



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2JBU  
Title : CRYSTAL STRUCTURE OF HUMAN INSULIN DEGRADING ENZYME  
COMPLEXED WITH CO-PURIFIED PEPTIDES.  
Authors : Im, H.; Shen, Y.; Tang, W.J.  
Deposited on : 2006-12-11  
Resolution : 3.00 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

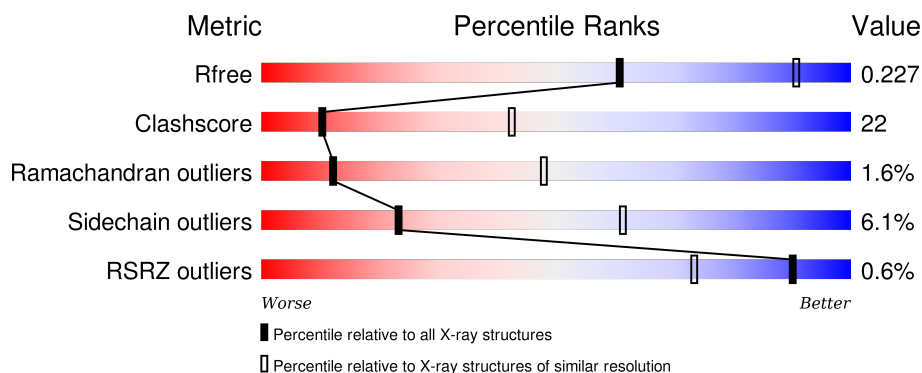
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	990	<div> <div style="width: 58%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> 58% 35% 5% .
1	B	990	<div> <div style="width: 55%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> 55% 37% . .
2	C	12	<div> <div style="width: 75%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 17%; background-color: grey;"></div> </div> 75% 8% 17%
2	D	12	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 17%; background-color: grey;"></div> </div> 67% 17% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	B	2017	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15899 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 INSULIN-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	1
			7859	5058	1318	1448	35			
1	B	961	Total	C	N	O	S	0	0	1
			7846	5049	1316	1446	35			

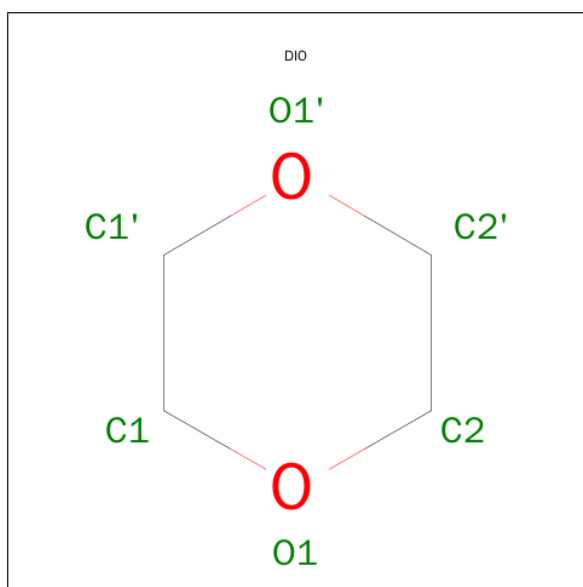
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLN	GLU	ENGINEERED MUTATION	UNP Q5T5N2
B	111	GLN	GLU	ENGINEERED MUTATION	UNP Q5T5N2

- Molecule 2 is a protein called CO-PURIFIED PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			51	30	10	11			
2	D	10	Total	C	N	O	0	0	0
			51	30	10	11			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		

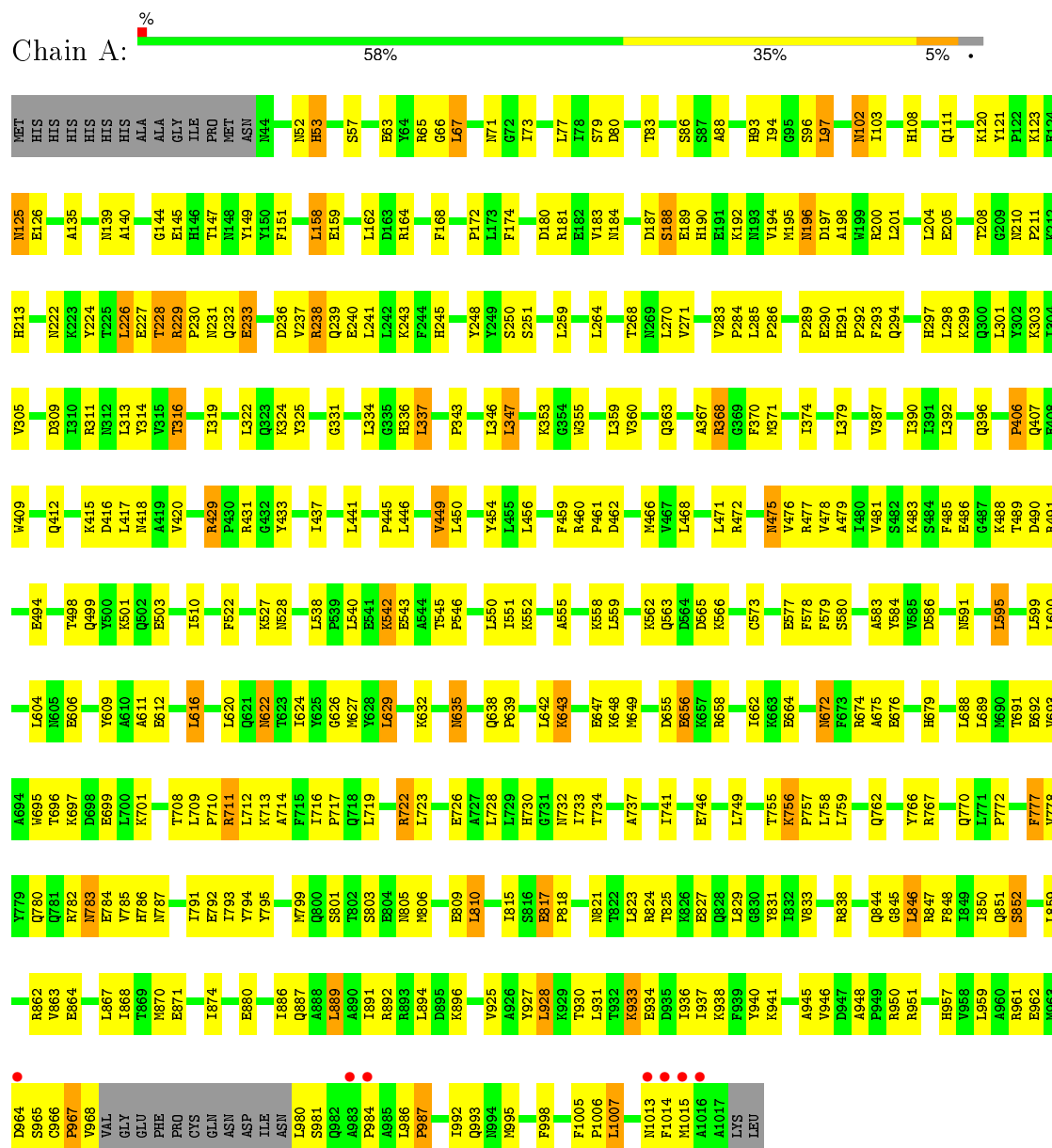
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	35	Total	O	0	0
			35	35		
4	D	1	Total	O	0	0
			1	1		

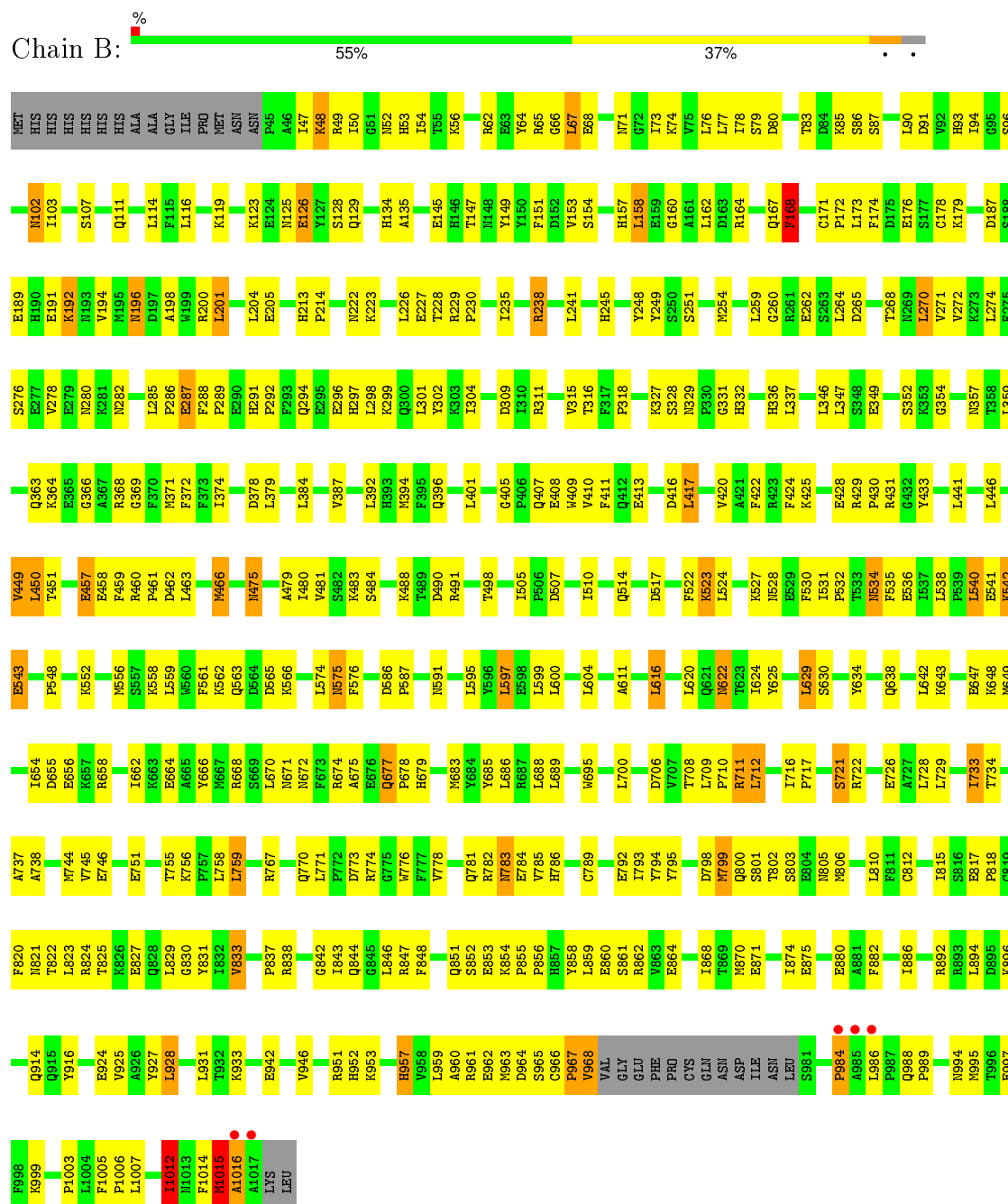
### 3 Residue-property plots

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: INSULIN-DEGRADING ENZYME



#### • Molecule 1: INSULIN-DEGRADING ENZYME



• Molecule 2: CO-PURIFIED PEPTIDE



• Molecule 2: CO-PURIFIED PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.28 Å   263.28 Å   90.73 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.86 – 3.00 49.75 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.86-3.00) 98.0 (49.75-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 3.01 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.186 , 0.240 0.180 , 0.227	Depositor DCC
$R_{free}$ test set	3670 reflections (5.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.3	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72861 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: DIO

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	0.51	0/8056	0.72	1/10896 (0.0%)
1	B	0.47	0/8043	0.69	1/10877 (0.0%)
2	C	0.93	0/49	0.72	0/64
2	D	0.77	0/49	0.72	0/64
All	All	0.49	0/16197	0.71	2/21901 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PHE	N-CA-C	-7.20	91.55	111.00
1	A	429	ARG	N-CA-C	-5.38	96.47	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7859	0	7788	310	0
1	B	7846	0	7776	372	0
2	C	51	0	51	3	0
2	D	51	0	51	3	0
3	A	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	2	0
4	A	44	0	0	2	0
4	B	35	0	0	4	0
4	D	1	0	0	0	0
All	All	15899	0	15682	679	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 22.

All (679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:LEU:HD23	1:B:928:LEU:HD21	1.30	1.12
1:A:538:LEU:HD23	1:A:734:THR:HG23	1.38	1.06
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.39	1.01
1:A:309:ASP:H	1:A:672:ASN:HD21	1.11	0.98
1:B:309:ASP:H	1:B:672:ASN:HD21	1.02	0.98
1:A:162:LEU:HD23	1:A:270:LEU:HD11	1.47	0.96
1:A:622:ASN:H	1:A:622:ASN:HD22	1.03	0.94
1:A:604:LEU:HD21	1:A:648:LYS:HG3	1.49	0.94
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.32	0.92
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.50	0.91
1:A:111:GLN:HE22	2:C:10:ALA:HB2	1.35	0.91
1:A:429:ARG:HH11	1:A:431:ARG:HB3	1.33	0.91
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.53	0.90
1:B:446:LEU:HD22	1:B:446:LEU:H	1.35	0.88
1:A:829:LEU:O	1:A:852:SER:HB2	1.73	0.88
1:B:309:ASP:H	1:B:672:ASN:ND2	1.69	0.88
1:B:1014:PHE:O	1:B:1015:MET:HB2	1.72	0.88
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.73	0.87
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.56	0.85
1:A:111:GLN:NE2	2:C:10:ALA:HB2	1.91	0.85
1:A:294:GLN:H	1:A:297:HIS:HD2	1.20	0.84
1:A:783:ASN:ND2	1:A:786:HIS:H	1.77	0.82
1:B:311:ARG:NH2	1:B:668:ARG:HE	1.77	0.82
1:B:540:LEU:HD12	1:B:563:GLN:OE1	1.81	0.80
1:B:783:ASN:ND2	1:B:786:HIS:H	1.79	0.80
1:A:125:ASN:HD22	1:A:125:ASN:H	1.30	0.80
1:B:65:ARG:HB2	1:B:264:LEU:HD13	1.64	0.80
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.63	0.79
1:B:534:ASN:HD21	1:B:536:GLU:HG2	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:OD1	1:A:491:ARG:HG3	1.84	0.78
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.20	0.77
1:B:815:ILE:HA	1:B:870:MET:HE2	1.66	0.77
1:A:309:ASP:H	1:A:672:ASN:ND2	1.82	0.77
1:B:196:ASN:ND2	1:B:198:ALA:H	1.81	0.77
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.68	0.76
1:A:316:THR:HG23	1:A:374:ILE:HG22	1.65	0.76
1:A:622:ASN:H	1:A:622:ASN:ND2	1.81	0.76
1:B:575:ASN:HD22	1:B:575:ASN:N	1.84	0.76
1:A:609:TYR:O	1:A:612:GLU:HB3	1.85	0.76
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.17	0.75
1:A:622:ASN:N	1:A:622:ASN:HD22	1.82	0.75
1:A:289:PRO:O	1:A:290:GLU:HB3	1.87	0.75
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.32	0.75
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.69	0.74
1:B:810:LEU:CD2	1:B:928:LEU:HD21	2.15	0.74
1:B:798:ASP:CG	1:B:799:MET:H	1.89	0.74
1:A:656:GLU:OE1	1:A:709:LEU:HD22	1.87	0.74
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.69	0.74
1:A:538:LEU:HD23	1:A:734:THR:CG2	2.16	0.73
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.23	0.73
1:B:689:LEU:HG	1:B:995:MET:HE1	1.70	0.73
1:A:196:ASN:HD22	1:A:197:ASP:N	1.86	0.73
1:A:71:ASN:HB2	1:A:251:SER:OG	1.88	0.72
1:B:90:LEU:HD11	1:B:254:MET:CE	2.19	0.72
1:B:782:ARG:HG3	1:B:959:LEU:HB2	1.71	0.72
1:B:960:ALA:HB3	1:B:963:MET:HB2	1.72	0.72
1:A:145:GLU:OE2	1:A:367:ALA:HB1	1.90	0.72
1:B:778:VAL:HG21	1:B:968:VAL:HG21	1.71	0.72
1:A:863:VAL:O	1:A:867:LEU:HD23	1.89	0.71
1:B:422:PHE:CZ	1:B:451:THR:HG22	2.24	0.71
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.36	0.71
1:B:604:LEU:HD21	1:B:648:LYS:HG3	1.70	0.71
1:B:534:ASN:HD22	1:B:534:ASN:C	1.93	0.71
1:A:392:LEU:O	1:A:396:GLN:HG3	1.91	0.71
1:B:677:GLN:HG3	1:B:786:HIS:CE1	2.26	0.71
1:B:805:ASN:ND2	1:B:844:GLN:HE22	1.89	0.71
1:A:236:ASP:CG	1:A:239:GLN:HG2	2.12	0.70
1:B:517:ASP:HB2	4:B:3016:HOH:O	1.90	0.70
1:A:205:GLU:HG3	3:A:2017:DIO:H1'2	1.74	0.69
1:B:574:LEU:C	1:B:575:ASN:HD22	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:HG22	1:B:47:ILE:O	1.90	0.69
1:B:172:PRO:HB2	1:B:174:PHE:CE1	2.27	0.69
1:B:311:ARG:HA	1:B:481:VAL:O	1.93	0.69
1:B:174:PHE:O	1:B:238:ARG:HD3	1.92	0.69
1:B:205:GLU:HG3	3:B:2017:DIO:H1'2	1.73	0.69
1:A:783:ASN:HD21	1:A:786:HIS:H	1.36	0.68
1:B:679:HIS:O	1:B:683:MET:HG3	1.93	0.68
1:B:770:GLN:HB3	1:B:1003:PRO:HG2	1.76	0.67
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.25	0.67
1:A:449:VAL:HG23	1:A:450:LEU:CD1	2.25	0.67
1:B:331:GLY:HA3	1:B:363:GLN:OE1	1.95	0.67
1:B:475:ASN:H	1:B:475:ASN:HD22	1.43	0.67
1:A:805:ASN:ND2	1:A:844:GLN:HE22	1.92	0.66
1:A:102:ASN:ND2	1:A:103:ILE:HG13	2.11	0.66
1:B:416:ASP:O	1:B:420:VAL:HG23	1.95	0.66
1:B:629:LEU:HD22	1:B:630:SER:N	2.09	0.66
1:B:446:LEU:CD2	1:B:446:LEU:H	2.08	0.66
1:B:200:ARG:NH2	1:B:498:THR:HA	2.11	0.66
1:B:600:LEU:HD21	1:B:649:MET:HB3	1.78	0.66
1:A:180:ASP:O	1:A:183:VAL:HG12	1.95	0.66
1:A:204:LEU:HG	3:A:2017:DIO:H22	1.78	0.65
1:A:538:LEU:CD2	1:A:734:THR:HG23	2.23	0.65
1:A:172:PRO:HB2	1:A:174:PHE:CE1	2.32	0.65
1:B:874:ILE:O	1:B:933:LYS:HE3	1.96	0.65
1:B:510:ILE:O	1:B:514:GLN:HG3	1.97	0.65
1:B:196:ASN:ND2	1:B:198:ALA:N	2.45	0.65
1:A:63:GLU:HB2	1:A:79:SER:HB3	1.77	0.65
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.77	0.65
1:B:967:PRO:HD3	4:B:3034:HOH:O	1.95	0.65
1:A:162:LEU:HD23	1:A:270:LEU:CD1	2.25	0.65
1:A:222:ASN:O	1:A:226:LEU:HB2	1.98	0.64
1:A:174:PHE:O	1:A:238:ARG:HD3	1.97	0.64
1:A:359:LEU:HD23	1:A:360:VAL:N	2.13	0.64
1:A:565:ASP:OD2	1:A:566:LYS:HE3	1.97	0.64
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.31	0.64
1:B:349:GLU:HA	1:B:349:GLU:OE2	1.97	0.64
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.78	0.64
1:B:599:LEU:CD2	1:B:662:ILE:HD12	2.22	0.64
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.79	0.64
1:B:711:ARG:CG	1:B:711:ARG:HH21	2.10	0.64
1:B:846:LEU:HD23	1:B:847:ARG:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ASN:HD22	1:B:475:ASN:N	1.96	0.64
1:A:846:LEU:HD23	1:A:847:ARG:N	2.12	0.63
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.80	0.63
1:A:874:ILE:O	1:A:933:LYS:HD3	1.98	0.63
1:B:245:HIS:O	1:B:249:TYR:HB2	1.98	0.63
1:B:733:ILE:HG13	1:B:737:ALA:HB3	1.78	0.63
1:B:407:GLN:HG3	1:B:409:TRP:NE1	2.14	0.63
1:B:622:ASN:H	1:B:622:ASN:HD22	1.46	0.63
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.81	0.63
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.80	0.63
1:B:298:LEU:HD21	1:B:318:PRO:HG2	1.80	0.63
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.80	0.62
1:A:196:ASN:C	1:A:196:ASN:HD22	2.02	0.62
1:B:597:LEU:HG	1:B:620:LEU:HG	1.81	0.62
1:B:80:ASP:O	1:B:83:THR:HG22	1.98	0.62
1:B:994:ASN:HB3	1:B:997:GLU:HB2	1.81	0.62
1:B:591:ASN:ND2	1:B:700:LEU:HD22	2.14	0.62
1:B:846:LEU:HD23	1:B:847:ARG:H	1.64	0.62
1:B:407:GLN:HG3	1:B:409:TRP:CD1	2.35	0.62
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.35	0.62
1:B:309:ASP:N	1:B:672:ASN:HD21	1.84	0.61
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.82	0.61
1:A:805:ASN:HD22	1:A:844:GLN:NE2	1.97	0.61
1:B:803:SER:HA	1:B:927:TYR:CE2	2.35	0.61
1:B:776:TRP:NE1	1:B:953:LYS:HE2	2.15	0.61
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.00	0.61
1:A:770:GLN:HA	1:A:1005:PHE:CE1	2.35	0.61
1:B:671:ASN:O	1:B:674:ARG:HG2	2.00	0.61
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.82	0.61
1:B:102:ASN:HD22	1:B:102:ASN:H	1.47	0.61
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.36	0.61
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.35	0.61
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.67	0.60
1:B:329:ASN:HB3	1:B:332:HIS:HB2	1.83	0.60
1:A:643:LYS:HE2	1:A:647:GLU:OE2	2.02	0.60
1:B:541:GLU:HB3	1:B:543:GLU:OE2	2.02	0.60
1:B:119:LYS:HB2	1:B:171:CYS:SG	2.41	0.60
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.82	0.60
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.83	0.60
1:B:789:CYS:SG	1:B:963:MET:SD	2.99	0.60
1:B:167:GLN:C	1:B:168:PHE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HB2	1:B:264:LEU:HD23	1.83	0.59
1:A:201:LEU:HD21	1:A:481:VAL:HG21	1.83	0.59
1:A:577:GLU:HG2	1:A:579:PHE:CZ	2.37	0.59
1:B:542:LYS:NZ	1:B:542:LYS:HB2	2.17	0.59
1:A:294:GLN:H	1:A:297:HIS:CD2	2.12	0.59
1:B:102:ASN:HD22	1:B:102:ASN:N	1.99	0.59
1:A:476:VAL:HG22	1:A:477:ARG:N	2.16	0.59
1:B:556:MET:HG2	1:B:746:GLU:HG2	1.84	0.59
1:A:545:THR:HB	1:A:546:PRO:HD2	1.85	0.59
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.01	0.59
1:B:854:LYS:HB2	1:B:859:LEU:HD21	1.84	0.59
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.85	0.59
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.67	0.59
1:B:428:GLU:HG2	1:B:433:TYR:CD1	2.38	0.59
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.18	0.59
1:A:709:LEU:HD11	1:A:713:LYS:HE3	1.85	0.59
1:A:777:PHE:N	1:A:777:PHE:CD1	2.71	0.59
1:B:683:MET:HA	1:B:792:GLU:OE2	2.02	0.58
1:A:552:LYS:NZ	1:A:746:GLU:OE1	2.35	0.58
1:A:67:LEU:C	1:A:67:LEU:HD12	2.23	0.58
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.58
1:A:870:MET:O	1:A:874:ILE:HG13	2.03	0.58
1:A:125:ASN:HD22	1:A:125:ASN:N	2.01	0.58
1:B:600:LEU:CD2	1:B:649:MET:HB3	2.33	0.58
1:A:550:LEU:N	1:A:1015:MET:SD	2.62	0.58
1:B:810:LEU:HD21	1:B:886:ILE:HG12	1.85	0.58
1:A:227:GLU:O	1:A:230:PRO:HD2	2.04	0.58
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.85	0.58
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.84	0.58
1:B:654:ILE:HD13	1:B:712:LEU:HD13	1.85	0.58
1:A:162:LEU:CD2	1:A:270:LEU:HD11	2.28	0.58
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.34	0.58
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.18	0.58
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.68	0.58
1:A:205:GLU:HG2	1:A:293:PHE:HZ	1.69	0.58
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.34	0.58
1:A:227:GLU:C	1:A:230:PRO:HD2	2.25	0.57
1:B:268:THR:O	1:B:272:VAL:HG23	2.04	0.57
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.39	0.57
1:A:197:ASP:O	1:A:201:LEU:HD13	2.03	0.57
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ASN:O	1:B:595:LEU:HB2	2.04	0.57
1:B:858:TYR:CZ	1:B:862:ARG:HD2	2.39	0.57
1:B:961:ARG:NH1	1:B:962:GLU:OE1	2.36	0.57
1:A:611:ALA:HB1	1:A:616:LEU:HB3	1.87	0.57
1:B:666:TYR:CZ	1:B:670:LEU:HD11	2.38	0.57
1:A:471:LEU:HD23	1:A:471:LEU:N	2.20	0.57
1:B:817:GLU:CB	1:B:818:PRO:HD3	2.34	0.57
1:A:778:VAL:HG21	1:A:968:VAL:HG11	1.86	0.57
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.19	0.57
1:B:384:LEU:O	1:B:384:LEU:HD12	2.04	0.57
1:B:831:TYR:CE2	2:D:12:ALA:HB2	2.39	0.57
1:B:54:ILE:HD12	1:B:446:LEU:O	2.05	0.56
1:B:534:ASN:ND2	1:B:536:GLU:H	2.02	0.56
1:A:159:GLU:HG3	1:A:270:LEU:HD21	1.86	0.56
1:B:675:ALA:HA	1:B:785:VAL:HG21	1.87	0.56
1:A:696:THR:OG1	1:A:699:GLU:HG3	2.03	0.56
1:B:147:THR:HG21	1:B:249:TYR:OH	2.05	0.56
1:A:980:LEU:N	4:A:3041:HOH:O	2.38	0.56
1:A:868:ILE:HD11	1:A:984:PRO:HB3	1.88	0.56
1:B:534:ASN:C	1:B:534:ASN:ND2	2.58	0.56
1:B:408:GLU:HB2	1:B:459:PHE:CE2	2.40	0.56
1:A:966:CYS:SG	1:A:967:PRO:HD2	2.45	0.56
1:B:387:VAL:HG21	1:B:480:ILE:HD13	1.87	0.56
1:B:864:GLU:OE1	1:B:951:ARG:NH2	2.35	0.56
1:A:767:ARG:HD3	1:A:1005:PHE:O	2.06	0.56
1:B:446:LEU:HD22	1:B:446:LEU:N	2.15	0.56
1:B:90:LEU:HD11	1:B:254:MET:HE2	1.86	0.56
1:A:479:ALA:HB2	3:A:2017:DIO:H12	1.88	0.56
1:B:706:ASP:O	1:B:708:THR:HG23	2.06	0.56
1:B:812:CYS:SG	1:B:837:PRO:HD3	2.45	0.56
1:B:160:GLY:O	1:B:164:ARG:HG3	2.05	0.56
1:A:181:ARG:O	1:A:184:ASN:HB2	2.06	0.56
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.88	0.56
1:B:538:LEU:H	1:B:538:LEU:HD12	1.70	0.56
1:A:204:LEU:O	1:A:208:THR:HG23	2.07	0.55
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.41	0.55
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.06	0.55
1:A:196:ASN:ND2	1:A:198:ALA:H	2.04	0.55
1:A:805:ASN:ND2	1:A:844:GLN:NE2	2.55	0.55
1:A:93:HIS:HD2	1:A:145:GLU:O	1.90	0.55
1:B:722:ARG:NH1	1:B:756:LYS:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLU:HG3	1:B:709:LEU:CD2	2.36	0.55
1:A:540:LEU:HD12	1:A:563:GLN:OE1	2.05	0.55
1:B:66:GLY:O	1:B:67:LEU:HB3	2.06	0.55
1:B:71:ASN:HB2	1:B:251:SER:OG	2.06	0.55
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.87	0.55
1:A:823:LEU:HD12	1:A:829:LEU:CD1	2.37	0.55
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.55	0.55
1:A:616:LEU:HD21	1:A:638:GLN:HG2	1.89	0.55
1:B:47:ILE:O	1:B:48:LYS:C	2.45	0.55
1:B:172:PRO:HB2	1:B:174:PHE:HE1	1.71	0.55
1:B:119:LYS:HD2	1:B:171:CYS:HB2	1.89	0.55
1:A:562:LYS:HD3	1:A:730:HIS:CE1	2.42	0.55
1:B:778:VAL:HG23	1:B:989:PRO:HB2	1.89	0.54
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.37	0.54
1:A:322:LEU:HD12	1:A:363:GLN:NE2	2.21	0.54
1:B:789:CYS:SG	1:B:856:PRO:HD3	2.48	0.54
1:B:479:ALA:HB2	3:B:2017:DIO:H12	1.90	0.54
1:B:868:ILE:HD11	1:B:984:PRO:HB3	1.89	0.54
1:A:236:ASP:OD1	1:A:239:GLN:HG2	2.08	0.54
1:A:868:ILE:CD1	1:A:984:PRO:HD3	2.38	0.54
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.43	0.54
1:B:316:THR:HG23	1:B:374:ILE:HG22	1.90	0.54
1:A:224:TYR:HA	1:A:228:THR:HB	1.89	0.54
1:A:240:GLU:OE2	1:A:243:LYS:HD2	2.08	0.54
1:A:102:ASN:HD22	1:A:102:ASN:N	2.06	0.54
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.42	0.54
1:A:77:LEU:HD11	1:A:268:THR:HA	1.90	0.54
1:A:200:ARG:NH2	1:A:498:THR:HA	2.23	0.54
1:B:111:GLN:HE21	2:D:10:ALA:HB2	1.73	0.54
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.90	0.53
1:B:134:HIS:HD2	1:B:157:HIS:CD2	2.26	0.53
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.43	0.53
1:A:655:ASP:HB3	1:A:658:ARG:HB2	1.90	0.53
1:B:49:ARG:HG2	1:B:50:ILE:H	1.74	0.53
1:A:196:ASN:O	1:A:200:ARG:HG3	2.09	0.53
1:A:86:SER:HB3	1:A:158:LEU:HG	1.91	0.53
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.89	0.53
1:B:449:VAL:HG23	1:B:450:LEU:H	1.74	0.53
1:B:417:LEU:HD21	1:B:531:ILE:HG12	1.89	0.53
1:B:287:GLU:OE1	1:B:289:PRO:HD3	2.09	0.53
1:A:331:GLY:HA3	1:A:363:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:LEU:HB2	1:B:833:VAL:HG11	1.91	0.53
1:B:540:LEU:HA	1:B:563:GLN:OE1	2.09	0.53
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.90	0.53
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.09	0.52
1:A:483:LYS:O	1:A:486:GLU:HB2	2.09	0.52
1:A:927:TYR:O	1:A:930:THR:HB	2.09	0.52
1:B:1014:PHE:O	1:B:1015:MET:CB	2.51	0.52
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.90	0.52
1:B:1012:ILE:HD11	1:B:1014:PHE:CE1	2.44	0.52
1:A:196:ASN:ND2	1:A:196:ASN:C	2.61	0.52
1:B:78:ILE:O	1:B:259:LEU:HA	2.10	0.52
1:A:231:ASN:O	1:A:233:GLU:N	2.36	0.52
1:B:409:TRP:CE2	1:B:410:VAL:HG23	2.44	0.52
1:A:558:LYS:HB3	1:A:726:GLU:HG3	1.91	0.52
1:B:392:LEU:O	1:B:396:GLN:HG3	2.10	0.52
1:A:407:GLN:HG3	1:A:409:TRP:CD1	2.44	0.52
1:B:733:ILE:CG1	1:B:737:ALA:HB3	2.39	0.52
1:B:119:LYS:CD	1:B:171:CYS:HB2	2.40	0.52
1:A:359:LEU:HD23	1:A:359:LEU:C	2.29	0.52
1:B:733:ILE:HG13	1:B:737:ALA:CB	2.40	0.52
1:B:179:LYS:HB3	1:B:179:LYS:HZ3	1.75	0.52
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.44	0.52
1:A:810:LEU:HD13	1:A:936:ILE:HG13	1.92	0.52
1:A:324:LYS:HE3	1:A:325:TYR:CZ	2.45	0.52
1:B:733:ILE:HG12	1:B:734:THR:N	2.25	0.51
1:B:48:LYS:HD2	1:B:68:GLU:CD	2.30	0.51
1:A:429:ARG:NH1	1:A:431:ARG:HB3	2.16	0.51
1:B:798:ASP:CG	1:B:799:MET:N	2.59	0.51
1:B:882:PHE:CE1	1:B:933:LYS:HA	2.46	0.51
1:B:179:LYS:HB3	1:B:179:LYS:NZ	2.24	0.51
1:B:806:MET:SD	1:B:924:GLU:HB3	2.50	0.51
1:B:968:VAL:HG22	1:B:989:PRO:HG3	1.92	0.51
1:A:231:ASN:C	1:A:233:GLU:H	2.13	0.51
1:B:831:TYR:HE2	2:D:12:ALA:HB2	1.75	0.51
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.92	0.51
1:B:196:ASN:HD22	1:B:198:ALA:N	2.09	0.51
1:B:86:SER:HB3	1:B:158:LEU:HG	1.93	0.51
1:A:499:GLN:OE1	1:A:499:GLN:HA	2.11	0.51
1:A:406:PRO:HG3	1:A:461:PRO:HB3	1.93	0.50
1:B:574:LEU:CD2	1:B:729:LEU:HD22	2.41	0.50
1:B:102:ASN:ND2	1:B:102:ASN:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HB3	1:A:1015:MET:HB2	1.92	0.50
1:A:723:LEU:HD12	1:A:755:THR:HG21	1.93	0.50
1:A:697:LYS:O	1:A:701:LYS:HG2	2.11	0.50
1:A:787:ASN:HB2	1:A:961:ARG:NH2	2.26	0.50
1:B:800:GLN:HA	1:B:805:ASN:HD21	1.75	0.50
1:B:407:GLN:O	1:B:410:VAL:HB	2.11	0.50
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.44	0.50
1:A:189:GLU:O	1:A:192:LYS:HG2	2.11	0.50
1:B:882:PHE:CZ	1:B:933:LYS:HA	2.46	0.50
1:A:183:VAL:HG23	1:A:226:LEU:HB3	1.94	0.50
1:B:449:VAL:HG23	1:B:450:LEU:N	2.27	0.50
1:A:733:ILE:HD11	1:A:741:ILE:HD12	1.93	0.50
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.77	0.50
1:A:791:ILE:HG21	1:A:859:LEU:HD23	1.93	0.50
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.46	0.50
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.47	0.50
1:B:328:SER:HB3	1:B:458:GLU:O	2.12	0.50
1:B:773:ASP:O	1:B:774:ARG:HB2	2.11	0.50
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.94	0.49
1:B:251:SER:HB3	1:B:278:VAL:CG1	2.39	0.49
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.95	0.49
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.94	0.49
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.15	0.49
1:B:158:LEU:O	1:B:158:LEU:HD23	2.12	0.49
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.93	0.49
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.94	0.49
1:A:555:ALA:HB1	1:A:757:PRO:HB3	1.93	0.49
1:A:827:GLU:OE2	1:A:862:ARG:NH1	2.45	0.49
1:A:578:PHE:HB2	1:A:627:MET:HB2	1.93	0.49
1:A:759:LEU:HD13	1:A:762:GLN:OE1	2.12	0.49
1:A:313:LEU:HD22	1:A:387:VAL:HG13	1.94	0.49
1:B:311:ARG:HH21	1:B:668:ARG:HE	1.56	0.49
1:A:313:LEU:HD12	1:A:314:TYR:N	2.28	0.49
1:A:799:MET:SD	1:A:1006:PRO:HG2	2.53	0.49
1:B:565:ASP:OD2	1:B:566:LYS:HG3	2.12	0.49
1:A:622:ASN:N	1:A:622:ASN:ND2	2.51	0.49
1:A:786:HIS:O	1:A:961:ARG:HB2	2.13	0.49
1:B:357:ASN:HB2	1:B:378:ASP:OD1	2.13	0.49
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.48	0.49
1:B:490:ASP:OD1	1:B:491:ARG:HG3	2.12	0.49
1:B:93:HIS:HD2	1:B:145:GLU:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:C	1:A:758:LEU:HD13	2.33	0.48
1:B:49:ARG:HG2	1:B:50:ILE:N	2.28	0.48
1:B:189:GLU:O	1:B:192:LYS:HG3	2.13	0.48
1:A:237:VAL:O	1:A:240:GLU:N	2.47	0.48
1:A:164:ARG:HG3	1:A:164:ARG:NH1	2.28	0.48
1:B:259:LEU:C	1:B:259:LEU:HD23	2.33	0.48
1:B:854:LYS:HA	1:B:854:LYS:HE2	1.95	0.48
1:B:311:ARG:NH2	1:B:668:ARG:NE	2.56	0.48
1:B:793:ILE:HG22	1:B:795:TYR:CE1	2.48	0.48
1:A:809:GLU:HB3	1:A:889:LEU:HD11	1.95	0.48
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	0.48
1:B:823:LEU:HD12	1:B:829:LEU:HD12	1.96	0.48
1:B:820:PHE:CZ	1:B:824:ARG:HD3	2.48	0.48
1:A:950:ARG:HB3	1:A:950:ARG:HH11	1.79	0.48
1:A:334:LEU:CD2	1:A:468:LEU:HD13	2.44	0.48
1:A:52:ASN:O	1:A:53:HIS:C	2.52	0.48
1:B:686:LEU:HD23	1:B:838:ARG:NH1	2.29	0.48
1:A:679:HIS:ND1	1:A:851:GLN:OE1	2.47	0.48
1:B:942:GLU:O	1:B:942:GLU:HG2	2.14	0.48
1:A:600:LEU:HD21	1:A:649:MET:HB3	1.95	0.48
1:B:294:GLN:O	1:B:298:LEU:HG	2.12	0.48
1:A:783:ASN:ND2	1:A:786:HIS:N	2.56	0.48
1:B:538:LEU:N	1:B:538:LEU:HD12	2.28	0.48
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.96	0.47
1:B:251:SER:OG	1:B:280:ASN:HB2	2.14	0.47
1:B:733:ILE:CG1	1:B:734:THR:N	2.77	0.47
1:B:56:LYS:NZ	1:B:62:ARG:O	2.38	0.47
1:B:204:LEU:CD2	1:B:304:ILE:HG12	2.44	0.47
1:A:314:TYR:HB2	1:A:479:ALA:HB3	1.95	0.47
1:B:475:ASN:ND2	1:B:475:ASN:N	2.62	0.47
1:B:802:THR:O	1:B:806:MET:HG2	2.14	0.47
1:B:821:ASN:O	1:B:825:THR:HB	2.13	0.47
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.95	0.47
1:B:575:ASN:ND2	1:B:575:ASN:N	2.55	0.47
1:B:622:ASN:H	1:B:622:ASN:ND2	2.12	0.47
1:B:868:ILE:O	1:B:871:GLU:HB3	2.15	0.47
1:B:871:GLU:O	1:B:875:GLU:HG3	2.15	0.47
1:B:914:GLN:HA	1:B:916:TYR:CE1	2.50	0.47
1:B:299:LYS:HA	1:B:505:ILE:HD12	1.96	0.47
1:A:674:ARG:HG3	1:A:674:ARG:HH11	1.80	0.47
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LEU:HD12	1:A:829:LEU:HD11	1.95	0.47
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.50	0.47
1:B:823:LEU:HD12	1:B:829:LEU:CD1	2.44	0.47
1:A:803:SER:HA	1:A:927:TYR:CE2	2.49	0.47
1:A:896:LYS:HD3	1:A:896:LYS:HA	1.59	0.47
1:B:123:LYS:HB3	1:B:126:GLU:HG2	1.97	0.47
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.47	0.47
1:B:830:GLY:HA3	1:B:851:GLN:O	2.15	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE2	2.50	0.47
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.97	0.47
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.97	0.47
1:A:80:ASP:O	1:A:83:THR:HG22	2.14	0.47
1:B:223:LYS:HE3	1:B:227:GLU:OE1	2.14	0.47
1:A:817:GLU:N	1:A:818:PRO:CD	2.77	0.47
1:B:789:CYS:O	1:B:851:GLN:HG3	2.15	0.47
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.17	0.47
1:B:643:LYS:O	1:B:647:GLU:HB2	2.15	0.47
1:B:151:PHE:CD1	1:B:151:PHE:C	2.88	0.47
1:A:123:LYS:HG2	1:A:125:ASN:ND2	2.30	0.47
1:A:558:LYS:HE3	1:A:558:LYS:HB2	1.80	0.47
1:A:880:GLU:HG3	1:B:327:LYS:HD3	1.97	0.47
1:A:722:ARG:CG	1:A:758:LEU:HD12	2.45	0.47
1:B:624:ILE:HG13	1:B:625:TYR:CD2	2.50	0.47
1:A:418:ASN:HB3	1:A:454:TYR:O	2.15	0.46
1:B:988:GLN:NE2	1:B:989:PRO:HD2	2.30	0.46
1:B:822:THR:O	1:B:827:GLU:HG3	2.15	0.46
1:B:49:ARG:CG	1:B:50:ILE:H	2.28	0.46
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.96	0.46
1:A:722:ARG:HG2	1:A:758:LEU:HD12	1.97	0.46
1:B:688:LEU:O	1:B:999:LYS:HE2	2.15	0.46
1:B:852:SER:OG	1:B:853:GLU:N	2.48	0.46
1:B:280:ASN:OD1	1:B:282:ASN:N	2.48	0.46
1:B:134:HIS:HD2	1:B:157:HIS:CG	2.34	0.46
1:B:103:ILE:HD11	1:B:235:ILE:HG21	1.98	0.46
1:B:815:ILE:HA	1:B:870:MET:CE	2.43	0.46
1:A:708:THR:OG1	1:A:711:ARG:HB2	2.15	0.46
1:A:174:PHE:CD2	1:A:241:LEU:HB3	2.51	0.46
1:A:838:ARG:O	1:A:844:GLN:HA	2.16	0.46
1:A:933:LYS:O	1:A:937:ILE:HG12	2.16	0.46
1:A:66:GLY:O	1:A:67:LEU:HB3	2.16	0.46
1:B:116:LEU:CD1	1:B:178:CYS:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG2	1:A:245:HIS:NE2	2.30	0.46
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.31	0.46
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.97	0.46
1:B:463:LEU:O	1:B:466:MET:HB3	2.16	0.46
1:A:551:ILE:HD11	1:A:559:LEU:CD2	2.46	0.45
1:B:751:GLU:O	1:B:751:GLU:HG2	2.16	0.45
1:B:928:LEU:O	1:B:928:LEU:HD22	2.16	0.45
1:A:194:VAL:HG12	1:A:195:MET:CE	2.47	0.45
1:B:196:ASN:HD21	1:B:198:ALA:H	1.61	0.45
1:B:800:GLN:CA	1:B:805:ASN:HD21	2.29	0.45
1:A:838:ARG:HG3	1:A:847:ARG:HD3	1.98	0.45
1:B:336:HIS:HD2	1:B:337:LEU:HD12	1.81	0.45
1:B:561:PHE:CG	1:B:562:LYS:N	2.85	0.45
1:B:655:ASP:HB3	1:B:658:ARG:HB2	1.98	0.45
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.31	0.45
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.81	0.45
1:A:817:GLU:CG	1:A:818:PRO:HD3	2.37	0.45
1:A:540:LEU:HD12	1:A:563:GLN:CD	2.36	0.45
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.99	0.45
1:B:417:LEU:HA	1:B:417:LEU:HD13	1.78	0.45
1:A:817:GLU:HG3	1:A:818:PRO:N	2.32	0.45
1:B:783:ASN:HD22	1:B:786:HIS:H	1.62	0.45
1:A:708:THR:HB	1:A:710:PRO:HD2	1.97	0.45
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.51	0.45
1:B:528:ASN:HB3	1:B:531:ILE:CD1	2.47	0.45
1:B:296:GLU:HG2	1:B:297:HIS:CD2	2.51	0.45
1:B:262:GLU:CD	1:B:262:GLU:H	2.19	0.45
1:B:1015:MET:O	1:B:1016:ALA:HB2	2.17	0.45
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.17	0.45
1:B:794:TYR:CE1	1:B:838:ARG:HD3	2.52	0.45
1:A:433:TYR:O	1:A:437:ILE:HG12	2.17	0.45
1:A:285:LEU:HD23	1:A:286:PRO:N	2.31	0.45
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.96	0.45
1:A:299:LYS:HD2	1:A:510:ILE:HG13	1.98	0.45
1:B:363:GLN:NE2	1:B:371:MET:HE1	2.31	0.45
1:A:472:ARG:HG2	1:A:472:ARG:NH1	2.32	0.45
1:A:583:ALA:HB3	1:A:626:GLY:HA2	1.99	0.45
1:A:573:CYS:SG	1:A:632:LYS:HD3	2.56	0.45
1:B:674:ARG:NH1	4:B:3025:HOH:O	2.28	0.45
1:A:871:GLU:OE2	1:A:941:LYS:HE3	2.17	0.45
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:ILE:CG2	1:B:795:TYR:CE1	3.01	0.44
1:A:674:ARG:HD3	1:A:784:GLU:OE2	2.17	0.44
1:B:116:LEU:HD12	1:B:178:CYS:HB3	1.99	0.44
1:B:379:LEU:HD13	1:B:384:LEU:HA	1.99	0.44
1:B:123:LYS:HE2	1:B:129:GLN:OE1	2.17	0.44
1:B:643:LYS:HB2	1:B:744:MET:SD	2.58	0.44
1:A:259:LEU:HD23	1:A:259:LEU:C	2.37	0.44
1:A:782:ARG:NH1	1:A:961:ARG:O	2.50	0.44
1:B:83:THR:OG1	1:B:85:LYS:O	2.32	0.44
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.52	0.44
1:A:756:LYS:HB3	1:A:756:LYS:HE2	1.71	0.44
1:A:147:THR:CG2	1:A:149:TYR:CE1	2.97	0.44
1:B:858:TYR:OH	1:B:862:ARG:HD2	2.17	0.44
1:B:548:PRO:HA	1:B:562:LYS:HB2	1.99	0.44
1:B:65:ARG:HH21	1:B:65:ARG:HG3	1.82	0.44
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.99	0.44
1:A:239:GLN:O	1:A:243:LYS:N	2.44	0.44
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.47	0.44
1:A:986:LEU:HA	1:A:987:PRO:HD3	1.85	0.44
1:B:191:GLU:HA	1:B:194:VAL:HG23	1.98	0.44
1:B:53:HIS:N	1:B:53:HIS:CD2	2.84	0.44
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.52	0.44
1:A:780:GLN:CD	1:A:959:LEU:HD11	2.38	0.44
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.17	0.44
1:A:174:PHE:CE2	1:A:241:LEU:HB3	2.53	0.44
1:B:855:PRO:HA	1:B:963:MET:HE1	2.00	0.44
1:A:102:ASN:HD22	1:A:102:ASN:H	1.65	0.44
1:A:459:PHE:CZ	1:A:461:PRO:HG3	2.53	0.44
1:B:721:SER:O	1:B:755:THR:HA	2.18	0.44
1:A:374:ILE:HD12	1:A:374:ILE:C	2.39	0.43
1:B:71:ASN:ND2	1:B:276:SER:HA	2.33	0.43
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.83	0.43
1:B:711:ARG:CG	1:B:711:ARG:NH2	2.75	0.43
1:A:65:ARG:HB2	1:A:264:LEU:HD13	2.00	0.43
1:B:201:LEU:HA	1:B:201:LEU:HD12	1.87	0.43
1:A:97:LEU:HB2	1:A:144:GLY:O	2.18	0.43
1:A:787:ASN:OD1	1:A:962:GLU:HG2	2.17	0.43
1:A:542:LYS:NZ	1:A:542:LYS:HB2	2.33	0.43
1:B:801:SER:H	1:B:805:ASN:ND2	2.15	0.43
1:B:784:GLU:O	1:B:961:ARG:HD3	2.18	0.43
1:B:538:LEU:H	1:B:538:LEU:CD1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:GLU:OE1	1:A:656:GLU:HA	2.18	0.43
1:B:168:PHE:CD1	1:B:168:PHE:N	2.86	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.73	0.43
1:B:759:LEU:HA	1:B:759:LEU:HD12	1.84	0.43
1:B:611:ALA:HB1	1:B:616:LEU:HB3	2.00	0.43
1:B:733:ILE:HD11	1:B:738:ALA:N	2.32	0.43
1:A:638:GLN:HB2	1:A:639:PRO:HD3	2.01	0.43
1:B:411:PHE:CD2	1:B:459:PHE:HB2	2.53	0.43
1:B:833:VAL:O	1:B:833:VAL:HG12	2.17	0.43
1:A:305:VAL:HG23	1:A:489:THR:HG21	2.00	0.43
1:B:843:ILE:HG22	1:B:844:GLN:H	1.82	0.43
1:B:407:GLN:HG3	1:B:409:TRP:HE1	1.82	0.43
1:A:151:PHE:C	1:A:151:PHE:CD1	2.92	0.43
1:B:116:LEU:HD13	1:B:178:CYS:SG	2.59	0.43
1:A:445:PRO:O	1:A:446:LEU:C	2.57	0.43
1:A:934:GLU:O	1:A:938:LYS:HG3	2.18	0.43
1:B:429:ARG:HH11	1:B:429:ARG:HG2	1.84	0.43
1:B:842:GLY:C	1:B:843:ILE:HD13	2.39	0.43
1:B:346:LEU:HD23	1:B:359:LEU:HD11	2.01	0.43
1:A:824:ARG:HB2	1:A:833:VAL:HG21	2.00	0.43
1:B:270:LEU:O	1:B:274:LEU:HG	2.19	0.43
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.51	0.43
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.54	0.43
1:B:228:THR:HG23	4:B:3007:HOH:O	2.18	0.43
1:B:860:GLU:OE1	1:B:957:HIS:CE1	2.72	0.43
1:B:174:PHE:HE2	1:B:241:LEU:HD22	1.84	0.43
1:A:714:ALA:O	1:A:717:PRO:HD2	2.19	0.43
1:A:200:ARG:HH21	1:A:498:THR:HA	1.82	0.42
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.42
1:B:162:LEU:HG	1:B:274:LEU:HD12	2.00	0.42
1:A:992:ILE:HD11	1:A:998:PHE:CE1	2.54	0.42
1:B:896:LYS:HA	1:B:896:LYS:HD3	1.68	0.42
1:B:304:ILE:HB	1:B:481:VAL:HG22	2.00	0.42
1:B:530:PHE:O	1:B:531:ILE:C	2.58	0.42
1:B:823:LEU:CB	1:B:833:VAL:HG11	2.49	0.42
1:B:153:VAL:HG22	1:B:154:SER:N	2.34	0.42
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.49	0.42
1:B:783:ASN:HD22	1:B:785:VAL:H	1.66	0.42
1:A:868:ILE:HD11	1:A:984:PRO:HD3	2.00	0.42
1:A:635:ASN:OD1	1:A:732:ASN:HB3	2.19	0.42
1:A:139:ASN:OD1	2:C:10:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:HIS:N	1:B:786:HIS:CD2	2.86	0.42
1:B:363:GLN:NE2	1:B:371:MET:CE	2.82	0.42
1:B:846:LEU:CD2	1:B:847:ARG:N	2.81	0.42
1:B:407:GLN:CG	1:B:409:TRP:HE1	2.31	0.42
1:A:965:SER:O	1:A:966:CYS:HB2	2.19	0.42
1:A:412:GLN:NE2	1:A:415:LYS:NZ	2.67	0.42
1:B:77:LEU:HD21	1:B:271:VAL:CG2	2.49	0.42
1:B:686:LEU:HA	1:B:686:LEU:HD12	1.80	0.42
1:B:196:ASN:HD22	1:B:196:ASN:C	2.23	0.42
1:B:329:ASN:CG	1:B:332:HIS:HD2	2.23	0.42
1:A:77:LEU:HD21	1:A:271:VAL:HG21	2.02	0.42
1:A:674:ARG:NH1	1:A:675:ALA:HB2	2.35	0.42
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.02	0.42
1:B:90:LEU:HD23	1:B:91:ASP:N	2.34	0.42
1:A:353:LYS:HD3	1:A:355:TRP:CZ3	2.54	0.42
1:A:347:LEU:O	1:A:347:LEU:HD22	2.20	0.42
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.87	0.42
1:B:882:PHE:CE2	1:B:886:ILE:HD11	2.55	0.42
1:A:600:LEU:HD11	1:A:648:LYS:HB3	2.00	0.42
1:B:459:PHE:O	1:B:461:PRO:HD2	2.20	0.42
1:A:810:LEU:HD12	1:A:931:LEU:HD23	2.01	0.42
1:A:791:ILE:HG22	1:A:850:ILE:O	2.20	0.42
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.01	0.42
1:B:424:PHE:CE1	1:B:535:PHE:CD2	3.08	0.42
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.89	0.42
1:A:527:LYS:HD3	1:A:528:ASN:N	2.34	0.42
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.35	0.42
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.55	0.42
1:B:886:ILE:HG23	1:B:928:LEU:HD13	2.01	0.42
1:A:783:ASN:ND2	1:A:785:VAL:H	2.18	0.42
1:B:422:PHE:CE2	1:B:451:THR:HG22	2.54	0.42
1:B:793:ILE:O	1:B:847:ARG:HA	2.20	0.42
1:A:792:GLU:HA	1:A:848:PHE:O	2.20	0.42
1:A:190:HIS:O	1:A:194:VAL:HG23	2.21	0.41
1:A:93:HIS:CD2	1:A:145:GLU:O	2.72	0.41
1:A:476:VAL:CG2	1:A:477:ARG:N	2.82	0.41
1:A:733:ILE:HG12	1:A:737:ALA:HB3	2.02	0.41
1:A:355:TRP:HB3	1:A:390:ILE:HD11	2.01	0.41
1:B:288:PHE:O	1:B:369:GLY:HA3	2.20	0.41
1:A:301:LEU:HA	1:A:478:VAL:O	2.20	0.41
1:A:121:TYR:HB3	1:A:126:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD23	1:B:90:LEU:C	2.40	0.41
1:B:125:ASN:ND2	1:B:817:GLU:OE1	2.54	0.41
1:A:815:ILE:HG22	1:A:870:MET:CE	2.50	0.41
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.55	0.41
1:B:708:THR:O	1:B:709:LEU:C	2.58	0.41
1:B:49:ARG:CG	1:B:50:ILE:N	2.83	0.41
1:A:343:PRO:HD3	1:A:606:GLU:HG2	2.02	0.41
1:A:821:ASN:O	1:A:825:THR:HB	2.20	0.41
1:A:551:ILE:HD11	1:A:559:LEU:HD21	2.02	0.41
1:B:301:LEU:HD12	1:B:302:TYR:H	1.85	0.41
1:B:168:PHE:HD1	1:B:168:PHE:N	2.18	0.41
1:B:862:ARG:CZ	1:B:862:ARG:HA	2.51	0.41
1:A:501:LYS:NZ	1:A:503:GLU:HG2	2.36	0.41
1:A:591:ASN:O	1:A:595:LEU:CD2	2.68	0.41
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.92	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.51	0.41
1:B:259:LEU:HD23	1:B:260:GLY:N	2.36	0.41
1:A:591:ASN:O	1:A:595:LEU:HD22	2.20	0.41
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.02	0.41
1:B:870:MET:O	1:B:874:ILE:HG13	2.20	0.41
1:B:591:ASN:HD21	1:B:700:LEU:HB3	1.86	0.41
1:B:119:LYS:CG	1:B:171:CYS:HB2	2.50	0.41
1:B:78:ILE:HB	1:B:259:LEU:HB2	2.03	0.41
1:A:283:VAL:HA	1:A:284:PRO:HD3	1.85	0.41
1:A:676:GLU:HA	1:A:676:GLU:OE2	2.21	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.75	0.41
1:A:108:HIS:O	1:A:111:GLN:HB3	2.21	0.41
1:A:168:PHE:O	1:A:172:PRO:HG3	2.20	0.41
1:A:767:ARG:HG2	1:A:1007:LEU:HD11	2.03	0.41
1:B:64:TYR:HD2	1:B:76:LEU:HD11	1.85	0.41
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.35	0.41
1:B:315:VAL:HG21	1:B:394:MET:SD	2.60	0.41
1:A:656:GLU:HB2	4:A:3030:HOH:O	2.21	0.41
1:A:102:ASN:ND2	1:A:102:ASN:H	2.19	0.41
1:B:542:LYS:HB2	1:B:542:LYS:HZ3	1.85	0.41
1:B:67:LEU:C	1:B:67:LEU:HD12	2.40	0.41
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.76	0.41
1:B:337:LEU:HD23	1:B:401:LEU:CD2	2.51	0.41
1:A:415:LYS:HA	1:A:456:LEU:HD12	2.03	0.41
1:B:352:SER:C	1:B:354:GLY:H	2.23	0.41
1:A:488:LYS:N	1:A:488:LYS:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:TYR:O	1:B:861:SER:OG	2.22	0.41
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.45	0.41
1:A:794:TYR:HE1	1:A:845:GLY:HA3	1.86	0.41
1:B:711:ARG:NH2	1:B:711:ARG:HG3	2.12	0.40
1:B:173:LEU:O	1:B:174:PHE:HB2	2.21	0.40
1:A:184:ASN:HA	1:A:184:ASN:HD22	1.70	0.40
1:B:722:ARG:HB3	1:B:758:LEU:HD12	2.04	0.40
1:B:821:ASN:HA	1:B:825:THR:OG1	2.20	0.40
1:A:928:LEU:HD22	1:A:928:LEU:O	2.20	0.40
1:B:96:SER:HA	1:B:107:SER:OG	2.21	0.40
1:B:534:ASN:HD22	1:B:535:PHE:N	2.18	0.40
1:B:846:LEU:HD22	1:B:848:PHE:CE1	2.56	0.40
1:B:285:LEU:HD22	1:B:286:PRO:CD	2.51	0.40
1:A:248:TYR:O	1:A:250:SER:N	2.49	0.40
1:B:576:PHE:CD1	1:B:576:PHE:N	2.89	0.40
1:B:523:LYS:HD2	1:B:523:LYS:N	2.35	0.40
1:A:111:GLN:NE2	1:A:140:ALA:HB3	2.35	0.40
1:A:93:HIS:CE1	1:A:368:ARG:HE	2.38	0.40
1:A:303:LYS:NZ	1:A:503:GLU:OE1	2.45	0.40
1:B:459:PHE:O	1:B:461:PRO:CD	2.69	0.40
1:B:196:ASN:ND2	1:B:196:ASN:C	2.75	0.40
1:B:856:PRO:HB2	1:B:957:HIS:CD2	2.57	0.40
1:B:591:ASN:ND2	1:B:700:LEU:CD2	2.84	0.40
1:A:311:ARG:NH1	1:A:379:LEU:O	2.43	0.40
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.54	0.40
1:B:576:PHE:CE2	1:B:745:VAL:HG21	2.56	0.40
1:A:319:ILE:HG13	1:A:371:MET:HB2	2.03	0.40
1:A:793:ILE:HG22	1:A:795:TYR:CE1	2.57	0.40
1:A:823:LEU:N	1:A:823:LEU:HD22	2.37	0.40
1:B:505:ILE:H	1:B:505:ILE:HG13	1.73	0.40
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.56	0.40
1:A:412:GLN:HE21	1:A:415:LYS:NZ	2.19	0.40
1:B:483:LYS:HD3	1:B:483:LYS:HA	1.97	0.40
1:A:210:ASN:HA	1:A:211:PRO:HD3	1.89	0.40
1:A:416:ASP:O	1:A:420:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	959/990 (97%)	885 (92%)	61 (6%)	13 (1%)	14	51
1	B	957/990 (97%)	861 (90%)	79 (8%)	17 (2%)	11	45
2	C	6/12 (50%)	5 (83%)	1 (17%)	0	100	100
2	D	6/12 (50%)	6 (100%)	0	0	100	100
All	All	1928/2004 (96%)	1757 (91%)	141 (7%)	30 (2%)	12	48

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	981	SER
1	B	48	LYS
1	B	52	ASN
1	B	984	PRO
1	B	1012	ILE
1	B	1015	MET
1	B	1016	ALA
1	B	721	SER
1	A	228	THR
1	A	232	GLN
1	A	233	GLU
1	A	368	ARG
1	A	672	ASN
1	A	987	PRO
1	B	484	SER
1	B	967	PRO
1	A	53	HIS
1	A	449	VAL
1	A	1014	PHE
1	B	67	LEU
1	A	96	SER
1	B	430	PRO

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Mol	Chain	Res	Type
1	B	965	SER
1	B	368	ARG
1	B	405	GLY
1	A	406	PRO
1	A	967	PRO
1	B	366	GLY
1	B	449	VAL
1	B	833	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	859/883 (97%)	808 (94%)	51 (6%)	24	63
1	B	858/883 (97%)	804 (94%)	54 (6%)	22	60
All	All	1717/1766 (97%)	1612 (94%)	105 (6%)	23	61

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	67	LEU
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	158	LEU
1	A	188	SER
1	A	196	ASN
1	A	226	LEU
1	A	229	ARG
1	A	238	ARG
1	A	316	THR
1	A	337	LEU
1	A	347	LEU
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	466	MET
1	A	475	ASN
1	A	494	GLU
1	A	542	LYS
1	A	543	GLU
1	A	595	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	635	ASN
1	A	642	LEU
1	A	643	LYS
1	A	656	GLU
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	722	ARG
1	A	728	LEU
1	A	756	LYS
1	A	772	PRO
1	A	777	PHE
1	A	783	ASN
1	A	801	SER
1	A	810	LEU
1	A	817	GLU
1	A	846	LEU
1	A	852	SER
1	A	889	LEU
1	A	928	LEU
1	A	933	LYS
1	A	957	HIS
1	A	964	ASP
1	A	993	GLN
1	A	1007	LEU
1	A	1013	ASN
1	B	74	LYS
1	B	87	SER
1	B	102	ASN
1	B	126	GLU
1	B	128	SER
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	168	PHE
1	B	192	LYS
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	238	ARG
1	B	265	ASP
1	B	270	LEU
1	B	287	GLU
1	B	347	LEU
1	B	417	LEU
1	B	431	ARG
1	B	450	LEU
1	B	457	GLU
1	B	466	MET
1	B	475	ASN
1	B	488	LYS
1	B	507	ASP
1	B	523	LYS
1	B	524	LEU
1	B	534	ASN
1	B	540	LEU
1	B	542	LYS
1	B	543	GLU
1	B	575	ASN
1	B	597	LEU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	677	GLN
1	B	678	PRO
1	B	711	ARG
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	759	LEU
1	B	783	ASN
1	B	799	MET
1	B	880	GLU
1	B	928	LEU
1	B	957	HIS

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Mol	Chain	Res	Type
1	B	964	ASP
1	B	966	CYS
1	B	968	VAL
1	B	1007	LEU
1	B	1012	ILE
1	B	1015	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	129	GLN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	332	HIS
1	A	336	HIS
1	A	363	GLN
1	A	412	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	736	GLN
1	A	743	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	887	GLN
1	A	914	GLN
1	A	922	ASN
1	B	52	ASN
1	B	53	HIS
1	B	93	HIS

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	134	HIS
1	B	157	HIS
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	332	HIS
1	B	336	HIS
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	475	ASN
1	B	502	GLN
1	B	515	ASN
1	B	534	ASN
1	B	575	ASN
1	B	591	ASN
1	B	622	ASN
1	B	672	ASN
1	B	718	GLN
1	B	783	ASN
1	B	786	HIS
1	B	805	ASN
1	B	828	GLN
1	B	887	GLN
1	B	917	ASN
1	B	922	ASN
1	B	957	HIS
1	B	982	GLN
1	B	988	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands 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	$\# Z  > 2$
3	DIO	A	2017	-	6,6,6	0.72	0	6,6,6	0.24	0
3	DIO	B	2017	-	6,6,6	0.73	0	6,6,6	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	2017	-	-	0/0/6/6	0/1/1/1
3	DIO	B	2017	-	-	0/0/6/6	0/1/1/1

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2017	DIO	3	0
3	B	2017	DIO	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	963/990 (97%)	-0.57	7 (0%) 89 70	15, 34, 60, 96	0
1	B	961/990 (97%)	-0.48	5 (0%) 91 76	19, 44, 71, 98	0
2	C	10/12 (83%)	0.03	0 100 100	30, 60, 73, 75	0
2	D	10/12 (83%)	-0.24	0 100 100	29, 61, 76, 80	0
All	All	1944/2004 (97%)	-0.52	12 (0%) 90 73	15, 39, 68, 98	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	985	ALA	3.4
1	A	1015	MET	3.3
1	B	984	PRO	3.2
1	A	1013	ASN	3.2
1	A	984	PRO	3.0
1	A	1014	PHE	2.9
1	B	1017	ALA	2.8
1	B	986	LEU	2.7
1	A	983	ALA	2.6
1	B	1016	ALA	2.3
1	A	964	ASP	2.2
1	A	1016	ALA	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DIO	B	2017	6/6	0.98	0.24	2.20	26,34,43,47	0
3	DIO	A	2017	6/6	0.98	0.23	1.36	45,55,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.