEU:CD2	2.49	0.41
2:D:240:GLU:C	2:D:242:PRO:HD3	2.40	0.41
2:B:50:LYS:HD3	2:B:137:GLN:HE21	1.86	0.41
1:A:26:GLU:OE2	1:A:26:GLU:HA	2.20	0.41
2:D:80:MET:O	2:D:80:MET:HG3	2.20	0.41
2:D:253:ASP:OD2	2:D:256:HIS:CG	2.71	0.41
2:B:325:ASN:HD22	2:B:326:ASP:N	2.18	0.41
1:A:422:GLU:H	1:A:422:GLU:CD	2.24	0.41
1:A:301:THR:HA	1:A:302:PRO:HD3	1.92	0.41
2:D:311:ALA:HA	3:F:7:LEU:HD23	2.03	0.41
2:B:176:PRO:HG2	2:B:310:ILE:HG21	2.03	0.41
1:A:297:ILE:HD12	1:A:297:ILE:H	1.85	0.41
2:B:140:ILE:HD11	3:E:7:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASN:ND2	1:C:265:PHE:HD1	2.19	0.41
2:D:206:LEU:HD12	2:D:206:LEU:HA	1.82	0.41
1:C:160:GLY:O	1:C:521:ILE:HA	2.20	0.41
2:D:323:VAL:O	2:D:332:THR:HA	2.20	0.41
1:C:150:LEU:HD12	1:C:151:LEU:N	2.36	0.41
1:A:416:MET:CE	1:A:424:VAL:HG13	2.50	0.41
1:C:184:ARG:O	1:C:185:LEU:C	2.58	0.41
2:D:284:VAL:HG12	2:D:287:ARG:NH1	2.35	0.41
1:C:43:THR:CG2	1:C:73:ASN:HD21	2.32	0.41
1:C:488:ALA:O	1:C:490:PRO:HD3	2.20	0.41
1:C:503:GLN:HA	1:C:503:GLN:OE1	2.20	0.41
1:C:150:LEU:HG	1:C:152:ILE:CD1	2.51	0.41
1:C:101:SER:HB3	5:C:567:HOH:O	2.21	0.41
1:C:75:PHE:N	1:C:75:PHE:CD1	2.89	0.41
1:C:217:ILE:H	1:C:217:ILE:CD1	2.28	0.41
2:B:242:PRO:HG3	2:B:259:TRP:CH2	2.56	0.41
1:A:421:ASN:HD22	1:A:423:ILE:HG22	1.86	0.41
1:C:412:ILE:HD12	1:C:412:ILE:N	2.36	0.41
1:C:65:VAL:HG13	1:C:69:ASP:HB3	2.03	0.41
2:B:178:ILE:HG13	2:B:307:VAL:HG22	2.03	0.41
2:D:199:CYS:O	2:D:202:CYS:HB2	2.19	0.41
1:A:31:ALA:HB1	1:A:509:ILE:HD12	2.03	0.41
2:D:236:GLN:O	2:D:240:GLU:HG3	2.21	0.41
1:A:486:GLY:HA3	2:B:22:LYS:NZ	2.35	0.41
2:D:54:ILE:HB	2:D:143:CYS:HA	2.02	0.41
1:A:413:ILE:HD13	1:A:472:VAL:CG1	2.51	0.41
1:A:418:ASN:HD22	1:A:419:PRO:N	2.19	0.41
1:C:194:GLU:O	1:C:195:HIS:C	2.58	0.41
2:B:330:LEU:HD23	2:B:330:LEU:N	2.35	0.41
1:A:315:VAL:HG13	1:A:321:GLY:C	2.41	0.41
1:A:189:PHE:HE1	1:A:345:VAL:HG12	1.86	0.40
1:C:189:PHE:CZ	1:C:192:LEU:HB2	2.56	0.40
2:B:139:HIS:HB2	2:B:140:ILE:HD12	2.03	0.40
2:B:140:ILE:HG21	2:B:307:VAL:HG13	2.03	0.40
1:C:119:PHE:O	1:C:119:PHE:CG	2.73	0.40
1:A:318:GLU:H	1:A:318:GLU:CD	2.24	0.40
1:C:314:PHE:CE2	1:C:324:PRO:HG3	2.56	0.40
1:C:432:VAL:HG22	1:C:443:PRO:HG2	2.03	0.40
1:C:416:MET:HG3	1:C:472:VAL:HG11	2.03	0.40
1:C:277:ASN:HD22	1:C:278:THR:N	2.19	0.40
1:A:84:ASN:HD22	1:A:87:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:C	1:A:375:ILE:H	2.23	0.40
2:D:204:LEU:O	2:D:206:LEU:N	2.42	0.40
2:B:82:THR:HG23	2:B:100:GLY:O	2.21	0.40
1:A:318:GLU:OE2	1:A:318:GLU:N	2.52	0.40
2:B:804:GLY:O	2:B:805:GLN:C	2.60	0.40
1:A:285:ILE:H	1:A:285:ILE:CD1	2.34	0.40
2:B:361:LEU:O	2:B:363:GLU:N	2.51	0.40
2:D:75:ILE:O	2:D:120:VAL:HA	2.21	0.40
2:B:31:THR:HG23	2:B:35:PHE:CB	2.46	0.40
2:B:97:LYS:HG3	2:B:98:ASP:N	2.37	0.40
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.79	0.40
1:C:236:THR:HB	1:C:239:GLU:CG	2.52	0.40
2:D:241:GLN:NE2	2:D:245:GLU:C	2.74	0.40
2:B:114:ARG:O	2:B:116:PRO:HD3	2.22	0.40
2:D:39:THR:C	2:D:41:SER:H	2.25	0.40
1:C:108:SER:HB3	1:C:111:ASN:ND2	2.36	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	518/531 (98%)	477 (92%)	30 (6%)	11 (2%)	9	16
1	C	508/531 (96%)	435 (86%)	56 (11%)	17 (3%)	5	7
2	B	404/434 (93%)	362 (90%)	33 (8%)	9 (2%)	8	15
2	D	385/434 (89%)	330 (86%)	41 (11%)	14 (4%)	4	6
3	E	11/26 (42%)	11 (100%)	0	0	100	100
3	F	8/26 (31%)	7 (88%)	1 (12%)	0	100	100
All	All	1834/1982 (92%)	1622 (88%)	161 (9%)	51 (3%)	6	10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	THR
2	B	384	THR
1	C	38	ALA
1	C	227	SER
1	C	228	GLU
1	C	333	ILE
2	D	242	PRO
2	D	275	GLY
2	D	374	LEU
2	D	601	ASN
1	A	38	ALA
1	A	277	ASN
2	B	58	GLY
2	B	92	PHE
2	B	319	ASN
2	B	607	GLN
2	B	802	VAL
1	C	262	GLU
1	C	445	VAL
1	C	446	SER
1	C	448	TYR
1	C	485	TYR
1	C	519	THR
2	D	905	VAL
1	A	317	LYS
2	B	362	GLN
1	C	195	HIS
1	C	197	GLN
2	D	319	ASN
1	A	253	LYS
2	B	116	PRO
1	C	518	ASN
2	D	40	GLU
2	D	205	GLU
1	A	37	ASN
1	A	262	GLU
1	A	280	GLN
1	A	367	SER
1	C	454	ILE
2	D	33	PRO
2	D	241	GLN
2	D	272	ASN

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Mol	Chain	Res	Type
2	D	274	ARG
2	D	351	GLN
1	C	190	PRO
1	C	198	SER
2	B	242	PRO
1	C	371	ALA
2	D	246	GLY
1	A	368	ILE
1	A	372	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/462 (96%)	427 (96%)	18 (4%)	38	67
1	C	435/462 (94%)	415 (95%)	20 (5%)	33	61
2	B	325/383 (85%)	308 (95%)	17 (5%)	29	54
2	D	278/383 (73%)	263 (95%)	15 (5%)	27	52
3	E	12/22 (54%)	12 (100%)	0	100	100
3	F	9/22 (41%)	9 (100%)	0	100	100
All	All	1504/1734 (87%)	1434 (95%)	70 (5%)	32	59

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	47	LYS
1	A	111	ASN
1	A	154	ARG
1	A	171	VAL
1	A	215	ILE
1	A	228	GLU
1	A	234	PRO
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	259	PRO
1	A	285	ILE
1	A	298	THR
1	A	329	ILE
1	A	405	ASP
1	A	418	ASN
1	A	423	ILE
1	A	424	VAL
1	A	441	ARG
2	B	14	GLU
2	B	31	THR
2	B	45	LEU
2	B	77	VAL
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	132	ASP
2	B	142	VAL
2	B	154	ILE
2	B	160	SER
2	B	166	ASP
2	B	182	THR
2	B	201	GLU
2	B	204	LEU
2	B	215	MET
2	B	325	ASN
1	C	69	ASP
1	C	72	ASN
1	C	97	ASN
1	C	99	ASP
1	C	103	SER
1	C	147	GLN
1	C	186	ASP
1	C	190	PRO
1	C	228	GLU
1	C	233	ILE
1	C	235	LYS
1	C	253	LYS
1	C	277	ASN
1	C	408	ASN
1	C	434	ARG
1	C	441	ARG

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Mol	Chain	Res	Type
1	C	446	SER
1	C	515	ILE
1	C	518	ASN
1	C	527	GLN
2	D	35	PHE
2	D	110	PHE
2	D	114	ARG
2	D	128	GLN
2	D	131	ASN
2	D	188	ASN
2	D	201	GLU
2	D	214	PRO
2	D	242	PRO
2	D	260	ILE
2	D	313	SER
2	D	353	ILE
2	D	354	GLN
2	D	362	GLN
2	D	366	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	48	ASN
1	A	77	GLN
1	A	84	ASN
1	A	111	ASN
1	A	115	ASN
1	A	224	GLN
1	A	264	ASN
1	A	271	ASN
1	A	277	ASN
1	A	322	ASN
1	A	344	ASN
1	A	359	ASN
1	A	370	GLN
1	A	408	ASN
1	A	418	ASN
1	A	421	ASN
1	A	447	ASN
1	A	503	GLN

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Mol	Chain	Res	Type
1	A	518	ASN
2	B	19	HIS
2	B	32	HIS
2	B	87	ASN
2	B	128	GLN
2	B	137	GLN
2	B	227	HIS
2	B	236	GLN
2	B	325	ASN
2	B	351	GLN
1	C	84	ASN
1	C	97	ASN
1	C	111	ASN
1	C	130	GLN
1	C	145	ASN
1	C	147	GLN
1	C	169	HIS
1	C	195	HIS
1	C	271	ASN
1	C	273	ASN
1	C	277	ASN
1	C	322	ASN
1	C	343	GLN
1	C	344	ASN
1	C	360	HIS
1	C	439	GLN
1	C	517	ASN
1	C	518	ASN
1	C	527	GLN
1	C	533	GLN
2	D	19	HIS
2	D	32	HIS
2	D	131	ASN
2	D	137	GLN
2	D	139	HIS
2	D	188	ASN
2	D	227	HIS
2	D	241	GLN
2	D	256	HIS
2	D	272	ASN
2	D	282	GLN
2	D	348	GLN

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Mol	Chain	Res	Type
2	D	362	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 2 ligands modelled in this entry, 2 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	521/531 (98%)	-0.02	26 (4%) 32 26	25, 52, 111, 130	0
1	C	511/531 (96%)	0.31	43 (8%) 14 9	38, 74, 122, 143	0
2	B	414/434 (95%)	-0.13	17 (4%) 41 33	25, 44, 107, 125	0
2	D	392/434 (90%)	0.83	79 (20%) 1 1	34, 82, 141, 160	0
3	E	13/26 (50%)	0.62	2 (15%) 3 1	58, 69, 83, 88	1 (7%)
3	F	10/26 (38%)	4.08	10 (100%) 0 0	105, 108, 110, 112	3 (30%)
All	All	1861/1982 (93%)	0.25	177 (9%) 10 6	25, 61, 126, 160	4 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	33	PRO	10.4
1	A	236	THR	8.3
2	D	707	ARG	7.6
2	D	259	TRP	6.9
2	D	31	THR	6.9
2	D	606	LEU	6.8
1	A	210	SER	6.7
2	D	219	ALA	6.3
2	D	34	ASP	6.3
3	F	5	PHE	6.2
1	A	229	THR	6.1
2	D	29	PRO	6.1
1	C	372	PRO	6.0
1	C	259	PRO	5.8
2	D	211	VAL	5.4
2	D	248	PRO	5.3
3	F	11	LYS	5.3
1	C	232	ARG	5.3
1	C	447	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	5.1
2	D	702	THR	5.1
1	C	334	ALA	5.0
1	A	200	ASP	5.0
1	A	234	PRO	5.0
2	D	32	HIS	4.9
2	D	28	GLY	4.8
2	D	352	ASN	4.8
3	F	9	GLN	4.7
2	D	24	LEU	4.7
2	D	18	ASN	4.6
3	F	6	SER	4.6
3	F	13	GLU	4.6
2	D	209	PRO	4.5
2	B	801	LEU	4.5
1	A	2	ALA	4.4
2	D	600	LYS	4.3
1	C	335	ASP	4.3
1	A	252	LEU	4.2
2	B	355	PHE	4.2
2	D	17	TRP	4.2
2	D	232	VAL	4.2
2	D	701	VAL	4.2
1	C	228	GLU	4.0
2	B	9	MET	4.0
1	C	245	ASP	4.0
2	D	20	VAL	3.9
2	D	40	GLU	3.8
2	D	207	TYR	3.8
1	C	333	ILE	3.7
1	A	237	TYR	3.7
3	F	12	LYS	3.7
2	B	702	THR	3.7
3	F	4	LEU	3.7
2	D	706	GLU	3.7
1	C	211	HIS	3.7
1	A	374	SER	3.7
1	C	370	GLN	3.6
2	D	36	GLU	3.6
2	B	211	VAL	3.5
2	D	601	ASN	3.5
2	D	25	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	299	LYS	3.5
2	D	210	GLN	3.5
2	D	287	ARG	3.5
1	C	215	ILE	3.4
1	A	208	ASP	3.4
2	D	383	ALA	3.4
1	A	259	PRO	3.4
2	D	208	PRO	3.4
2	D	244	GLY	3.3
2	D	237	TRP	3.3
2	D	364	VAL	3.2
1	C	278	THR	3.2
2	D	46	LEU	3.2
2	D	228	CYS	3.1
1	C	451	GLU	3.1
1	A	1	MET	3.1
2	B	210	GLN	3.1
2	D	47	ASP	3.1
3	F	10	GLN	3.1
2	B	384	THR	3.0
2	B	707	ARG	3.0
2	D	234	MET	3.0
1	C	9	LYS	3.0
2	D	23	PHE	3.0
1	A	308	ALA	3.0
2	D	30	PHE	3.0
1	A	232	ARG	3.0
2	D	247	VAL	3.0
1	C	221	TYR	2.9
2	D	607	GLN	2.9
1	C	449	GLN	2.9
1	A	260	GLU	2.9
3	F	7	LEU	2.9
1	A	8	LEU	2.9
2	D	251	GLY	2.8
2	D	220	SER	2.8
1	C	292	ASP	2.8
2	D	708	THR	2.8
2	D	710	PRO	2.8
1	C	251	ILE	2.7
2	D	285	VAL	2.7
2	D	255	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	448	TYR	2.7
1	A	233	ILE	2.7
2	B	803	ASP	2.7
2	D	256	HIS	2.7
1	C	261	ASP	2.7
2	D	379	PRO	2.7
2	D	603	THR	2.6
1	A	310	ALA	2.6
2	D	243	PHE	2.6
1	A	3	GLN	2.6
1	C	37	ASN	2.6
2	D	35	PHE	2.6
2	D	384	THR	2.5
2	D	238	PRO	2.5
2	D	353	ILE	2.5
3	E	10	GLN	2.5
2	D	21	LYS	2.5
2	B	701	VAL	2.5
2	B	349	LEU	2.5
2	B	601	ASN	2.5
1	A	261	ASP	2.5
1	C	249	GLN	2.5
3	E	13	GLU	2.5
2	D	204	LEU	2.5
1	C	191	GLU	2.4
2	D	704	ILE	2.4
1	C	219	ALA	2.4
2	D	117	ASN	2.4
2	D	900	LEU	2.4
1	C	193	ARG	2.4
2	B	341	GLU	2.4
2	D	22	LYS	2.4
1	C	343	GLN	2.3
1	A	5	GLY	2.3
2	D	222	PRO	2.3
1	C	480	HIS	2.3
1	C	107	GLU	2.3
2	D	377	LYS	2.3
2	D	44	PHE	2.3
2	D	602	ARG	2.3
2	D	26	ARG	2.3
1	A	226	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	380	ALA	2.3
1	C	450	VAL	2.3
1	A	230	ASN	2.3
2	D	375	GLN	2.3
2	B	166	ASP	2.2
2	B	370	ASN	2.2
1	A	243	PHE	2.2
1	A	372	PRO	2.2
2	D	95	ARG	2.2
1	C	230	ASN	2.2
1	C	263	GLU	2.2
1	C	199	TYR	2.2
2	D	206	LEU	2.2
3	F	8	LYS	2.2
2	D	350	PRO	2.2
1	C	212	THR	2.2
1	C	443	PRO	2.2
1	C	84	ASN	2.2
2	D	278	TYR	2.1
2	D	227	HIS	2.1
1	C	250	GLY	2.1
1	C	336	SER	2.1
1	C	253	LYS	2.1
1	C	36	ILE	2.1
2	D	703	SER	2.1
2	D	1007	PHE	2.0
2	D	260	ILE	2.0
2	D	381	ILE	2.0
1	C	268	ALA	2.0
2	B	703	SER	2.0
2	B	381	ILE	2.0
1	A	4	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	B	1014	1/1	0.99	0.08	-1.40	49,49,49,49	0
4	ZN	D	1014	1/1	0.98	0.09	-2.92	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.