



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:55 pm BST

PDB ID : 3QG5  
Title : The Mre11:Rad50 complex forms an ATP dependent molecular clamp in DNA double-strand break repair  
Authors : Lammens, K.  
Deposited on : 2011-01-24  
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

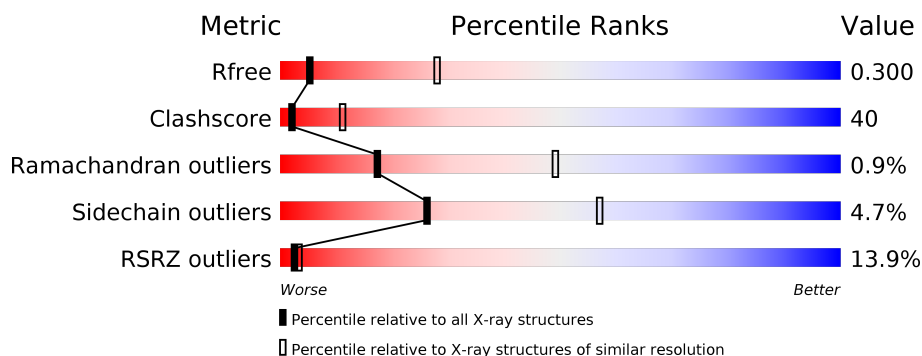
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 respectively. 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	365	
1	B	365	
2	C	379	
2	D	379	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11601 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 rad50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	Se	95	0	0
			2799	1784	486	525	4			
1	B	349	Total	C	N	O	Se	371	0	0
			2799	1784	486	525	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	GLY	-	LINKER	UNP Q9X1X1
A	679	GLY	-	LINKER	UNP Q9X1X1
A	680	ALA	-	LINKER	UNP Q9X1X1
A	681	GLY	-	LINKER	UNP Q9X1X1
A	682	GLY	-	LINKER	UNP Q9X1X1
A	683	ALA	-	LINKER	UNP Q9X1X1
A	684	GLY	-	LINKER	UNP Q9X1X1
A	685	GLY	-	LINKER	UNP Q9X1X1
B	678	GLY	-	LINKER	UNP Q9X1X1
B	679	GLY	-	LINKER	UNP Q9X1X1
B	680	ALA	-	LINKER	UNP Q9X1X1
B	681	GLY	-	LINKER	UNP Q9X1X1
B	682	GLY	-	LINKER	UNP Q9X1X1
B	683	ALA	-	LINKER	UNP Q9X1X1
B	684	GLY	-	LINKER	UNP Q9X1X1
B	685	GLY	-	LINKER	UNP Q9X1X1

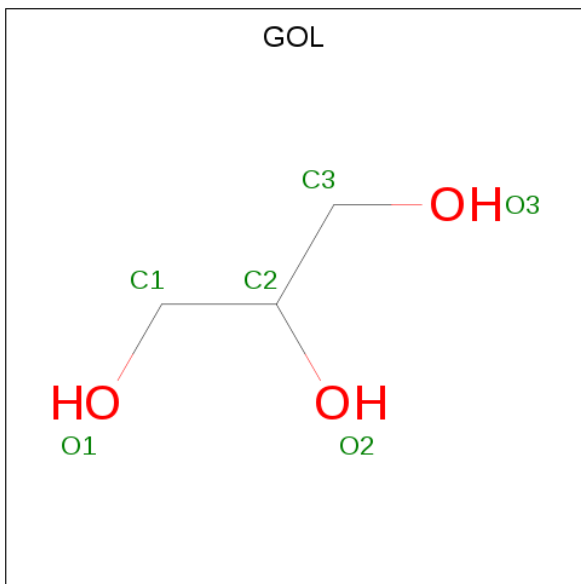
- Molecule 2 is a protein called Mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	362	Total	C	N	O	S Se	127	0	0
			2985	1915	505	558	1 6			
2	D	366	Total	C	N	O	S Se	114	0	0
			3006	1928	512	559	1 6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	MSE	-	INITIATING METHIONINE	UNP Q9X1X0
D	7	MSE	-	INITIATING METHIONINE	UNP Q9X1X0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

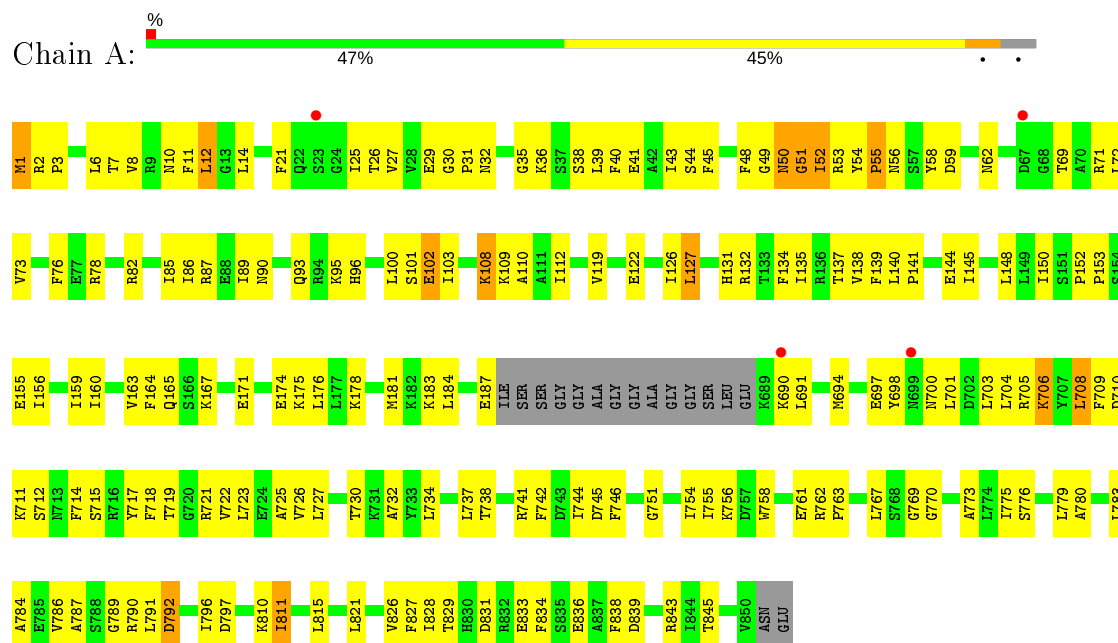


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

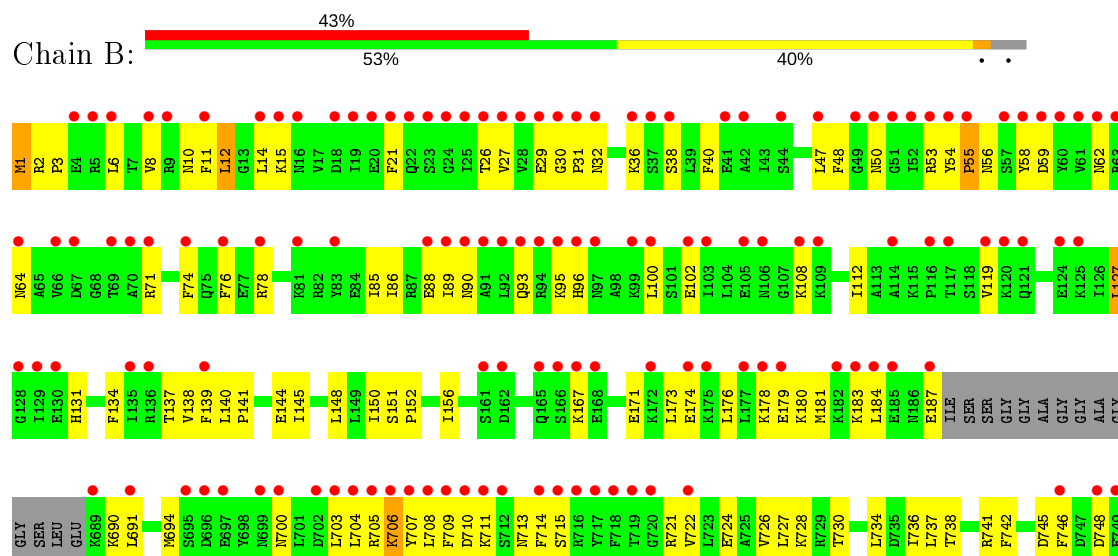
### 3 Residue-property plots [i](#)

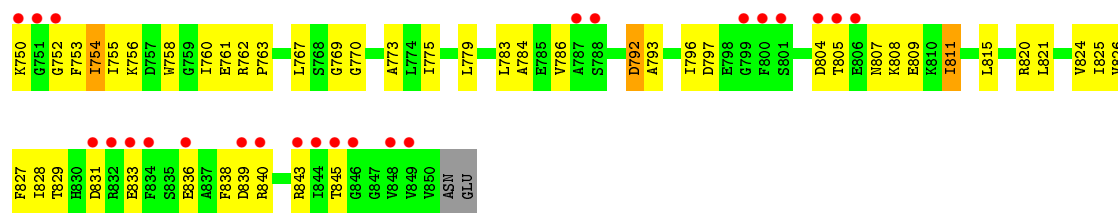
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: rad50

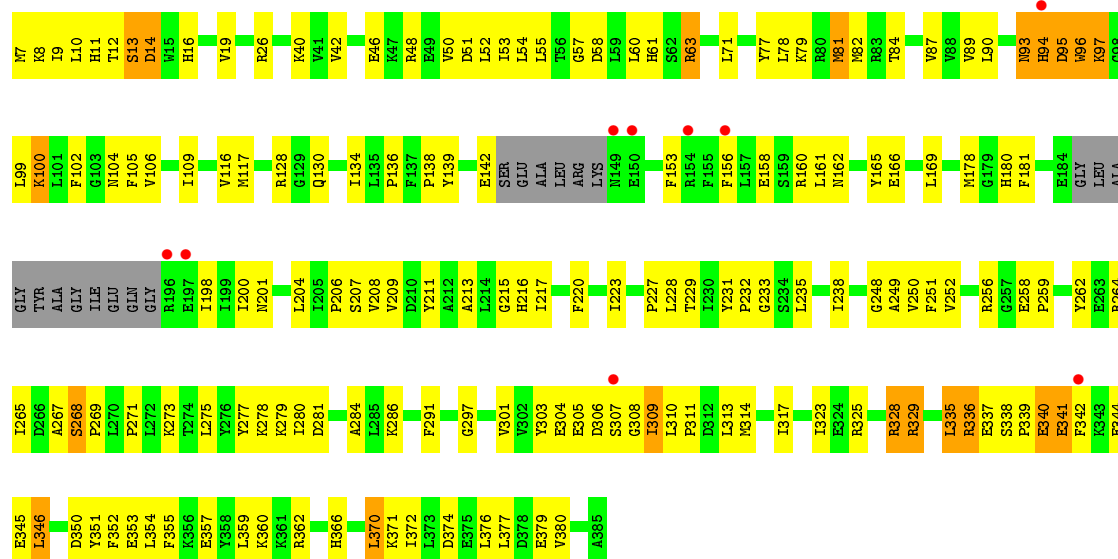


#### • Molecule 1: rad50

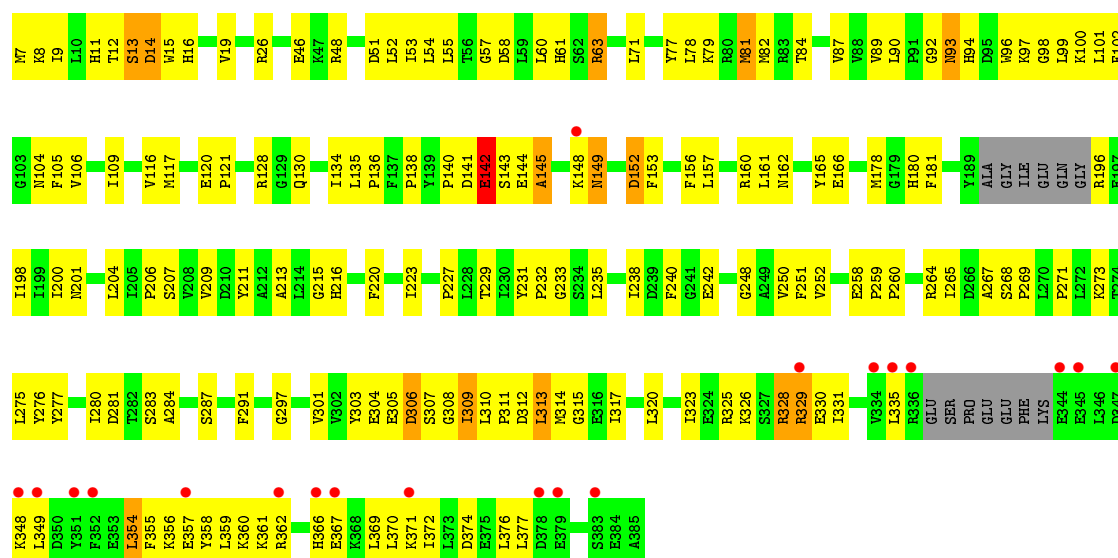




● Molecule 2: Mre11



● Molecule 2: Mre11



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.19 Å   187.00 Å   300.17 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.40) 98.9 (20.00-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.44 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.258   ,   0.295 0.269   ,   0.300	Depositor DCC
$R_{free}$ test set	2020 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.26	0/2837	0.43	0/3797
1	B	0.25	0/2837	0.42	0/3797
2	C	0.29	0/3041	0.55	3/4086 (0.1%)
2	D	0.29	0/3061	0.62	7/4112 (0.2%)
All	All	0.27	0/11776	0.51	10/15792 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	329	ARG	NE-CZ-NH1	-12.34	114.13	120.30
2	C	329	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	D	329	ARG	NE-CZ-NH2	12.10	126.35	120.30
2	C	329	ARG	NE-CZ-NH1	11.94	126.27	120.30
2	D	196	ARG	NE-CZ-NH1	-11.60	114.50	120.30
2	D	196	ARG	NE-CZ-NH2	11.23	125.92	120.30
2	D	93	ASN	N-CA-CB	6.20	121.76	110.60
2	D	329	ARG	CD-NE-CZ	6.06	132.08	123.60
2	C	329	ARG	CD-NE-CZ	5.98	131.98	123.60
2	D	196	ARG	CD-NE-CZ	5.74	131.63	123.60

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	2799	0	2870	253	0
1	B	2799	0	2870	179	0
2	C	2985	0	3006	254	0
2	D	3006	0	3038	265	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
All	All	11601	0	11800	869	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 40.

All (869) 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:174:GLU:HG2	1:A:709:PHE:CE1	1.61	1.34
2:D:306:ASP:HB2	2:D:325:ARG:NH1	1.40	1.30
1:A:3:PRO:HB2	1:A:21:PHE:CE1	1.67	1.29
2:D:306:ASP:CB	2:D:325:ARG:NH1	1.96	1.27
2:D:14:ASP:OD2	2:D:57:GLY:HA3	1.29	1.27
2:D:306:ASP:CB	2:D:325:ARG:HH11	1.50	1.24
2:D:148:LYS:HB3	2:D:152:ASP:CB	1.66	1.23
2:C:340:GLU:O	2:C:341:GLU:HG2	1.39	1.22
2:C:346:LEU:O	2:C:346:LEU:HD12	1.39	1.20
1:A:25:ILE:HD11	1:A:827:PHE:CE1	1.76	1.19
1:B:26:THR:CB	1:B:826:VAL:HG12	1.72	1.19
1:B:26:THR:HB	1:B:826:VAL:CG1	1.74	1.18
1:A:3:PRO:HB2	1:A:21:PHE:CD1	1.81	1.15
2:C:40:LYS:NZ	2:C:268:SER:OG	1.79	1.15
2:C:308:GLY:HA2	2:C:309:ILE:HB	1.27	1.15
2:D:148:LYS:HD2	2:D:152:ASP:CG	1.68	1.14
1:B:738:THR:HG21	1:B:742:PHE:HD2	1.04	1.14
2:D:149:ASN:O	2:D:153:PHE:HB3	1.50	1.10
2:D:142:GLU:HG2	2:D:143:SER:N	1.66	1.10
2:C:308:GLY:CA	2:C:309:ILE:HB	1.83	1.09
2:C:93:ASN:HB2	2:C:139:TYR:HB3	1.14	1.08
1:A:25:ILE:HD11	1:A:827:PHE:HE1	1.07	1.06
1:A:174:GLU:HA	1:A:709:PHE:HZ	1.15	1.06
2:D:149:ASN:HA	2:D:153:PHE:HB2	1.09	1.06
1:B:26:THR:O	1:B:826:VAL:HA	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:ND2	1:A:93:GLN:OE1	1.89	1.05
1:B:746:PHE:CE1	1:B:752:GLY:O	2.08	1.05
2:C:338:SER:N	2:C:339:PRO:HD3	1.67	1.05
1:B:741:ARG:CZ	1:B:742:PHE:CZ	2.40	1.05
2:D:149:ASN:HD22	2:D:153:PHE:CB	1.68	1.05
1:A:722:VAL:HG23	1:A:726:VAL:CG2	1.86	1.05
2:D:149:ASN:HD22	2:D:153:PHE:HB3	1.22	1.05
2:D:79:LYS:HA	2:D:82:MSE:HE2	1.39	1.03
1:B:762:ARG:HH12	2:D:283:SER:HA	1.21	1.02
1:A:722:VAL:O	1:A:726:VAL:HB	1.58	1.02
1:A:722:VAL:HG23	1:A:726:VAL:HG21	1.06	1.02
2:C:79:LYS:HA	2:C:82:MSE:HE2	1.41	1.01
1:A:714:PHE:CE1	2:C:355:PHE:HA	1.96	1.01
2:D:14:ASP:HB3	2:D:58:ASP:N	1.77	0.99
1:B:738:THR:HG21	1:B:742:PHE:CD2	1.96	0.99
1:A:708:LEU:HD23	1:A:708:LEU:C	1.81	0.98
2:D:148:LYS:HB3	2:D:152:ASP:HB3	1.44	0.98
1:A:723:LEU:CD2	1:A:746:PHE:CD2	2.46	0.98
1:A:714:PHE:CZ	2:C:355:PHE:HB2	1.97	0.98
1:A:721:ARG:HG3	2:C:354:LEU:HD11	1.46	0.98
2:D:13:SER:HB2	2:D:232:PRO:HB2	1.46	0.98
2:D:149:ASN:CA	2:D:153:PHE:HB2	1.94	0.97
1:A:174:GLU:HG2	1:A:709:PHE:HE1	0.85	0.96
1:A:174:GLU:HA	1:A:709:PHE:CZ	1.99	0.96
2:D:148:LYS:CA	2:D:152:ASP:HB2	1.96	0.96
2:D:144:GLU:OE2	2:D:152:ASP:HB3	1.65	0.95
1:B:746:PHE:CD1	1:B:752:GLY:O	2.20	0.94
1:A:174:GLU:CG	1:A:709:PHE:HE1	1.80	0.94
1:A:722:VAL:CG2	1:A:726:VAL:HG21	1.97	0.94
1:A:3:PRO:HB2	1:A:21:PHE:HE1	1.26	0.93
2:D:92:GLY:O	2:D:94:HIS:CD2	2.21	0.93
2:C:11:HIS:CE1	2:C:232:PRO:HG2	2.04	0.93
2:C:161:LEU:HD13	2:C:204:LEU:HB3	1.50	0.93
2:D:148:LYS:O	2:D:152:ASP:CB	2.16	0.93
1:B:174:GLU:HG2	1:B:709:PHE:CE1	2.03	0.92
2:C:96:TRP:HE1	2:C:99:LEU:HB2	1.33	0.92
2:D:306:ASP:OD1	2:D:306:ASP:C	2.07	0.92
2:D:148:LYS:HB3	2:D:152:ASP:HB2	1.49	0.92
2:D:161:LEU:HD13	2:D:204:LEU:HB3	1.51	0.92
1:A:89:ILE:HB	1:A:96:HIS:HD2	1.34	0.92
2:C:308:GLY:HA2	2:C:309:ILE:CB	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:ASP:HB3	2:D:325:ARG:NH1	1.84	0.91
1:B:713:ASN:HB3	2:D:358:TYR:OH	1.71	0.91
2:D:142:GLU:HG2	2:D:143:SER:H	1.36	0.91
2:D:149:ASN:ND2	2:D:153:PHE:CB	2.33	0.91
2:C:11:HIS:CE1	2:C:232:PRO:CG	2.53	0.91
1:B:89:ILE:HB	1:B:96:HIS:HD2	1.33	0.90
1:B:174:GLU:HG2	1:B:709:PHE:HE1	1.35	0.90
2:C:96:TRP:NE1	2:C:99:LEU:HB2	1.85	0.90
1:A:719:THR:O	1:A:722:VAL:HG12	1.70	0.90
1:B:746:PHE:HE2	1:B:748:ASP:OD1	1.54	0.90
2:D:149:ASN:HA	2:D:153:PHE:CB	1.99	0.90
1:B:741:ARG:CZ	1:B:742:PHE:HZ	1.83	0.89
2:C:13:SER:HB2	2:C:232:PRO:HB2	1.53	0.89
2:D:149:ASN:ND2	2:D:153:PHE:CG	2.41	0.89
1:A:723:LEU:HD23	1:A:746:PHE:CD2	2.06	0.88
2:C:306:ASP:HA	2:C:325:ARG:HH11	1.38	0.88
1:A:3:PRO:CB	1:A:21:PHE:CE1	2.56	0.87
2:D:148:LYS:CB	2:D:152:ASP:HB2	2.02	0.87
1:A:708:LEU:HB2	2:C:355:PHE:CZ	2.10	0.87
2:D:148:LYS:CB	2:D:152:ASP:CB	2.51	0.87
1:B:78:ARG:HD3	1:B:127:LEU:HD22	1.57	0.87
2:D:153:PHE:HZ	2:D:198:ILE:HD12	1.37	0.87
1:A:25:ILE:CD1	1:A:827:PHE:HE1	1.85	0.87
2:C:335:LEU:O	2:C:336:ARG:HG2	1.74	0.87
2:D:12:THR:HG22	2:D:55:LEU:HD23	1.56	0.86
1:A:50:ASN:O	1:A:131:HIS:NE2	2.08	0.86
1:A:714:PHE:CG	2:C:355:PHE:HD1	1.92	0.86
2:D:360:LYS:HA	2:D:366:HIS:HB3	1.56	0.86
1:A:78:ARG:HD3	1:A:127:LEU:HD22	1.55	0.86
1:A:714:PHE:CE1	2:C:355:PHE:CA	2.59	0.85
2:D:280:ILE:O	2:D:307:SER:HB3	1.76	0.85
2:D:280:ILE:N	2:D:307:SER:OG	2.09	0.85
1:A:706:LYS:HE3	1:A:706:LYS:HA	1.59	0.85
2:C:93:ASN:HB2	2:C:139:TYR:CB	2.03	0.85
2:C:11:HIS:ND1	2:C:232:PRO:HG3	1.92	0.84
1:A:714:PHE:CD2	2:C:355:PHE:HD1	1.94	0.84
2:D:148:LYS:O	2:D:152:ASP:HB2	1.77	0.84
2:D:11:HIS:CE1	2:D:213:ALA:HB1	2.13	0.84
2:D:12:THR:CG2	2:D:55:LEU:CD2	2.57	0.83
1:B:755:ILE:HD13	1:B:767:LEU:HD11	1.58	0.83
1:A:174:GLU:CG	1:A:709:PHE:CE1	2.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:ASP:OD2	2:D:57:GLY:CA	2.23	0.83
1:A:723:LEU:HD21	1:A:746:PHE:CD2	2.13	0.82
1:B:706:LYS:HE3	1:B:706:LYS:HA	1.59	0.82
2:D:310:LEU:H	2:D:310:LEU:HD23	1.45	0.82
1:B:746:PHE:CE2	1:B:748:ASP:OD1	2.33	0.82
2:D:60:LEU:HD12	2:D:96:TRP:CZ2	2.14	0.82
1:A:708:LEU:O	1:A:708:LEU:HD23	1.80	0.81
1:A:708:LEU:HA	2:C:355:PHE:CE1	2.16	0.81
2:C:40:LYS:HZ2	2:C:268:SER:HG	1.26	0.81
2:D:96:TRP:CZ2	2:D:99:LEU:HD22	2.16	0.81
1:A:3:PRO:CB	1:A:21:PHE:CD1	2.63	0.81
2:C:13:SER:OG	2:C:232:PRO:HD2	1.81	0.80
1:B:151:SER:O	1:B:752:GLY:HA2	1.80	0.80
1:A:738:THR:HG22	1:A:741:ARG:HB3	1.62	0.80
1:B:758:TRP:HZ2	2:D:276:TYR:O	1.65	0.80
2:D:148:LYS:O	2:D:152:ASP:CA	2.29	0.80
1:B:738:THR:HG22	1:B:741:ARG:HB3	1.62	0.79
2:C:11:HIS:ND1	2:C:232:PRO:CG	2.46	0.79
2:D:141:ASP:O	2:D:142:GLU:HB3	1.83	0.79
2:D:94:HIS:HB3	2:D:96:TRP:CZ3	2.18	0.79
1:A:3:PRO:O	1:A:21:PHE:HD1	1.66	0.78
1:B:758:TRP:CZ2	2:D:276:TYR:O	2.36	0.78
2:D:149:ASN:O	2:D:153:PHE:CB	2.30	0.78
1:A:719:THR:O	1:A:722:VAL:CG1	2.31	0.78
2:C:340:GLU:O	2:C:341:GLU:CG	2.27	0.78
2:C:96:TRP:HZ3	2:D:97:LYS:HD3	1.47	0.78
1:A:714:PHE:CG	2:C:355:PHE:CD1	2.71	0.78
2:C:63:ARG:HB2	2:C:94:HIS:O	1.83	0.78
2:D:148:LYS:O	2:D:153:PHE:N	2.17	0.78
1:A:722:VAL:O	1:A:726:VAL:CB	2.30	0.77
2:D:94:HIS:ND1	2:D:96:TRP:HZ3	1.83	0.77
1:B:805:THR:HA	1:B:808:LYS:HG3	1.65	0.77
1:A:49:GLY:HA2	1:A:87:ARG:NH2	2.00	0.77
1:B:26:THR:O	1:B:826:VAL:CA	2.31	0.77
1:A:704:LEU:HD22	2:C:372:ILE:CD1	2.13	0.77
1:B:820:ARG:HD2	2:D:328:ARG:HH12	1.48	0.77
1:B:758:TRP:HD1	2:D:287:SER:OG	1.66	0.76
2:C:338:SER:N	2:C:339:PRO:CD	2.47	0.76
2:D:54:LEU:HG	2:D:178:MSE:HE2	1.68	0.76
1:A:706:LYS:HE2	1:A:710:ASP:CG	2.06	0.75
2:C:268:SER:N	2:C:269:PRO:CD	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:HIS:HB3	2:D:250:VAL:HG13	1.67	0.75
1:B:40:PHE:CZ	1:B:139:PHE:HB2	2.22	0.75
1:B:29:GLU:O	1:B:843:ARG:HA	1.86	0.75
2:D:14:ASP:HB3	2:D:58:ASP:CA	2.17	0.75
1:A:29:GLU:O	1:A:843:ARG:HA	1.87	0.75
2:D:153:PHE:CZ	2:D:198:ILE:HD12	2.21	0.75
1:B:705:ARG:O	1:B:709:PHE:HD2	1.69	0.75
1:A:3:PRO:CB	1:A:21:PHE:HE1	1.98	0.74
1:B:711:LYS:HA	1:B:715:SER:HB3	1.70	0.74
1:A:714:PHE:HE1	2:C:355:PHE:HA	1.51	0.74
1:A:52:ILE:HD11	1:A:135:ILE:HD12	1.69	0.74
1:B:703:LEU:HD12	1:B:704:LEU:N	2.03	0.74
1:A:708:LEU:CD2	1:A:708:LEU:C	2.54	0.74
2:C:54:LEU:HG	2:C:178:MSE:HE2	1.67	0.74
2:C:311:PRO:O	2:C:313:LEU:HD12	1.88	0.73
2:D:16:HIS:O	2:D:19:VAL:HG12	1.87	0.73
2:D:12:THR:CG2	2:D:55:LEU:HD23	2.17	0.73
2:C:311:PRO:O	2:C:313:LEU:CD1	2.36	0.73
1:A:40:PHE:CZ	1:A:139:PHE:HB2	2.23	0.73
2:D:148:LYS:C	2:D:152:ASP:HB2	2.09	0.73
1:A:714:PHE:CD2	2:C:355:PHE:CD1	2.76	0.73
1:B:758:TRP:HD1	2:D:287:SER:HG	1.32	0.73
2:D:148:LYS:O	2:D:152:ASP:N	2.22	0.73
2:D:306:ASP:CA	2:D:325:ARG:HH11	2.02	0.73
1:B:704:LEU:HD22	2:D:372:ILE:HD11	1.71	0.72
1:B:762:ARG:NH1	2:D:283:SER:HA	2.01	0.72
2:C:14:ASP:OD1	2:C:57:GLY:HA3	1.90	0.72
1:A:174:GLU:HG2	1:A:709:PHE:CZ	2.25	0.72
1:A:703:LEU:HD12	1:A:704:LEU:N	2.04	0.72
2:C:337:GLU:C	2:C:339:PRO:HD3	2.09	0.72
1:A:25:ILE:HD11	1:A:827:PHE:CD1	2.25	0.72
2:D:26:ARG:NH2	2:D:314:MSE:O	2.22	0.72
1:B:721:ARG:HH22	2:D:349:LEU:HD23	1.55	0.72
2:C:346:LEU:O	2:C:346:LEU:CD1	2.30	0.72
1:A:26:THR:HB	1:A:826:VAL:HG12	1.72	0.72
1:A:738:THR:HG21	1:A:742:PHE:HD2	1.55	0.72
2:C:116:VAL:HG11	2:C:136:PRO:HB3	1.71	0.72
2:D:16:HIS:CD2	2:D:238:ILE:HD11	2.24	0.71
2:D:92:GLY:O	2:D:94:HIS:HD2	1.70	0.71
2:D:134:ILE:HD12	2:D:178:MSE:HE3	1.72	0.71
2:D:306:ASP:CB	2:D:325:ARG:HH12	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:ASN:CB	2:C:139:TYR:HB3	2.08	0.71
1:A:714:PHE:CZ	2:C:355:PHE:CB	2.71	0.71
1:A:714:PHE:CD1	2:C:355:PHE:HD1	2.09	0.71
2:C:328:ARG:HG3	2:C:328:ARG:HH21	1.54	0.71
2:C:328:ARG:CG	2:C:328:ARG:HH21	2.04	0.70
2:C:8:LYS:HB3	2:C:251:PHE:HE1	1.57	0.70
2:D:148:LYS:CD	2:D:152:ASP:CG	2.55	0.70
1:B:140:LEU:HB3	1:B:145:ILE:HD11	1.71	0.70
2:D:144:GLU:O	2:D:145:ALA:HB3	1.91	0.70
2:D:14:ASP:CB	2:D:58:ASP:N	2.53	0.70
2:D:116:VAL:HG11	2:D:136:PRO:HB3	1.71	0.70
1:B:29:GLU:OE1	1:B:29:GLU:C	2.30	0.70
1:B:26:THR:HB	1:B:826:VAL:HG12	0.82	0.70
2:D:148:LYS:HD2	2:D:152:ASP:OD1	1.91	0.70
1:A:140:LEU:HB3	1:A:145:ILE:HD11	1.72	0.70
1:A:174:GLU:CA	1:A:709:PHE:HZ	2.00	0.70
1:A:789:GLY:HA2	2:C:346:LEU:HD11	1.73	0.70
1:A:3:PRO:O	1:A:21:PHE:CD1	2.45	0.70
1:B:26:THR:N	1:B:825:ILE:O	2.20	0.70
2:C:309:ILE:HG22	2:C:309:ILE:O	1.90	0.69
2:C:96:TRP:CD1	2:C:99:LEU:HB2	2.27	0.69
1:B:738:THR:CG2	1:B:742:PHE:HD2	1.95	0.69
2:D:148:LYS:HD2	2:D:152:ASP:OD2	1.91	0.69
2:C:346:LEU:HD12	2:C:346:LEU:C	2.13	0.69
2:D:8:LYS:HB3	2:D:251:PHE:HE1	1.58	0.69
2:D:14:ASP:HB3	2:D:58:ASP:H	1.56	0.69
2:D:153:PHE:HZ	2:D:198:ILE:CD1	2.05	0.69
2:D:311:PRO:O	2:D:313:LEU:HD13	1.93	0.69
2:C:134:ILE:HD12	2:C:178:MSE:HE3	1.73	0.69
1:A:708:LEU:HA	2:C:355:PHE:HE1	1.57	0.69
2:D:328:ARG:HG3	2:D:328:ARG:HH21	1.56	0.69
2:D:313:LEU:HD13	2:D:313:LEU:N	2.08	0.69
1:A:770:GLY:N	1:A:811:ILE:HD12	2.08	0.69
1:A:52:ILE:CD1	1:A:135:ILE:HD12	2.23	0.68
2:C:280:ILE:HB	2:C:310:LEU:HD21	1.75	0.68
2:D:14:ASP:CB	2:D:58:ASP:H	2.06	0.68
1:A:6:LEU:HG	1:A:43:ILE:HG12	1.74	0.68
2:C:360:LYS:HA	2:C:366:HIS:CB	2.23	0.68
2:D:328:ARG:CG	2:D:328:ARG:HH21	2.06	0.68
2:D:149:ASN:ND2	2:D:153:PHE:HB3	1.99	0.68
2:D:358:TYR:CE1	2:D:362:ARG:HD3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:GLY:N	1:B:811:ILE:HD12	2.08	0.68
1:A:48:PHE:CG	1:A:131:HIS:HB2	2.28	0.68
2:D:235:LEU:O	2:D:269:PRO:HG3	1.95	0.67
2:D:313:LEU:O	2:D:317:ILE:N	2.27	0.67
2:D:63:ARG:HB3	2:D:94:HIS:ND1	2.09	0.67
2:C:63:ARG:HB3	2:C:95:ASP:HA	1.76	0.67
2:D:14:ASP:CG	2:D:58:ASP:H	1.97	0.67
1:A:69:THR:HG22	1:A:90:ASN:HB2	1.77	0.67
1:A:714:PHE:CD1	2:C:355:PHE:CD1	2.82	0.67
1:A:100:LEU:HD22	1:A:112:ILE:HD12	1.75	0.67
1:B:703:LEU:HD11	2:D:369:LEU:HD21	1.77	0.67
1:A:184:LEU:HG	1:A:698:TYR:HB2	1.77	0.67
1:B:29:GLU:CD	1:B:30:GLY:N	2.48	0.67
2:D:13:SER:OG	2:D:232:PRO:HD2	1.95	0.67
2:D:312:ASP:OD2	2:D:315:GLY:HA3	1.94	0.67
1:A:3:PRO:HB2	1:A:21:PHE:HD1	1.54	0.66
2:C:16:HIS:O	2:C:19:VAL:HG12	1.95	0.66
1:A:721:ARG:O	1:A:725:ALA:HB3	1.95	0.66
2:D:306:ASP:HB2	2:D:325:ARG:HH12	1.51	0.66
2:C:313:LEU:HD12	2:C:313:LEU:N	2.10	0.66
1:B:758:TRP:NE1	2:D:277:TYR:CZ	2.63	0.66
1:A:721:ARG:HG3	2:C:354:LEU:CD1	2.23	0.66
2:C:63:ARG:HD2	2:C:94:HIS:HB3	1.78	0.66
2:D:306:ASP:O	2:D:306:ASP:OD1	2.13	0.66
1:A:714:PHE:CE2	2:C:355:PHE:HD1	2.14	0.66
2:D:78:LEU:O	2:D:82:MSE:HG3	1.96	0.66
1:B:704:LEU:HD13	2:D:369:LEU:HB3	1.78	0.65
1:A:176:LEU:HD21	2:C:379:GLU:HG2	1.78	0.65
1:B:100:LEU:HD22	1:B:112:ILE:HD12	1.78	0.65
2:C:12:THR:HG22	2:C:249:ALA:HB2	1.78	0.65
2:D:153:PHE:O	2:D:157:LEU:HG	1.97	0.65
1:B:820:ARG:HH21	2:D:328:ARG:NH1	1.94	0.65
1:A:52:ILE:CG1	1:A:135:ILE:HD12	2.27	0.65
1:A:82:ARG:HG3	1:A:103:ILE:HB	1.79	0.65
2:C:104:ASN:HB2	2:C:117:MSE:HE1	1.78	0.65
2:C:340:GLU:OE1	2:C:341:GLU:N	2.30	0.65
2:D:148:LYS:CD	2:D:152:ASP:OD1	2.44	0.65
1:A:722:VAL:HA	1:A:726:VAL:HG23	1.80	0.64
2:C:10:LEU:HB2	2:C:50:VAL:HG11	1.79	0.64
1:A:51:GLY:C	1:A:52:ILE:HG13	2.16	0.64
2:C:360:LYS:HA	2:C:366:HIS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:ALA:CB	2:C:269:PRO:HD3	2.27	0.64
2:C:306:ASP:CA	2:C:325:ARG:HH11	2.10	0.64
2:C:335:LEU:O	2:C:336:ARG:CG	2.46	0.64
2:D:12:THR:CG2	2:D:55:LEU:HD22	2.27	0.64
1:B:89:ILE:HB	1:B:96:HIS:CD2	2.25	0.64
2:D:12:THR:HG21	2:D:55:LEU:CD2	2.26	0.64
1:B:746:PHE:HD1	1:B:753:PHE:HA	1.61	0.64
2:C:336:ARG:HG3	2:C:337:GLU:N	2.13	0.64
1:A:723:LEU:HD21	1:A:746:PHE:CE2	2.33	0.63
2:C:355:PHE:CE2	2:C:359:LEU:HD21	2.33	0.63
2:D:92:GLY:O	2:D:93:ASN:OD1	2.16	0.63
1:A:30:GLY:H	1:A:36:LYS:HD3	1.63	0.63
1:B:762:ARG:NH2	2:D:283:SER:OG	2.31	0.63
2:C:63:ARG:CB	2:C:94:HIS:O	2.46	0.63
1:B:30:GLY:H	1:B:36:LYS:HD3	1.63	0.63
1:B:705:ARG:HG3	1:B:709:PHE:CE2	2.34	0.63
2:C:308:GLY:HA3	2:C:309:ILE:HB	1.76	0.63
2:C:78:LEU:O	2:C:82:MSE:HG3	1.98	0.63
1:A:744:ILE:HG22	1:A:755:ILE:HG13	1.80	0.63
2:D:104:ASN:HB2	2:D:117:MSE:HE1	1.79	0.63
2:D:14:ASP:HB3	2:D:58:ASP:C	2.18	0.63
2:C:267:ALA:HB3	2:C:269:PRO:HD3	1.81	0.62
2:D:13:SER:HB2	2:D:232:PRO:CB	2.27	0.62
2:C:96:TRP:CZ3	2:D:97:LYS:HD3	2.31	0.62
2:D:144:GLU:HG3	2:D:148:LYS:HB2	1.80	0.62
1:A:89:ILE:HB	1:A:96:HIS:CD2	2.26	0.62
1:B:804:ASP:O	1:B:808:LYS:HG2	1.99	0.62
2:D:313:LEU:N	2:D:313:LEU:CD1	2.62	0.62
1:A:101:SER:HB2	1:A:109:LYS:HB3	1.82	0.62
2:C:105:PHE:HE2	2:D:106:VAL:HG11	1.65	0.62
1:A:137:THR:HG23	1:A:784:ALA:HB1	1.81	0.61
2:D:357:GLU:HG3	2:D:360:LYS:NZ	2.15	0.61
1:A:165:GLN:CD	2:C:352:PHE:HE2	2.03	0.61
1:A:12:LEU:O	1:A:38:SER:HB3	2.00	0.61
1:B:12:LEU:O	1:B:38:SER:HB3	2.00	0.61
2:D:152:ASP:O	2:D:156:PHE:CB	2.49	0.61
1:B:137:THR:HG23	1:B:784:ALA:HB1	1.81	0.61
2:C:307:SER:O	2:C:310:LEU:CD2	2.49	0.61
2:D:9:ILE:HB	2:D:252:VAL:HG13	1.81	0.61
2:C:26:ARG:NH2	2:C:314:MSE:O	2.33	0.61
1:A:738:THR:HG21	1:A:742:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PHE:CZ	1:B:138:VAL:HG11	2.36	0.61
1:A:52:ILE:HG12	1:A:135:ILE:HD12	1.83	0.60
2:C:350:ASP:OD1	2:C:353:GLU:HB3	2.01	0.60
1:B:755:ILE:CD1	1:B:767:LEU:HD11	2.30	0.60
2:D:148:LYS:HB3	2:D:152:ASP:CG	2.21	0.60
2:D:144:GLU:OE2	2:D:148:LYS:HB3	2.00	0.60
2:C:81:MSE:HB3	2:C:87:VAL:HG11	1.82	0.60
1:A:171:GLU:O	1:A:174:GLU:HB3	2.02	0.60
1:A:1:MSE:HG3	1:A:76:PHE:HB2	1.84	0.60
1:B:36:LYS:HD2	1:B:829:THR:O	2.01	0.60
2:C:342:PHE:O	2:C:344:GLU:HG2	2.02	0.60
2:D:313:LEU:HD13	2:D:313:LEU:H	1.65	0.60
2:D:326:LYS:HG3	2:D:330:GLU:HB2	1.84	0.60
1:B:741:ARG:HG3	1:B:758:TRP:CE2	2.37	0.60
1:B:12:LEU:HD11	1:B:53:ARG:NE	2.16	0.60
1:A:36:LYS:HD2	1:A:829:THR:O	2.01	0.60
1:A:727:LEU:HD13	1:A:745:ASP:HA	1.82	0.60
2:C:10:LEU:HD13	2:C:10:LEU:C	2.22	0.59
2:C:340:GLU:C	2:C:341:GLU:HG2	2.21	0.59
2:D:356:LYS:HG3	2:D:370:LEU:HD11	1.84	0.59
1:A:134:PHE:CZ	1:A:138:VAL:HG11	2.37	0.59
2:C:11:HIS:HB3	2:C:250:VAL:HG13	1.83	0.59
1:A:2:ARG:HG3	1:A:792:ASP:CB	2.33	0.59
1:A:711:LYS:O	1:A:715:SER:HB3	2.01	0.59
1:A:48:PHE:CZ	1:A:131:HIS:HA	2.37	0.59
1:A:183:LYS:O	1:A:187:GLU:HG2	2.03	0.59
1:B:811:ILE:HD13	1:B:811:ILE:N	2.17	0.59
1:A:164:PHE:CG	1:A:718:PHE:HZ	2.21	0.58
1:A:811:ILE:N	1:A:811:ILE:HD13	2.17	0.58
1:B:2:ARG:HG3	1:B:792:ASP:CB	2.33	0.58
2:D:144:GLU:O	2:D:145:ALA:CB	2.51	0.58
1:B:708:LEU:HB2	2:D:355:PHE:CZ	2.38	0.58
1:A:721:ARG:CG	2:C:354:LEU:HD11	2.29	0.58
1:B:760:ILE:HD11	2:D:291:PHE:HA	1.84	0.58
1:A:3:PRO:CB	1:A:21:PHE:HD1	2.12	0.58
1:A:45:PHE:CE1	1:A:49:GLY:O	2.56	0.58
1:B:171:GLU:O	1:B:174:GLU:HB3	2.02	0.58
1:B:746:PHE:CD1	1:B:753:PHE:HA	2.38	0.58
1:A:704:LEU:HD22	2:C:372:ILE:HD12	1.85	0.58
2:D:81:MSE:HB3	2:D:87:VAL:HG11	1.84	0.58
2:C:181:PHE:CG	2:C:200:ILE:HD12	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:HIS:O	2:C:370:LEU:HD23	2.03	0.58
2:D:16:HIS:O	2:D:19:VAL:CG1	2.51	0.58
2:C:313:LEU:H	2:C:313:LEU:CD1	2.16	0.58
1:A:714:PHE:CE1	2:C:355:PHE:CB	2.87	0.58
2:C:211:TYR:HE2	2:C:213:ALA:HB2	1.68	0.58
1:A:145:ILE:HG22	1:A:776:SER:OG	2.04	0.57
1:A:722:VAL:CG2	1:A:726:VAL:CG2	2.70	0.57
1:A:741:ARG:HG3	1:A:758:TRP:CE2	2.38	0.57
1:B:2:ARG:HG3	1:B:792:ASP:HB3	1.86	0.57
2:D:12:THR:HG21	2:D:55:LEU:HD22	1.84	0.57
1:B:741:ARG:HD3	1:B:742:PHE:CD2	2.40	0.57
1:B:750:LYS:HD2	1:B:754:ILE:HD11	1.87	0.57
2:C:11:HIS:HE1	2:C:232:PRO:CG	2.13	0.57
2:D:280:ILE:HB	2:D:307:SER:HB2	1.87	0.57
2:C:102:PHE:CE2	2:C:106:VAL:HG21	2.40	0.57
1:A:714:PHE:CE2	2:C:355:PHE:CD1	2.92	0.57
2:D:369:LEU:O	2:D:372:ILE:HG13	2.03	0.57
1:A:773:ALA:HB1	1:A:815:LEU:HD21	1.86	0.57
1:B:756:LYS:HA	1:B:761:GLU:HA	1.86	0.57
1:B:773:ALA:HB1	1:B:815:LEU:HD21	1.87	0.57
2:D:335:LEU:HD13	2:D:335:LEU:O	2.04	0.57
1:B:183:LYS:O	1:B:187:GLU:HG2	2.03	0.57
1:B:1:MSE:HG3	1:B:76:PHE:HB2	1.85	0.57
1:A:723:LEU:O	1:A:727:LEU:HB2	2.04	0.56
2:D:304:GLU:HG3	2:D:305:GLU:H	1.70	0.56
1:A:755:ILE:HD13	1:A:767:LEU:HD11	1.87	0.56
2:C:313:LEU:O	2:C:317:ILE:N	2.34	0.56
2:D:310:LEU:N	2:D:310:LEU:HD23	2.17	0.56
1:A:2:ARG:HG3	1:A:792:ASP:HB3	1.88	0.56
2:C:40:LYS:NZ	2:C:268:SER:HG	1.86	0.56
2:D:54:LEU:HG	2:D:178:MSE:CE	2.36	0.56
2:D:211:TYR:HE2	2:D:213:ALA:HB2	1.71	0.56
2:D:306:ASP:HB3	2:D:325:ARG:HH11	1.48	0.56
1:A:31:PRO:HD3	1:A:845:THR:HG22	1.87	0.56
1:B:152:PRO:O	1:B:156:ILE:HG13	2.06	0.56
1:B:90:ASN:HD22	1:B:93:GLN:NE2	2.04	0.56
2:C:96:TRP:CZ3	2:D:97:LYS:CD	2.88	0.56
2:C:96:TRP:HZ3	2:D:97:LYS:CD	2.16	0.56
1:A:152:PRO:O	1:A:156:ILE:HG13	2.05	0.56
2:C:13:SER:HB2	2:C:233:GLY:N	2.21	0.56
2:C:181:PHE:CD2	2:C:200:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:ILE:O	2:D:376:LEU:HG	2.06	0.56
1:B:26:THR:O	1:B:827:PHE:N	2.38	0.56
1:A:756:LYS:HA	1:A:761:GLU:HA	1.87	0.56
1:B:178:LYS:HA	1:B:181:MSE:HE2	1.88	0.56
1:B:3:PRO:O	1:B:21:PHE:HB2	2.05	0.55
2:C:11:HIS:NE2	2:C:213:ALA:HB1	2.21	0.55
1:B:31:PRO:HD3	1:B:845:THR:HG22	1.87	0.55
2:C:335:LEU:O	2:C:336:ARG:CB	2.55	0.55
1:A:155:GLU:O	1:A:159:ILE:HG12	2.05	0.55
1:A:721:ARG:O	1:A:725:ALA:CB	2.54	0.55
1:A:7:THR:HB	1:A:73:VAL:HG22	1.89	0.55
2:C:313:LEU:HD12	2:C:313:LEU:H	1.69	0.55
2:C:55:LEU:HD12	2:C:89:VAL:HG22	1.88	0.55
1:A:163:VAL:HG13	1:A:164:PHE:CD1	2.41	0.55
1:A:722:VAL:O	1:A:726:VAL:N	2.39	0.55
1:B:736:ILE:HD13	1:B:821:LEU:HD23	1.89	0.55
1:B:805:THR:HA	1:B:808:LYS:CG	2.36	0.55
1:A:148:LEU:HD23	1:A:148:LEU:O	2.07	0.55
2:C:54:LEU:HG	2:C:178:MSE:CE	2.36	0.55
2:C:215:GLY:O	2:C:216:HIS:HB3	2.07	0.55
2:D:207:SER:HA	2:D:227:PRO:HG3	1.89	0.55
1:A:711:LYS:HA	1:A:715:SER:HB3	1.87	0.55
2:D:55:LEU:HD12	2:D:89:VAL:HG22	1.89	0.55
1:A:49:GLY:HA2	1:A:87:ARG:HH22	1.71	0.54
2:C:16:HIS:CD2	2:C:238:ILE:HD11	2.42	0.54
2:C:357:GLU:HA	2:C:360:LYS:HG2	1.88	0.54
1:A:711:LYS:HA	1:A:715:SER:CB	2.37	0.54
1:B:29:GLU:OE1	1:B:30:GLY:N	2.40	0.54
2:C:158:GLU:HA	2:C:161:LEU:HD12	1.89	0.54
2:C:207:SER:HA	2:C:227:PRO:HG3	1.89	0.54
1:B:156:ILE:HD12	1:B:746:PHE:CE1	2.41	0.54
2:C:109:ILE:CD1	2:D:106:VAL:HG13	2.36	0.54
1:A:14:LEU:HD21	1:A:39:LEU:HD23	1.90	0.54
1:B:703:LEU:HD11	2:D:369:LEU:CD2	2.37	0.54
2:C:9:ILE:HB	2:C:252:VAL:HG13	1.89	0.54
2:D:181:PHE:CD2	2:D:200:ILE:HD12	2.43	0.54
1:B:734:LEU:HB3	1:B:742:PHE:O	2.08	0.54
2:D:328:ARG:NH2	2:D:328:ARG:CG	2.69	0.54
1:B:722:VAL:O	1:B:726:VAL:HB	2.08	0.54
2:D:181:PHE:CG	2:D:200:ILE:HD12	2.42	0.54
2:D:357:GLU:HA	2:D:360:LYS:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:HIS:O	2:C:19:VAL:CG1	2.55	0.54
1:A:178:LYS:HA	1:A:181:MSE:HE2	1.89	0.54
1:B:27:VAL:HG12	1:B:840:ARG:O	2.08	0.54
1:A:708:LEU:CB	2:C:355:PHE:CZ	2.88	0.54
2:D:7:MSE:HE1	2:D:52:LEU:HB2	1.90	0.54
1:A:762:ARG:NH1	2:C:286:LYS:HD3	2.23	0.54
2:C:13:SER:CB	2:C:233:GLY:N	2.70	0.54
1:A:717:TYR:CD2	2:C:354:LEU:HD21	2.43	0.54
1:B:820:ARG:NH2	2:D:328:ARG:NH1	2.56	0.54
2:D:215:GLY:O	2:D:216:HIS:HB3	2.07	0.53
1:B:741:ARG:HG3	1:B:758:TRP:CZ2	2.43	0.53
1:B:833:GLU:O	1:B:836:GLU:HG3	2.08	0.53
1:B:820:ARG:CD	2:D:328:ARG:HH12	2.21	0.53
2:D:94:HIS:ND1	2:D:96:TRP:CZ3	2.70	0.53
1:B:727:LEU:HD13	1:B:745:ASP:HA	1.90	0.53
1:A:833:GLU:O	1:A:836:GLU:HG3	2.08	0.53
2:C:346:LEU:C	2:C:346:LEU:CD1	2.76	0.53
2:C:280:ILE:CB	2:C:310:LEU:HD21	2.37	0.53
2:C:307:SER:O	2:C:310:LEU:HD21	2.09	0.53
2:C:96:TRP:CD1	2:C:96:TRP:O	2.61	0.53
1:B:148:LEU:O	1:B:148:LEU:HD23	2.09	0.53
2:C:273:LYS:HG2	2:C:291:PHE:CZ	2.43	0.53
2:D:54:LEU:CG	2:D:178:MSE:HE2	2.39	0.53
2:C:102:PHE:CE2	2:C:106:VAL:CG2	2.92	0.53
2:C:128:ARG:HB2	2:C:130:GLN:HE22	1.73	0.53
2:D:313:LEU:HB2	2:D:320:LEU:HD23	1.90	0.53
1:A:31:PRO:HD2	1:A:845:THR:HA	1.91	0.53
1:A:49:GLY:CA	1:A:87:ARG:HH22	2.22	0.53
1:B:721:ARG:NH2	2:D:349:LEU:HD23	2.23	0.53
2:C:308:GLY:HA2	2:C:309:ILE:CG1	2.38	0.53
2:D:268:SER:N	2:D:269:PRO:CD	2.71	0.53
2:C:93:ASN:CB	2:C:139:TYR:CD2	2.91	0.52
1:A:102:GLU:O	1:A:102:GLU:HG3	2.09	0.52
1:B:1:MSE:CG	1:B:76:PHE:HB2	2.39	0.52
2:C:280:ILE:H	2:C:307:SER:CB	2.22	0.52
1:A:175:LYS:HA	1:A:178:LYS:NZ	2.25	0.52
1:A:27:VAL:HG11	1:A:838:PHE:HB2	1.90	0.52
2:C:12:THR:HG22	2:C:249:ALA:CB	2.40	0.52
2:D:11:HIS:CE1	2:D:213:ALA:CB	2.88	0.52
2:D:149:ASN:C	2:D:149:ASN:HD22	2.06	0.52
2:C:201:ASN:HB3	2:C:204:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PHE:CE1	2:C:355:PHE:HD1	2.27	0.52
1:B:156:ILE:HD13	1:B:753:PHE:CE2	2.45	0.52
1:B:26:THR:CG2	1:B:826:VAL:HG12	2.39	0.52
1:A:714:PHE:HE2	2:C:351:TYR:CE1	2.28	0.52
2:D:156:PHE:O	2:D:160:ARG:HD3	2.09	0.52
1:A:717:TYR:CE2	2:C:354:LEU:HD21	2.44	0.52
2:C:10:LEU:HD21	2:C:265:ILE:HD12	1.92	0.52
2:C:11:HIS:O	2:C:249:ALA:HB1	2.10	0.52
1:A:714:PHE:CE1	2:C:355:PHE:CD1	2.98	0.52
2:C:46:GLU:HG2	2:C:84:THR:OG1	2.08	0.52
2:D:273:LYS:HG2	2:D:291:PHE:CZ	2.45	0.52
1:B:178:LYS:NZ	1:B:178:LYS:HB3	2.25	0.52
2:C:268:SER:N	2:C:269:PRO:HD3	2.23	0.52
2:C:7:MSE:HE1	2:C:52:LEU:HB2	1.91	0.52
1:A:12:LEU:HD11	1:A:53:ARG:NE	2.25	0.51
1:A:164:PHE:CB	1:A:718:PHE:HZ	2.23	0.51
2:D:98:GLY:O	2:D:101:LEU:HB2	2.10	0.51
2:D:360:LYS:HA	2:D:366:HIS:CB	2.36	0.51
1:A:131:HIS:O	1:A:135:ILE:HG12	2.10	0.51
2:C:13:SER:CB	2:C:232:PRO:HB2	2.33	0.51
2:D:301:VAL:CG2	2:D:323:ILE:HG12	2.40	0.51
2:D:46:GLU:HG2	2:D:84:THR:OG1	2.09	0.51
1:A:48:PHE:CD1	1:A:131:HIS:HB2	2.46	0.51
1:B:178:LYS:HB3	1:B:178:LYS:HZ3	1.74	0.51
2:C:79:LYS:HG3	2:D:105:PHE:HE1	1.75	0.51
1:A:164:PHE:HB2	1:A:718:PHE:HZ	1.75	0.51
1:B:809:GLU:HB3	1:B:833:GLU:OE2	2.11	0.51
2:D:128:ARG:HB2	2:D:130:GLN:HE22	1.75	0.51
1:A:108:LYS:HD2	1:A:109:LYS:O	2.10	0.51
1:A:1:MSE:CG	1:A:76:PHE:HB2	2.40	0.51
1:A:3:PRO:O	1:A:21:PHE:HB2	2.10	0.51
2:D:16:HIS:CD2	2:D:238:ILE:CD1	2.94	0.51
2:D:348:LYS:C	2:D:349:LEU:HD22	2.31	0.51
1:A:184:LEU:CD1	1:A:698:TYR:HB2	2.41	0.51
2:D:201:ASN:HB3	2:D:204:LEU:HG	1.92	0.51
2:C:372:ILE:O	2:C:376:LEU:HG	2.11	0.51
2:D:223:ILE:HB	2:D:229:THR:HB	1.93	0.51
1:A:178:LYS:NZ	1:A:178:LYS:HB3	2.25	0.50
2:C:97:LYS:O	2:C:100:LYS:HG3	2.10	0.50
2:C:313:LEU:CD1	2:C:313:LEU:N	2.72	0.50
1:A:790:ARG:HG2	2:C:345:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PRO:HD2	1:B:845:THR:HA	1.92	0.50
2:C:223:ILE:HB	2:C:229:THR:HB	1.92	0.50
1:B:738:THR:CG2	1:B:741:ARG:HB3	2.37	0.50
2:C:93:ASN:HB3	2:C:139:TYR:CD2	2.46	0.50
2:D:152:ASP:O	2:D:156:PHE:HB3	2.12	0.50
2:D:280:ILE:O	2:D:307:SER:CB	2.54	0.50
2:D:357:GLU:HG3	2:D:360:LYS:HZ1	1.77	0.50
2:D:9:ILE:HB	2:D:252:VAL:CG1	2.40	0.50
1:A:730:THR:HG21	1:A:744:ILE:HD11	1.93	0.50
2:C:11:HIS:ND1	2:C:232:PRO:HG2	2.16	0.50
2:C:304:GLU:HG3	2:C:305:GLU:H	1.77	0.50
1:A:714:PHE:CZ	2:C:355:PHE:HD1	2.30	0.50
2:D:301:VAL:HG22	2:D:323:ILE:HG12	1.92	0.50
1:B:758:TRP:CH2	2:D:276:TYR:N	2.78	0.50
2:C:153:PHE:CZ	2:C:198:ILE:HD12	2.47	0.50
2:C:268:SER:N	2:C:269:PRO:HD2	2.25	0.50
2:C:281:ASP:H	2:C:284:ALA:HB3	1.77	0.50
2:D:102:PHE:CE2	2:D:106:VAL:HG21	2.47	0.50
1:B:724:GLU:O	1:B:728:LYS:HB2	2.11	0.50
2:C:301:VAL:HG22	2:C:323:ILE:HG12	1.94	0.50
2:D:152:ASP:O	2:D:156:PHE:HB2	2.11	0.50
1:A:810:LYS:HE3	2:C:279:LYS:NZ	2.27	0.49
2:C:11:HIS:CE1	2:C:232:PRO:HG3	2.32	0.49
2:D:99:LEU:O	2:D:102:PHE:HB3	2.12	0.49
1:A:741:ARG:HG3	1:A:758:TRP:CZ2	2.47	0.49
1:A:95:LYS:NZ	1:A:95:LYS:HB2	2.26	0.49
1:B:156:ILE:CD1	1:B:746:PHE:CE1	2.95	0.49
2:C:19:VAL:HG23	2:C:61:HIS:CE1	2.46	0.49
2:D:281:ASP:H	2:D:284:ALA:HB3	1.75	0.49
1:A:25:ILE:HG23	1:A:25:ILE:O	2.12	0.49
2:C:54:LEU:CG	2:C:178:MSE:HE2	2.39	0.49
2:C:328:ARG:NH2	2:C:328:ARG:CG	2.68	0.49
2:D:148:LYS:HA	2:D:152:ASP:HB2	1.87	0.49
2:C:10:LEU:HD13	2:C:11:HIS:N	2.27	0.49
2:C:116:VAL:CG1	2:C:136:PRO:HB3	2.41	0.49
2:C:309:ILE:CG2	2:C:309:ILE:O	2.60	0.49
1:B:100:LEU:HB2	1:B:119:VAL:HG13	1.95	0.49
2:C:306:ASP:HA	2:C:325:ARG:NH1	2.18	0.49
1:A:184:LEU:HB3	1:A:698:TYR:HD1	1.78	0.49
1:A:723:LEU:HD23	1:A:746:PHE:CG	2.48	0.49
1:B:1:MSE:HG2	1:B:2:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HB3	1:A:167:LYS:NZ	2.27	0.49
2:C:13:SER:HB2	2:C:232:PRO:CB	2.36	0.49
1:A:1:MSE:HG2	1:A:2:ARG:N	2.28	0.48
1:A:723:LEU:HD23	1:A:746:PHE:HD2	1.74	0.48
1:A:174:GLU:OE1	1:A:175:LYS:HD3	2.13	0.48
1:A:35:GLY:O	1:A:39:LEU:HB2	2.13	0.48
1:B:15:LYS:CE	1:B:64:ASN:HD22	2.26	0.48
1:B:762:ARG:HH22	2:D:283:SER:C	2.15	0.48
2:C:301:VAL:CG2	2:C:323:ILE:HG12	2.42	0.48
2:C:307:SER:O	2:C:310:LEU:HG	2.13	0.48
1:A:100:LEU:HB2	1:A:119:VAL:HG13	1.94	0.48
1:A:738:THR:CG2	1:A:741:ARG:HB3	2.36	0.48
2:C:48:ARG:HD3	2:C:251:PHE:CE2	2.48	0.48
2:D:149:ASN:C	2:D:149:ASN:ND2	2.64	0.48
2:D:358:TYR:CZ	2:D:362:ARG:HD3	2.48	0.48
1:B:167:LYS:NZ	1:B:167:LYS:HB3	2.28	0.48
1:B:690:LYS:O	1:B:694:MSE:HG3	2.14	0.48
1:B:746:PHE:HB2	1:B:753:PHE:CD1	2.48	0.48
1:B:783:LEU:O	1:B:786:VAL:HG12	2.13	0.48
1:A:691:LEU:HA	1:A:694:MSE:HE2	1.95	0.48
2:C:235:LEU:O	2:C:269:PRO:HG3	2.13	0.48
1:B:745:ASP:O	1:B:754:ILE:HB	2.12	0.48
1:B:48:PHE:CG	1:B:131:HIS:HB2	2.48	0.48
1:B:32:ASN:HA	1:B:36:LYS:HZ1	1.79	0.48
1:B:691:LEU:HA	1:B:694:MSE:HE2	1.96	0.48
2:C:109:ILE:HD11	2:D:109:ILE:HD11	1.95	0.48
2:D:63:ARG:HD3	2:D:94:HIS:CE1	2.49	0.48
1:B:734:LEU:HD11	1:B:775:ILE:HA	1.96	0.48
1:B:95:LYS:HB2	1:B:95:LYS:NZ	2.29	0.48
2:C:278:LYS:NZ	2:C:305:GLU:HG3	2.28	0.48
2:C:7:MSE:CE	2:C:52:LEU:HB2	2.44	0.48
1:B:1:MSE:HG3	1:B:76:PHE:CD2	2.49	0.48
2:C:10:LEU:CD1	2:C:12:THR:HG23	2.44	0.48
2:D:144:GLU:OE2	2:D:152:ASP:CB	2.52	0.48
1:B:703:LEU:O	1:B:707:TYR:CD2	2.66	0.47
2:C:42:VAL:HG22	2:C:81:MSE:SE	2.64	0.47
2:D:15:TRP:O	2:D:16:HIS:HB2	2.13	0.47
2:D:258:GLU:HB3	2:D:259:PRO:HD2	1.96	0.47
2:D:267:ALA:O	2:D:268:SER:OG	2.30	0.47
1:A:137:THR:CG2	1:A:791:LEU:HD11	2.43	0.47
2:C:280:ILE:N	2:C:307:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:ASP:HB3	2:D:58:ASP:O	2.14	0.47
1:B:58:TYR:HA	1:B:89:ILE:HD11	1.95	0.47
2:D:7:MSE:CE	2:D:52:LEU:HB2	2.44	0.47
1:A:101:SER:HA	1:A:110:ALA:O	2.14	0.47
1:A:1:MSE:HG3	1:A:76:PHE:CD2	2.47	0.47
1:B:714:PHE:CE1	2:D:354:LEU:HD13	2.50	0.47
2:C:277:TYR:O	2:C:303:TYR:HA	2.13	0.47
2:D:102:PHE:CE2	2:D:106:VAL:CG2	2.98	0.47
2:D:277:TYR:O	2:D:303:TYR:HA	2.14	0.47
1:A:690:LYS:O	1:A:694:MSE:HG3	2.14	0.47
1:A:783:LEU:O	1:A:786:VAL:HG12	2.14	0.47
1:B:179:GLU:O	1:B:183:LYS:HG2	2.15	0.47
2:C:258:GLU:HB3	2:C:259:PRO:HD2	1.96	0.47
1:A:78:ARG:HD3	1:A:127:LEU:CD2	2.36	0.47
1:B:173:LEU:HD23	1:B:173:LEU:O	2.15	0.47
1:B:703:LEU:HD13	1:B:707:TYR:HE2	1.79	0.47
1:B:71:ARG:CZ	1:B:86:ILE:HG21	2.45	0.47
2:D:19:VAL:HG23	2:D:61:HIS:CE1	2.50	0.47
1:A:708:LEU:CA	2:C:355:PHE:CZ	2.98	0.47
2:C:267:ALA:C	2:C:269:PRO:HD3	2.35	0.47
1:A:734:LEU:HD11	1:A:775:ILE:HA	1.97	0.47
2:D:116:VAL:CG1	2:D:136:PRO:HB3	2.42	0.47
2:D:271:PRO:O	2:D:297:GLY:HA3	2.15	0.47
1:A:102:GLU:HB3	1:A:112:ILE:HD11	1.97	0.47
1:A:58:TYR:HA	1:A:89:ILE:HD11	1.95	0.47
2:D:313:LEU:HB3	2:D:317:ILE:HD12	1.97	0.47
1:A:52:ILE:HD13	1:A:135:ILE:HG23	1.97	0.47
1:A:11:PHE:CE1	1:A:12:LEU:HD23	2.50	0.46
1:A:706:LYS:HE2	1:A:710:ASP:OD1	2.14	0.46
2:D:48:ARG:HD3	2:D:251:PHE:CE2	2.50	0.46
2:C:95:ASP:N	2:C:95:ASP:OD1	2.45	0.46
2:D:141:ASP:O	2:D:142:GLU:CB	2.58	0.46
2:D:148:LYS:HD3	2:D:152:ASP:OD1	2.14	0.46
1:A:714:PHE:CZ	2:C:355:PHE:CD1	3.03	0.46
1:B:736:ILE:O	1:B:820:ARG:NH2	2.49	0.46
2:D:206:PRO:HB2	2:D:209:VAL:HG13	1.97	0.46
1:A:174:GLU:CG	1:A:709:PHE:CZ	2.95	0.46
2:C:53:ILE:HG21	2:C:81:MSE:HG3	1.97	0.46
2:D:149:ASN:ND2	2:D:153:PHE:CD2	2.84	0.46
1:A:122:GLU:O	1:A:126:ILE:HG13	2.15	0.46
1:A:184:LEU:CG	1:A:698:TYR:HB2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:GLU:O	1:A:701:LEU:HG	2.16	0.46
1:B:15:LYS:HE3	1:B:64:ASN:HD22	1.79	0.46
2:C:206:PRO:HB2	2:C:209:VAL:HG13	1.97	0.46
2:C:248:GLY:HA3	2:C:265:ILE:O	2.16	0.46
2:C:355:PHE:O	2:C:359:LEU:HD13	2.15	0.46
1:B:762:ARG:HH22	2:D:283:SER:CA	2.28	0.46
1:B:141:PRO:HG2	1:B:144:GLU:HB2	1.98	0.46
1:A:141:PRO:HG2	1:A:144:GLU:HB2	1.98	0.46
2:D:142:GLU:CG	2:D:143:SER:N	2.54	0.46
2:D:377:LEU:O	2:D:377:LEU:HD13	2.16	0.46
1:A:156:ILE:O	1:A:160:ILE:HG12	2.15	0.46
1:A:164:PHE:CZ	1:A:787:ALA:HB2	2.51	0.46
1:B:726:VAL:CG2	1:B:786:VAL:HG11	2.46	0.46
2:D:77:TYR:O	2:D:81:MSE:HB2	2.16	0.46
1:A:779:LEU:HD23	1:A:779:LEU:O	2.16	0.45
1:B:176:LEU:HG	1:B:180:LYS:NZ	2.32	0.45
1:B:706:LYS:HE2	1:B:710:ASP:OD1	2.16	0.45
1:B:779:LEU:HD23	1:B:779:LEU:O	2.16	0.45
2:C:215:GLY:O	2:C:216:HIS:CB	2.64	0.45
2:C:377:LEU:O	2:C:380:VAL:HG12	2.16	0.45
2:D:248:GLY:HA3	2:D:265:ILE:O	2.16	0.45
1:A:71:ARG:CZ	1:A:86:ILE:HG21	2.46	0.45
1:B:29:GLU:CD	1:B:29:GLU:C	2.75	0.45
1:B:738:THR:CG2	1:B:742:PHE:CD2	2.83	0.45
2:C:340:GLU:C	2:C:341:GLU:CG	2.82	0.45
2:C:77:TYR:O	2:C:81:MSE:HB2	2.17	0.45
2:C:105:PHE:CE2	2:D:106:VAL:HG11	2.49	0.45
1:B:47:LEU:HD11	1:B:74:PHE:CE2	2.51	0.45
2:D:304:GLU:OE1	2:D:328:ARG:HD3	2.16	0.45
2:D:117:MSE:HE3	2:D:117:MSE:HB2	1.93	0.45
1:A:810:LYS:HE3	2:C:279:LYS:HZ1	1.82	0.45
1:B:838:PHE:O	1:B:839:ASP:C	2.55	0.45
2:D:149:ASN:CA	2:D:153:PHE:CB	2.74	0.45
1:A:730:THR:O	1:A:734:LEU:HD23	2.16	0.45
2:C:153:PHE:HZ	2:C:198:ILE:HD12	1.82	0.45
2:D:53:ILE:HB	2:D:87:VAL:HG12	1.99	0.45
1:A:3:PRO:CG	1:A:21:PHE:CD1	2.99	0.44
1:A:745:ASP:HB2	1:A:754:ILE:HD11	1.99	0.44
1:B:71:ARG:HD2	1:B:88:GLU:OE2	2.17	0.44
1:A:160:ILE:HG13	1:A:722:VAL:HG11	1.99	0.44
2:C:271:PRO:O	2:C:297:GLY:HA3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:TRP:CE2	2:D:99:LEU:HD22	2.52	0.44
1:B:184:LEU:HD21	1:B:694:MSE:HB3	1.99	0.44
1:B:705:ARG:HG3	1:B:709:PHE:CD2	2.52	0.44
2:C:96:TRP:CD1	2:C:99:LEU:CB	2.99	0.44
2:D:148:LYS:C	2:D:152:ASP:CB	2.79	0.44
1:B:11:PHE:CE1	1:B:12:LEU:HD23	2.53	0.44
1:B:730:THR:O	1:B:734:LEU:HD23	2.18	0.44
2:C:162:ASN:O	2:C:166:GLU:HG2	2.18	0.44
2:C:220:PHE:CG	2:C:264:ARG:NH1	2.86	0.44
2:C:8:LYS:HB3	2:C:251:PHE:CE1	2.45	0.44
2:D:366:HIS:CE1	2:D:367:GLU:HG2	2.52	0.44
1:A:78:ARG:HG3	1:A:127:LEU:HD13	2.00	0.44
1:A:3:PRO:C	1:A:21:PHE:HD1	2.21	0.44
2:C:109:ILE:HD12	2:D:106:VAL:HG13	1.99	0.44
2:D:12:THR:HG22	2:D:55:LEU:CD2	2.27	0.44
2:D:357:GLU:HG3	2:D:360:LYS:HZ2	1.83	0.44
1:A:3:PRO:HG2	1:A:21:PHE:CD1	2.53	0.44
1:A:55:PRO:HG2	1:A:56:ASN:H	1.83	0.44
1:A:714:PHE:HE1	2:C:355:PHE:CA	2.15	0.44
1:A:732:ALA:HB1	2:C:342:PHE:CD1	2.53	0.44
2:D:63:ARG:H	2:D:63:ARG:HG2	1.46	0.44
2:D:14:ASP:CG	2:D:58:ASP:N	2.68	0.44
1:A:755:ILE:HG23	1:A:762:ARG:O	2.18	0.44
1:B:703:LEU:HD13	1:B:707:TYR:CE2	2.52	0.44
2:C:211:TYR:CE2	2:C:213:ALA:HB2	2.52	0.44
1:B:179:GLU:OE2	1:B:183:LYS:HE2	2.18	0.43
1:B:27:VAL:HG11	1:B:838:PHE:HB2	1.99	0.43
2:D:305:GLU:OE1	2:D:305:GLU:HA	2.17	0.43
1:A:108:LYS:HB3	1:A:108:LYS:HE3	1.78	0.43
1:A:769:GLY:HA3	1:A:811:ILE:HD11	2.00	0.43
1:A:838:PHE:O	1:A:839:ASP:C	2.54	0.43
2:D:303:TYR:O	2:D:325:ARG:HA	2.17	0.43
2:D:60:LEU:HD11	2:D:71:LEU:HD23	2.00	0.43
1:A:184:LEU:HD21	1:A:694:MSE:HB3	2.00	0.43
1:A:27:VAL:HG13	1:A:27:VAL:O	2.18	0.43
1:A:45:PHE:CD1	1:A:49:GLY:O	2.72	0.43
1:A:783:LEU:HD23	1:A:783:LEU:O	2.18	0.43
2:C:303:TYR:O	2:C:325:ARG:HA	2.19	0.43
1:A:708:LEU:CA	2:C:355:PHE:CE1	2.96	0.43
1:B:758:TRP:CH2	2:D:276:TYR:O	2.71	0.43
1:A:90:ASN:HB3	1:A:93:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ILE:HD11	1:B:775:ILE:HD13	2.01	0.43
2:C:267:ALA:O	2:C:268:SER:CB	2.66	0.43
1:B:55:PRO:HG2	1:B:56:ASN:H	1.83	0.43
2:C:345:GLU:HA	2:C:345:GLU:OE1	2.19	0.43
2:D:308:GLY:HA2	2:D:309:ILE:C	2.38	0.43
1:A:10:ASN:O	1:A:62:ASN:HB2	2.19	0.43
1:A:174:GLU:CA	1:A:709:PHE:CZ	2.86	0.43
1:A:828:ILE:HG22	1:A:828:ILE:O	2.18	0.43
2:C:10:LEU:CD2	2:C:265:ILE:HD12	2.48	0.43
2:C:371:LYS:HA	2:C:374:ASP:OD2	2.19	0.43
2:D:19:VAL:HB	2:D:61:HIS:CG	2.54	0.43
1:A:52:ILE:O	1:A:52:ILE:HG22	2.19	0.43
1:B:769:GLY:HA3	1:B:811:ILE:HD11	1.99	0.43
2:C:10:LEU:CD1	2:C:10:LEU:C	2.87	0.43
2:D:162:ASN:O	2:D:166:GLU:HG2	2.19	0.43
2:D:215:GLY:O	2:D:216:HIS:CB	2.64	0.43
2:D:275:LEU:HD11	2:D:291:PHE:CE2	2.53	0.43
1:A:108:LYS:HD2	1:A:109:LYS:N	2.34	0.43
1:B:12:LEU:HD13	1:B:54:TYR:HE2	1.83	0.43
1:A:797:ASP:HB3	1:A:828:ILE:HB	2.01	0.43
1:B:797:ASP:HB3	1:B:828:ILE:HB	2.00	0.43
2:C:128:ARG:HB2	2:C:130:GLN:NE2	2.32	0.43
2:D:149:ASN:O	2:D:149:ASN:ND2	2.43	0.43
2:D:275:LEU:HB2	2:D:301:VAL:HG12	2.01	0.43
2:D:328:ARG:HA	2:D:331:ILE:HG22	2.01	0.43
2:C:53:ILE:HB	2:C:87:VAL:HG12	2.00	0.43
2:D:207:SER:HA	2:D:227:PRO:CG	2.48	0.42
2:D:313:LEU:CB	2:D:320:LEU:HD23	2.48	0.42
2:C:51:ASP:OD1	2:C:128:ARG:HD3	2.18	0.42
1:A:153:PRO:HD3	1:A:751:GLY:O	2.18	0.42
1:A:754:ILE:HD12	1:A:754:ILE:O	2.19	0.42
1:B:6:LEU:O	1:B:6:LEU:HD13	2.18	0.42
2:D:220:PHE:CG	2:D:264:ARG:NH1	2.88	0.42
2:D:94:HIS:CB	2:D:96:TRP:CZ3	2.97	0.42
1:A:71:ARG:NH1	1:A:86:ILE:HD13	2.34	0.42
1:B:708:LEU:HD23	1:B:708:LEU:C	2.40	0.42
1:B:762:ARG:NH2	2:D:283:SER:O	2.50	0.42
2:D:51:ASP:OD1	2:D:128:ARG:HD3	2.19	0.42
1:A:85:ILE:HG12	1:A:100:LEU:HA	2.02	0.42
1:B:56:ASN:HB3	1:B:59:ASP:OD2	2.20	0.42
2:C:275:LEU:HB2	2:C:301:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:360:LYS:HA	2:C:366:HIS:HB2	1.98	0.42
2:C:63:ARG:HD2	2:C:94:HIS:CB	2.46	0.42
2:D:371:LYS:HA	2:D:374:ASP:OD2	2.19	0.42
2:D:53:ILE:HG21	2:D:81:MSE:HG3	2.02	0.42
1:A:51:GLY:O	1:A:52:ILE:HG13	2.19	0.42
1:A:56:ASN:HB3	1:A:59:ASP:OD2	2.20	0.42
1:A:164:PHE:HB2	1:A:718:PHE:CZ	2.52	0.42
1:B:78:ARG:HG3	1:B:127:LEU:HD13	2.02	0.42
2:C:134:ILE:O	2:C:136:PRO:HD3	2.20	0.42
2:C:14:ASP:HB3	2:C:58:ASP:N	2.35	0.42
1:A:145:ILE:HG23	1:A:780:ALA:HB2	2.02	0.42
1:B:140:LEU:O	1:B:796:ILE:HA	2.19	0.42
1:B:746:PHE:HB2	1:B:753:PHE:HD1	1.85	0.42
1:B:156:ILE:CD1	1:B:753:PHE:CE2	3.02	0.42
1:B:828:ILE:O	1:B:828:ILE:HG22	2.20	0.42
1:B:71:ARG:NH1	1:B:86:ILE:HD13	2.34	0.42
2:D:8:LYS:HB3	2:D:251:PHE:CE1	2.46	0.42
1:A:721:ARG:O	1:A:725:ALA:N	2.51	0.42
1:B:793:ALA:HA	1:B:824:VAL:O	2.19	0.42
2:D:120:GLU:HA	2:D:121:PRO:HD3	1.82	0.42
2:D:149:ASN:ND2	2:D:153:PHE:HB2	2.29	0.42
1:A:12:LEU:HD13	1:A:54:TYR:HE2	1.84	0.42
1:B:746:PHE:CE1	1:B:752:GLY:C	2.88	0.42
1:B:95:LYS:HB2	1:B:95:LYS:HZ1	1.83	0.42
2:D:63:ARG:O	2:D:96:TRP:HE3	2.03	0.42
1:A:78:ARG:CG	1:A:127:LEU:HD13	2.49	0.41
1:A:7:THR:O	1:A:72:LEU:HA	2.20	0.41
1:A:762:ARG:HG3	1:A:763:PRO:HD2	2.02	0.41
2:C:102:PHE:C	2:C:102:PHE:CD2	2.92	0.41
2:C:11:HIS:HD2	2:C:54:LEU:HB3	1.85	0.41
2:C:207:SER:HA	2:C:227:PRO:CG	2.49	0.41
1:A:176:LEU:HD21	2:C:379:GLU:CG	2.47	0.41
1:A:6:LEU:O	1:A:6:LEU:HD13	2.20	0.41
1:A:705:ARG:HG2	1:A:706:LYS:N	2.35	0.41
1:A:708:LEU:HD23	1:A:709:PHE:N	2.32	0.41
1:A:8:VAL:HG11	1:A:14:LEU:HD22	2.02	0.41
2:D:149:ASN:C	2:D:153:PHE:CB	2.87	0.41
1:A:178:LYS:HZ3	1:A:178:LYS:HB3	1.84	0.41
2:C:217:ILE:O	2:C:233:GLY:HA2	2.20	0.41
2:C:273:LYS:HG3	2:C:275:LEU:CD1	2.51	0.41
2:D:128:ARG:HB2	2:D:130:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:SER:CB	2:D:233:GLY:N	2.84	0.41
2:D:144:GLU:OE2	2:D:148:LYS:CB	2.69	0.41
2:D:259:PRO:HA	2:D:260:PRO:HD3	1.87	0.41
2:D:273:LYS:HG3	2:D:275:LEU:CD1	2.51	0.41
1:B:50:ASN:HB2	1:B:131:HIS:CE1	2.56	0.41
2:C:97:LYS:HA	2:C:100:LYS:HG3	2.03	0.41
1:A:140:LEU:O	1:A:796:ILE:HA	2.20	0.41
1:A:165:GLN:CD	2:C:352:PHE:CE2	2.90	0.41
1:A:78:ARG:CD	1:A:127:LEU:HD13	2.50	0.41
2:C:11:HIS:HD2	2:C:54:LEU:CB	2.34	0.41
2:C:275:LEU:HD11	2:C:291:PHE:CE2	2.55	0.41
1:B:85:ILE:HD11	1:B:100:LEU:HG	2.02	0.41
1:B:703:LEU:O	1:B:707:TYR:HD2	2.04	0.41
1:B:78:ARG:NE	1:B:78:ARG:HA	2.36	0.41
1:B:804:ASP:OD1	1:B:807:ASN:HB2	2.21	0.41
1:B:8:VAL:HG11	1:B:14:LEU:HD22	2.01	0.41
2:C:280:ILE:CB	2:C:310:LEU:CD2	2.99	0.41
2:C:366:HIS:C	2:C:370:LEU:HD23	2.40	0.41
2:D:180:HIS:CE1	2:D:216:HIS:HB2	2.56	0.41
2:D:206:PRO:O	2:D:227:PRO:HG2	2.20	0.41
1:A:32:ASN:HA	1:A:36:LYS:HZ1	1.84	0.41
1:B:737:LEU:HD21	1:B:821:LEU:HG	2.03	0.41
2:C:60:LEU:HD11	2:C:71:LEU:HD23	2.03	0.41
1:B:706:LYS:HE3	1:B:706:LYS:CA	2.41	0.41
2:C:117:MSE:HE3	2:C:117:MSE:HB2	1.91	0.41
2:C:169:LEU:HD21	2:C:208:VAL:HG11	2.03	0.41
2:C:13:SER:H	2:C:232:PRO:HB2	1.86	0.41
2:C:366:HIS:HB2	2:C:370:LEU:HD21	2.02	0.41
2:D:90:LEU:HD11	2:D:138:PRO:HB3	2.02	0.41
1:A:700:ASN:O	1:A:703:LEU:HG	2.20	0.41
1:A:706:LYS:HE2	1:A:710:ASP:OD2	2.19	0.41
1:A:706:LYS:HE3	1:A:706:LYS:CA	2.41	0.41
2:C:220:PHE:HD1	2:C:231:TYR:O	2.04	0.41
2:C:228:LEU:HD21	2:C:262:TYR:CD2	2.56	0.41
2:D:361:LYS:HB2	2:D:361:LYS:NZ	2.36	0.41
2:D:19:VAL:HG23	2:D:61:HIS:NE2	2.36	0.41
1:B:700:ASN:O	1:B:703:LEU:HG	2.20	0.41
1:B:90:ASN:ND2	1:B:93:GLN:HG3	2.36	0.41
2:C:9:ILE:HB	2:C:252:VAL:CG1	2.50	0.41
2:C:206:PRO:O	2:C:227:PRO:HG2	2.21	0.41
2:C:90:LEU:HD11	2:C:138:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:PHE:C	2:D:242:GLU:H	2.24	0.41
1:A:132:ARG:HD3	1:A:132:ARG:C	2.41	0.40
1:A:41:GLU:OE2	1:A:52:ILE:N	2.43	0.40
1:A:95:LYS:NZ	1:A:95:LYS:CB	2.84	0.40
1:B:762:ARG:HG3	1:B:763:PRO:HD2	2.02	0.40
2:C:14:ASP:HB3	2:C:58:ASP:H	1.86	0.40
2:C:156:PHE:O	2:C:160:ARG:HD3	2.21	0.40
2:C:180:HIS:CE1	2:C:216:HIS:HB2	2.56	0.40
2:D:135:LEU:HD22	2:D:135:LEU:N	2.36	0.40
1:A:148:LEU:HD23	1:A:148:LEU:C	2.42	0.40
1:A:737:LEU:HD21	1:A:821:LEU:HG	2.04	0.40
2:C:11:HIS:HE1	2:C:232:PRO:HG2	1.71	0.40
1:A:714:PHE:HE2	2:C:351:TYR:CZ	2.39	0.40
2:C:105:PHE:HE2	2:D:106:VAL:CG1	2.32	0.40
2:C:14:ASP:N	2:C:14:ASP:OD1	2.55	0.40
2:C:278:LYS:HZ3	2:C:305:GLU:HG3	1.85	0.40
2:D:148:LYS:O	2:D:152:ASP:C	2.58	0.40
1:A:834:PHE:O	1:A:838:PHE:CE2	2.75	0.40
1:A:85:ILE:HD11	1:A:100:LEU:HG	2.04	0.40
1:B:10:ASN:O	1:B:62:ASN:HB2	2.20	0.40
2:D:220:PHE:HD1	2:D:231:TYR:O	2.04	0.40
2:C:307:SER:O	2:C:310:LEU:CG	2.70	0.40
2:D:134:ILE:O	2:D:136:PRO:HD3	2.22	0.40
2:D:93:ASN:C	2:D:93:ASN:OD1	2.60	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	345/365 (94%)	314 (91%)	27 (8%)	4 (1%)	13 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	345/365 (94%)	315 (91%)	28 (8%)	2 (1%)	25	57
2	C	356/379 (94%)	330 (93%)	23 (6%)	3 (1%)	19	51
2	D	360/379 (95%)	330 (92%)	27 (8%)	3 (1%)	19	51
All	All	1406/1488 (94%)	1289 (92%)	105 (8%)	12 (1%)	17	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	268	SER
2	C	309	ILE
1	A	51	GLY
2	C	336	ARG
2	D	145	ALA
1	A	52	ILE
1	B	55	PRO
2	D	140	PRO
2	D	142	GLU
1	A	55	PRO
1	A	150	ILE
1	B	150	ILE

### 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	303/307 (99%)	290 (96%)	13 (4%)	29	59
1	B	303/307 (99%)	293 (97%)	10 (3%)	38	66
2	C	331/335 (99%)	310 (94%)	21 (6%)	18	47
2	D	331/335 (99%)	315 (95%)	16 (5%)	25	56
All	All	1268/1284 (99%)	1208 (95%)	60 (5%)	26	57

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	12	LEU
1	A	44	SER
1	A	50	ASN
1	A	102	GLU
1	A	108	LYS
1	A	127	LEU
1	A	706	LYS
1	A	708	LEU
1	A	712	SER
1	A	792	ASP
1	A	811	ILE
1	A	831	ASP
1	B	1	MSE
1	B	12	LEU
1	B	102	GLU
1	B	108	LYS
1	B	127	LEU
1	B	706	LYS
1	B	754	ILE
1	B	792	ASP
1	B	811	ILE
1	B	831	ASP
2	C	13	SER
2	C	14	ASP
2	C	63	ARG
2	C	81	MSE
2	C	93	ASN
2	C	94	HIS
2	C	95	ASP
2	C	96	TRP
2	C	97	LYS
2	C	100	LYS
2	C	142	GLU
2	C	165	TYR
2	C	256	ARG
2	C	328	ARG
2	C	329	ARG
2	C	335	LEU
2	C	340	GLU
2	C	341	GLU
2	C	346	LEU
2	C	362	ARG

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Mol	Chain	Res	Type
2	C	370	LEU
2	D	13	SER
2	D	14	ASP
2	D	63	ARG
2	D	81	MSE
2	D	100	LYS
2	D	142	GLU
2	D	149	ASN
2	D	152	ASP
2	D	165	TYR
2	D	306	ASP
2	D	309	ILE
2	D	313	LEU
2	D	328	ARG
2	D	329	ARG
2	D	354	LEU
2	D	359	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	96	HIS
1	A	121	GLN
1	B	64	ASN
1	B	93	GLN
1	B	96	HIS
1	B	121	GLN
2	C	93	ASN
2	C	180	HIS
2	C	216	HIS
2	C	366	HIS
2	D	72	HIS
2	D	149	ASN
2	D	216	HIS

### 5.3.3 RNA ⓘ

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](#)

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	GOL	A	3968	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	D	3968	-	5,5,5	0.41	0	5,5,5	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	GOL	A	3968	-	-	2/4/4/4	-
3	GOL	D	3968	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3968	GOL	O1-C1-C2-C3
3	D	3968	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	3968	GOL	O1-C1-C2-O2
3	D	3968	GOL	O1-C1-C2-O2

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	345/365 (94%)	-0.37	4 (1%) 79 77	30, 83, 211, 328	75 (21%)
1	B	318/365 (87%)	2.30	158 (49%) 0 0	51, 134, 217, 391	277 (87%)
2	C	354/379 (93%)	-0.31	9 (2%) 57 55	33, 87, 193, 279	85 (24%)
2	D	355/379 (93%)	-0.15	20 (5%) 24 25	30, 88, 225, 363	81 (22%)
All	All	1372/1488 (92%)	0.32	191 (13%) 2 3	30, 100, 213, 391	518 (37%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	702	ASP	16.4
1	B	187	GLU	11.8
1	B	16	ASN	11.0
1	B	845	THR	10.3
1	B	103	ILE	9.9
1	B	22	GLN	9.2
1	B	699	ASN	7.9
1	B	42	ALA	7.8
1	B	95	LYS	7.6
1	B	715	SER	7.5
1	B	801	SER	7.5
1	B	695	SER	7.4
1	B	182	LYS	7.3
1	B	799	GLY	7.2
1	B	719	THR	7.1
1	B	162	ASP	6.9
1	B	124	GLU	6.9
1	B	94	ARG	6.9
1	B	97	ASN	6.8
1	B	57	SER	6.6
1	B	703	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	800	PHE	6.5
1	B	120	LYS	6.5
1	B	31	PRO	6.4
1	B	700	ASN	6.4
1	B	99	LYS	6.4
1	B	60	TYR	6.4
1	B	185	GLU	6.3
1	B	102	GLU	6.2
1	B	91	ALA	6.2
1	B	174	GLU	6.1
2	D	336	ARG	6.1
1	B	92	LEU	6.0
1	B	697	GLU	5.9
1	B	66	VAL	5.8
1	B	846	GLY	5.8
1	B	96	HIS	5.8
1	B	106	ASN	5.7
1	B	161	SER	5.7
1	B	183	LYS	5.7
1	B	129	ILE	5.6
1	B	38	SER	5.6
1	B	839	ASP	5.6
1	B	50	ASN	5.5
1	B	136	ARG	5.4
2	C	196	ARG	5.4
2	D	345	GLU	5.4
1	B	23	SER	5.3
1	B	24	GLY	5.3
1	B	69	THR	5.3
1	B	130	GLU	5.2
1	B	696	ASP	5.2
1	B	844	ILE	5.2
1	B	179	GLU	5.1
1	B	90	ASN	5.1
1	B	168	GLU	5.1
2	D	335	LEU	5.0
1	B	44	SER	5.0
1	B	117	THR	5.0
1	B	691	LEU	5.0
1	B	67	ASP	4.9
1	B	30	GLY	4.8
1	B	70	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	167	LYS	4.7
2	D	344	GLU	4.7
1	B	83	TYR	4.7
2	C	150	GLU	4.6
1	B	20	GLU	4.6
1	B	59	ASP	4.6
1	B	64	ASN	4.6
1	B	55	PRO	4.4
1	B	108	LYS	4.4
1	B	836	GLU	4.4
1	B	175	LYS	4.3
1	B	707	TYR	4.3
1	B	27	VAL	4.2
1	B	47	LEU	4.2
1	B	114	ALA	4.2
1	B	58	TYR	4.2
1	B	9	ARG	4.1
1	B	81	LYS	4.1
1	B	109	LYS	4.0
1	B	54	TYR	4.0
1	B	804	ASP	4.0
1	B	61	VAL	3.9
1	B	100	LEU	3.9
1	B	139	PHE	3.9
1	B	128	GLY	3.8
1	B	184	LEU	3.8
1	B	88	GLU	3.7
1	B	710	ASP	3.7
1	B	105	GLU	3.7
1	B	74	PHE	3.6
1	B	748	ASP	3.6
1	B	49	GLY	3.6
1	B	752	GLY	3.5
1	B	177	LEU	3.5
1	B	15	LYS	3.5
1	B	165	GLN	3.5
1	B	121	GLN	3.4
1	B	843	ARG	3.4
1	B	714	PHE	3.3
1	B	125	LYS	3.3
1	B	716	ARG	3.3
1	B	746	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	307	SER	3.3
1	B	166	SER	3.3
1	B	832	ARG	3.3
1	B	93	GLN	3.2
2	C	197	GLU	3.2
2	C	149	ASN	3.1
1	B	172	LYS	3.1
1	B	135	ILE	3.1
1	B	806	GLU	3.1
2	D	371	LYS	3.1
2	D	351	TYR	3.0
1	B	18	ASP	3.0
1	B	833	GLU	3.0
1	B	71	ARG	3.0
2	D	362	ARG	2.9
1	B	89	ILE	2.9
1	B	25	ILE	2.9
2	C	156	PHE	2.9
1	B	28	VAL	2.9
1	B	11	PHE	2.8
1	B	53	ARG	2.8
1	B	718	PHE	2.8
1	B	849	VAL	2.8
1	B	119	VAL	2.7
2	D	378	ASP	2.7
1	B	63	ARG	2.7
2	D	347	ASP	2.6
2	C	342	PHE	2.6
1	B	722	VAL	2.6
2	D	379	GLU	2.6
1	B	76	PHE	2.6
1	B	709	PHE	2.5
1	B	14	LEU	2.5
1	B	708	LEU	2.5
1	B	8	VAL	2.5
1	B	689	LYS	2.5
1	B	788	SER	2.5
1	B	840	ARG	2.5
1	A	67	ASP	2.5
1	B	19	ILE	2.5
1	B	749	GLU	2.5
1	B	51	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	52	ILE	2.5
2	D	357	GLU	2.4
2	D	367	GLU	2.4
1	B	787	ALA	2.4
1	B	712	SER	2.4
1	A	23	SER	2.3
2	D	348	LYS	2.3
1	B	717	TYR	2.3
1	B	36	LYS	2.3
1	B	32	ASN	2.3
1	B	848	VAL	2.3
1	B	62	ASN	2.3
2	D	329	ARG	2.3
1	B	711	LYS	2.3
1	B	4	GLU	2.3
1	B	720	GLY	2.3
1	A	699	ASN	2.3
1	B	705	ARG	2.3
1	B	6	LEU	2.2
2	D	334	VAL	2.2
1	B	706	LYS	2.2
1	B	5	ARG	2.2
1	B	704	LEU	2.2
2	D	366	HIS	2.2
1	B	29	GLU	2.2
1	B	831	ASP	2.2
1	B	178	LYS	2.2
2	C	94	HIS	2.2
1	B	41	GLU	2.1
1	B	116	PRO	2.1
1	B	21	PHE	2.1
2	D	349	LEU	2.1
1	A	690	LYS	2.1
1	B	751	GLY	2.1
1	B	805	THR	2.1
2	C	154	ARG	2.1
1	B	37	SER	2.1
2	D	383	SER	2.1
1	B	78	ARG	2.1
2	D	148	LYS	2.1
1	B	26	THR	2.1
1	B	750	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	834	PHE	2.1
2	D	352	PHE	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	3968	6/6	0.85	0.28	56,83,86,86	0
3	GOL	A	3968	6/6	0.95	0.17	53,55,58,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.