



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:40 am BST

PDB ID : 2FWR  
Title : Structure of Archaeoglobus Fulgidis XPB  
Authors : Fan, L.; Arvai, A.S.; Tainer, J.A.  
Deposited on : 2006-02-02  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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

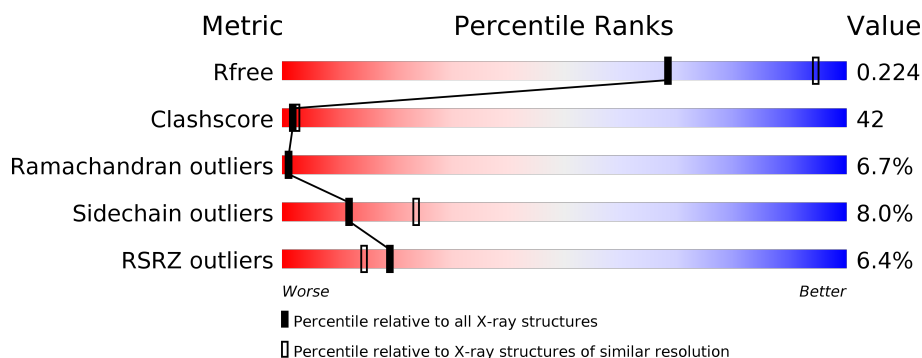
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	472	<div> <div>7%</div> <div> <div>39%</div> <div>45%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	472	<div> <div>5%</div> <div> <div>43%</div> <div>40%</div> <div>6%</div> <div>10%</div> </div> </div>
1	C	472	<div> <div>4%</div> <div> <div>33%</div> <div>44%</div> <div>10%</div> <div>12%</div> </div> </div>
1	D	472	<div> <div>8%</div> <div> <div>31%</div> <div>50%</div> <div>10%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14769 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 DNA repair protein RAD25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3513	2242	627	638	6			
1	B	423	Total	C	N	O	S	0	0	0
			3419	2181	611	619	8			
1	C	414	Total	C	N	O	S	0	0	0
			3317	2119	589	604	5			
1	D	428	Total	C	N	O	S	0	0	0
			3402	2169	604	623	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O29889
A	2	GLY	-	CLONING ARTIFACT	UNP O29889
A	3	SER	-	CLONING ARTIFACT	UNP O29889
A	4	SER	-	CLONING ARTIFACT	UNP O29889
A	5	HIS	-	EXPRESSION TAG	UNP O29889
A	6	HIS	-	EXPRESSION TAG	UNP O29889
A	7	HIS	-	EXPRESSION TAG	UNP O29889
A	8	HIS	-	EXPRESSION TAG	UNP O29889
A	9	HIS	-	EXPRESSION TAG	UNP O29889
A	10	HIS	-	EXPRESSION TAG	UNP O29889
A	11	SER	-	CLONING ARTIFACT	UNP O29889
A	12	SER	-	CLONING ARTIFACT	UNP O29889
A	13	GLY	-	CLONING ARTIFACT	UNP O29889
A	14	LEU	-	CLONING ARTIFACT	UNP O29889
A	15	VAL	-	CLONING ARTIFACT	UNP O29889
A	16	PRO	-	CLONING ARTIFACT	UNP O29889
A	17	ARG	-	CLONING ARTIFACT	UNP O29889
A	18	GLY	-	CLONING ARTIFACT	UNP O29889
A	19	SER	-	CLONING ARTIFACT	UNP O29889
A	20	HIS	-	CLONING ARTIFACT	UNP O29889
B	1	MET	-	INITIATING METHIONINE	UNP O29889

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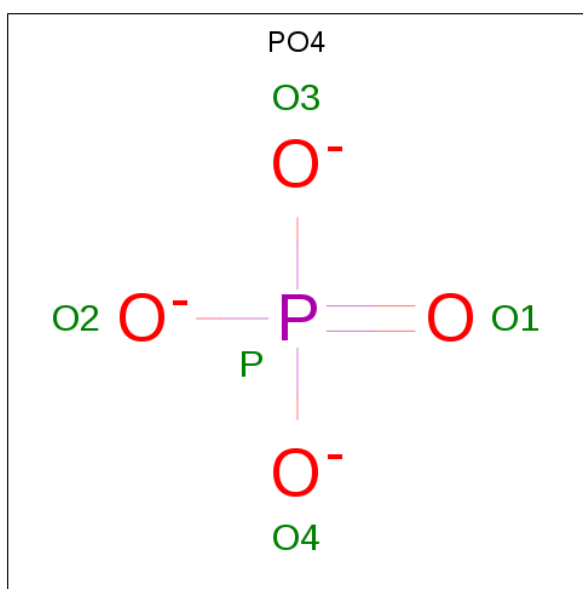
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	CLONING ARTIFACT	UNP 029889
B	3	SER	-	CLONING ARTIFACT	UNP 029889
B	4	SER	-	CLONING ARTIFACT	UNP 029889
B	5	HIS	-	EXPRESSION TAG	UNP 029889
B	6	HIS	-	EXPRESSION TAG	UNP 029889
B	7	HIS	-	EXPRESSION TAG	UNP 029889
B	8	HIS	-	EXPRESSION TAG	UNP 029889
B	9	HIS	-	EXPRESSION TAG	UNP 029889
B	10	HIS	-	EXPRESSION TAG	UNP 029889
B	11	SER	-	CLONING ARTIFACT	UNP 029889
B	12	SER	-	CLONING ARTIFACT	UNP 029889
B	13	GLY	-	CLONING ARTIFACT	UNP 029889
B	14	LEU	-	CLONING ARTIFACT	UNP 029889
B	15	VAL	-	CLONING ARTIFACT	UNP 029889
B	16	PRO	-	CLONING ARTIFACT	UNP 029889
B	17	ARG	-	CLONING ARTIFACT	UNP 029889
B	18	GLY	-	CLONING ARTIFACT	UNP 029889
B	19	SER	-	CLONING ARTIFACT	UNP 029889
B	20	HIS	-	CLONING ARTIFACT	UNP 029889
C	1	MET	-	INITIATING METHIONINE	UNP 029889
C	2	GLY	-	CLONING ARTIFACT	UNP 029889
C	3	SER	-	CLONING ARTIFACT	UNP 029889
C	4	SER	-	CLONING ARTIFACT	UNP 029889
C	5	HIS	-	EXPRESSION TAG	UNP 029889
C	6	HIS	-	EXPRESSION TAG	UNP 029889
C	7	HIS	-	EXPRESSION TAG	UNP 029889
C	8	HIS	-	EXPRESSION TAG	UNP 029889
C	9	HIS	-	EXPRESSION TAG	UNP 029889
C	10	HIS	-	EXPRESSION TAG	UNP 029889
C	11	SER	-	CLONING ARTIFACT	UNP 029889
C	12	SER	-	CLONING ARTIFACT	UNP 029889
C	13	GLY	-	CLONING ARTIFACT	UNP 029889
C	14	LEU	-	CLONING ARTIFACT	UNP 029889
C	15	VAL	-	CLONING ARTIFACT	UNP 029889
C	16	PRO	-	CLONING ARTIFACT	UNP 029889
C	17	ARG	-	CLONING ARTIFACT	UNP 029889
C	18	GLY	-	CLONING ARTIFACT	UNP 029889
C	19	SER	-	CLONING ARTIFACT	UNP 029889
C	20	HIS	-	CLONING ARTIFACT	UNP 029889
D	1	MET	-	INITIATING METHIONINE	UNP 029889
D	2	GLY	-	CLONING ARTIFACT	UNP 029889
D	3	SER	-	CLONING ARTIFACT	UNP 029889

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	CLONING ARTIFACT	UNP O29889
D	5	HIS	-	EXPRESSION TAG	UNP O29889
D	6	HIS	-	EXPRESSION TAG	UNP O29889
D	7	HIS	-	EXPRESSION TAG	UNP O29889
D	8	HIS	-	EXPRESSION TAG	UNP O29889
D	9	HIS	-	EXPRESSION TAG	UNP O29889
D	10	HIS	-	EXPRESSION TAG	UNP O29889
D	11	SER	-	CLONING ARTIFACT	UNP O29889
D	12	SER	-	CLONING ARTIFACT	UNP O29889
D	13	GLY	-	CLONING ARTIFACT	UNP O29889
D	14	LEU	-	CLONING ARTIFACT	UNP O29889
D	15	VAL	-	CLONING ARTIFACT	UNP O29889
D	16	PRO	-	CLONING ARTIFACT	UNP O29889
D	17	ARG	-	CLONING ARTIFACT	UNP O29889
D	18	GLY	-	CLONING ARTIFACT	UNP O29889
D	19	SER	-	CLONING ARTIFACT	UNP O29889
D	20	HIS	-	CLONING ARTIFACT	UNP O29889

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



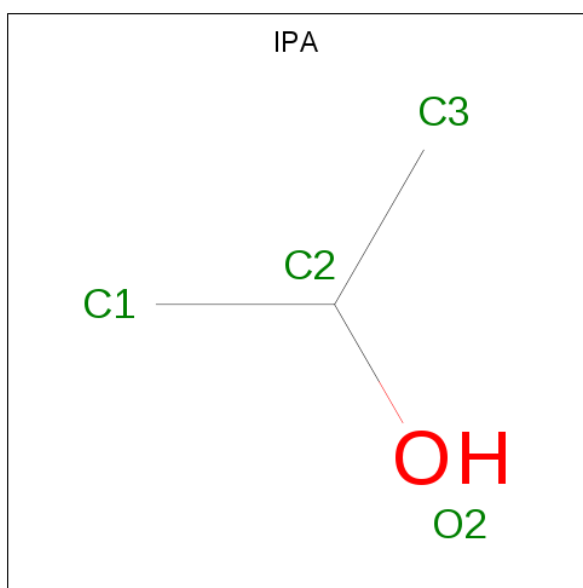
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		

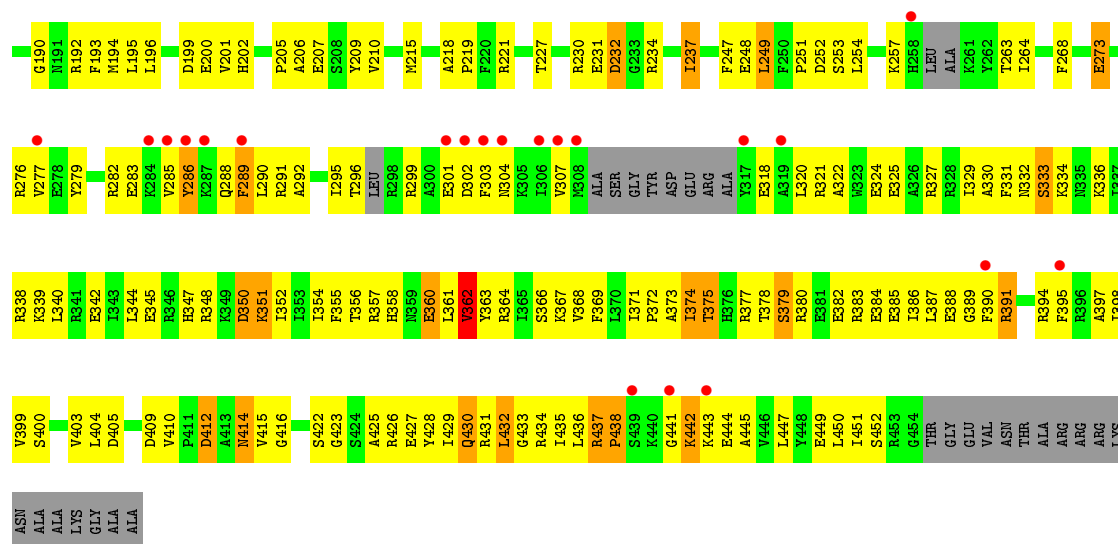
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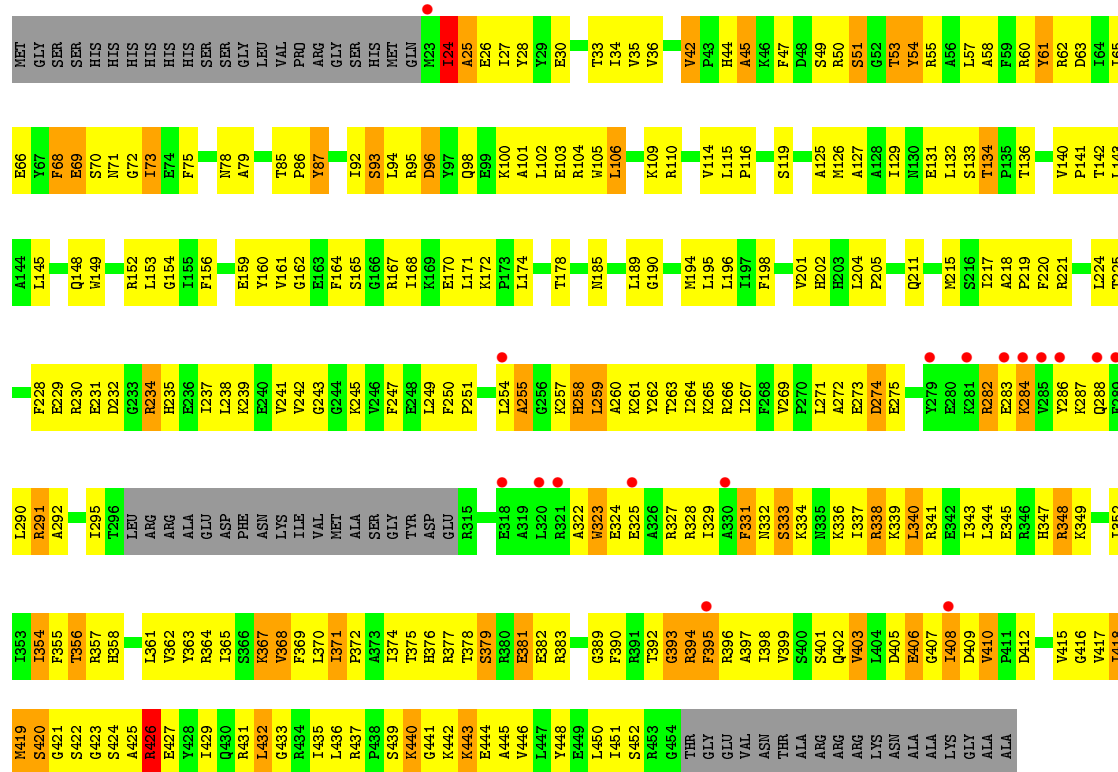
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	299	Total 299	O 299	0	0
4	C	261	Total 261	O 261	0	0
4	D	220	Total 220	O 220	0	0



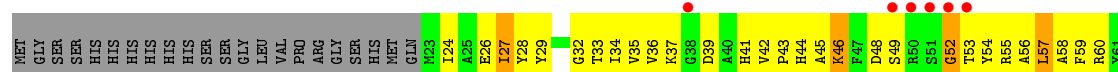




• Molecule 1: DNA repair protein RAD25



• Molecule 1: DNA repair protein RAD25



GLY	I408	R346	K284	S216	L137	R62
ALA	D409	H347	V285	I217	I138	D63
	V410		V286	A218	V139	I64
	P411	D350	K287	P219	V140	I65
	A413	K351	Q288	R221	P141	E66
	N414	I352	F289	L222	T142	Y67
	V415	I353	L290		F68	F69
	G415	I354	R291	T225	L143	S70
	V417	F355	A292	A226	W149	N71
	I418	T356	R293	A227	K150	G72
	M419	R357	G294	T227	E151	I73
	S420	H358	I295	F228	R152	E74
	G421	N359	T296	E229	L153	F75
	S422	E360	LEU	R230	G154	V76
	G423	L361	ARG	E231	I155	D77
	S424	V362	ARG	D232	E158	N78
	A425	R363	ALA	G233	E159	A79
	R426	R364	GLU	R234	Y160	A80
	E427	I365	ASP		V161	D81
	Y428	S366	PHE	I237	G162	P82
	I429	K367	ASN	L238	E163	I83
	Q430	V368	K305	K239	F164	P84
	R431	F369	I306		S165	T85
	L432	L370	V307	V242	G166	P86
		I371	N308	G243	R167	
	I435	P372	A309		L168	E91
	L436	A373	S310	V246	K169	I92
	R437	I374	G311		E170	S93
	P438	T375	V312	L249	L171	I94
	S439	H376	ASP	F250	K172	R95
	K440	R377	GLU	P251	P173	D86
	G441	T378	ARG	D252	L174	Y97
	K442	S379	A316	S253	T175	Q98
	E443	R380	V317	L254	V176	E99
		E381	E318	A255	S177	K100
	L447	E382	A319	G256	T178	A101
	Y448	R383	L320	K257	Y179	L102
	E449	E384	R321	H258	D180	
	L450	L387	A322	L259		W105
	I451	E388	K323	K261	V184	L106
	S452	G389	E324		K109	K109
	R453	F390	A326	L264	R110	R110
	G454	R391	R327	K265	G111	G111
	T455	T392	K328	A266	C112	C112
	E457	R394	I329	I267	M194	I113
	V458	F395	F331	F268	L195	V114
	N459	R396	N332	V269	F198	L115
	T460	A397	S333	E273		P116
	A461	I398		D274	V201	T117
	ARG	V399	K336	E275		G118
	ARG	S400	I337	R276		K121
	ARG	Q402	R338	V277		
	LYS	V403	K339	E278		L132
	ASN	L404	I340	Y279		S133
	ALA	D405		E280		T134
	LYS	E406	T343	R281		P135
		G407	I344	R282		T136
			E345	E283		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.09 Å 97.96 Å 113.73 Å 79.03° 85.54° 89.69°	Depositor
Resolution (Å)	29.35 – 2.60 29.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (29.35-2.60) 84.7 (29.35-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.300 0.211 , 0.224	Depositor DCC
$R_{free}$ test set	2888 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 102.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: PO4, IPA

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	0.49	0/3583	0.69	0/4827
1	B	0.48	0/3484	0.68	1/4688 (0.0%)
1	C	0.44	0/3383	0.67	0/4562
1	D	0.43	0/3466	0.65	0/4673
All	All	0.46	0/13916	0.67	1/18750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	GLY	N-CA-C	5.20	126.10	113.10

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	3513	0	3546	303	0
1	B	3419	0	3446	243	0
1	C	3317	0	3324	302	0
1	D	3402	0	3401	310	0
2	A	5	0	0	0	0
2	B	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	12	0	24	6	0
4	A	286	0	0	14	1
4	B	299	0	0	10	3
4	C	261	0	0	12	0
4	D	220	0	0	12	1
All	All	14769	0	13741	1153	4

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 42.

All (1153) 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:D:438:PRO:HB3	1:D:444:GLU:HA	1.31	1.08
1:A:333:SER:HB3	1:A:336:LYS:HG3	1.36	1.07
1:C:24:ILE:H	1:C:24:ILE:HD12	1.20	1.03
1:D:356:THR:HG23	1:D:362:VAL:HG22	1.38	1.01
1:D:95:ARG:HB3	1:D:259:LEU:HD11	1.39	1.01
1:A:377:ARG:HG3	1:A:378:THR:H	1.23	1.01
1:A:438:PRO:HB2	1:A:443:LYS:HA	1.42	1.00
1:A:398:ILE:HD13	1:A:399:VAL:N	1.76	0.98
1:A:285:VAL:HG23	1:A:286:TYR:H	1.29	0.98
1:A:386:ILE:H	1:A:386:ILE:HD12	1.29	0.97
1:A:391:ARG:HB2	1:A:411:PRO:HG3	1.44	0.97
1:C:375:THR:HG22	1:C:378:THR:HG23	1.46	0.97
1:D:306:ILE:HG23	1:D:307:VAL:H	1.31	0.96
1:A:100:LYS:HZ2	1:A:104:ARG:HH21	1.11	0.96
1:D:132:LEU:HD23	1:D:458:VAL:HG21	1.47	0.95
1:C:408:ILE:HG23	1:C:409:ASP:H	1.32	0.94
1:C:148:GLN:HE21	1:C:152:ARG:HH12	1.15	0.94
1:D:132:LEU:HA	1:D:458:VAL:HG21	1.49	0.93
1:D:407:GLY:O	1:D:410:VAL:HG13	1.68	0.93
1:D:408:ILE:HG22	1:D:409:ASP:H	1.31	0.92
1:A:100:LYS:NZ	1:A:104:ARG:HH21	1.68	0.92
1:C:334:LYS:O	1:C:338:ARG:HD3	1.69	0.91
1:B:290:LEU:HB3	1:B:296:THR:HA	1.52	0.90
1:A:134:THR:HG22	4:A:2827:HOH:O	1.71	0.89
1:A:285:VAL:HG21	1:A:322:ALA:CB	2.02	0.89
1:C:325:GLU:HG3	1:C:329:ILE:HD13	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLY:HA2	1:C:392:THR:HG22	1.52	0.89
1:D:162:GLY:HA3	1:D:172:LYS:HD3	1.55	0.89
1:C:282:ARG:O	1:C:286:TYR:HB2	1.73	0.88
1:C:42:VAL:HG12	1:C:44:HIS:H	1.38	0.88
1:A:398:ILE:HD13	1:A:399:VAL:H	1.36	0.88
1:D:418:ILE:HD11	1:D:447:LEU:HD11	1.57	0.87
1:B:288:GLN:O	1:B:292:ALA:HB2	1.75	0.86
1:D:370:LEU:HD13	1:D:370:LEU:H	1.40	0.86
1:C:30:GLU:O	1:C:33:THR:HG22	1.76	0.86
1:A:405:ASP:HB2	1:A:435:ILE:HD11	1.56	0.86
1:B:352:ILE:HG22	1:B:415:VAL:HB	1.56	0.86
1:A:103:GLU:HG3	1:A:426:ARG:NH1	1.90	0.85
1:D:329:ILE:HD12	1:D:330:ALA:N	1.92	0.85
1:A:377:ARG:HG3	1:A:378:THR:N	1.90	0.84
1:D:380:ARG:O	1:D:384:GLU:HG2	1.75	0.84
1:D:405:ASP:HB3	1:D:435:ILE:HD11	1.59	0.84
1:A:66:GLU:HA	1:A:297:LEU:HD12	1.61	0.82
1:C:361:LEU:HD11	1:C:419:MET:HG3	1.61	0.82
1:D:329:ILE:HD12	1:D:330:ALA:H	1.41	0.82
1:C:27:ILE:HG13	1:C:27:ILE:O	1.79	0.82
1:C:26:GLU:HG3	1:C:78:ASN:HD22	1.44	0.81
1:C:403:VAL:HG21	1:C:431:ARG:NH2	1.94	0.81
1:D:102:LEU:O	1:D:106:LEU:HD13	1.81	0.81
1:C:383:ARG:HH22	1:C:402:GLN:NE2	1.79	0.81
1:A:89:ASP:HB3	4:A:2548:HOH:O	1.78	0.81
1:C:205:PRO:HB2	1:C:230:ARG:HH11	1.46	0.81
1:C:354:ILE:HG12	1:C:399:VAL:HG23	1.62	0.81
1:A:103:GLU:HG3	1:A:426:ARG:HH11	1.44	0.80
1:C:115:LEU:HD23	1:C:249:LEU:HB3	1.60	0.80
1:C:259:LEU:HD11	1:C:262:TYR:CE2	2.16	0.80
1:C:62:ARG:O	1:C:66:GLU:HG3	1.82	0.79
1:B:115:LEU:O	1:B:121:LYS:HE3	1.83	0.79
1:A:259:LEU:HD13	1:A:260:ALA:N	1.98	0.79
1:B:377:ARG:HD2	1:B:377:ARG:O	1.83	0.79
1:D:132:LEU:HA	1:D:458:VAL:CG2	2.11	0.79
1:A:358:HIS:O	1:A:362:VAL:HG23	1.83	0.79
1:A:207:GLU:HG2	3:A:6002:IPA:H12	1.62	0.79
1:D:352:ILE:HD12	1:D:353:ILE:N	1.98	0.79
1:A:295:ILE:HB	1:A:299:ARG:H	1.48	0.78
1:B:333:SER:HB3	1:B:336:LYS:HG2	1.64	0.78
1:B:389:GLY:O	1:B:394:ARG:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:THR:CG2	1:D:362:VAL:HG22	2.12	0.78
1:D:100:LYS:HD3	1:D:426:ARG:HH22	1.49	0.78
1:C:272:ALA:HB3	1:C:275:GLU:HG3	1.67	0.77
1:B:121:LYS:HG3	2:B:4002:PO4:O4	1.85	0.77
1:D:232:ASP:OD1	1:D:234:ARG:HG3	1.84	0.77
1:C:420:SER:HB3	1:C:450:LEU:O	1.84	0.77
1:D:379:SER:HB3	1:D:382:GLU:HB2	1.67	0.76
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.67	0.76
1:D:321:ARG:O	1:D:325:GLU:HB2	1.84	0.76
1:C:257:LYS:NZ	1:C:260:ALA:HB3	2.00	0.76
1:D:205:PRO:HA	1:D:237:ILE:HD11	1.68	0.76
1:A:285:VAL:HG21	1:A:322:ALA:HB3	1.64	0.76
1:A:122:THR:HG21	1:A:152:ARG:CD	2.15	0.76
1:B:99:GLU:O	1:B:103:GLU:HG2	1.86	0.75
1:C:205:PRO:HA	1:C:237:ILE:HD11	1.67	0.75
1:C:95:ARG:HB2	1:C:98:GLN:HG3	1.69	0.75
1:C:115:LEU:HD21	1:C:247:PHE:HE1	1.50	0.75
1:D:325:GLU:O	1:D:329:ILE:HG13	1.85	0.75
1:D:388:GLU:HA	1:D:391:ARG:CG	2.17	0.75
1:B:27:ILE:HG22	1:B:36:VAL:HG22	1.68	0.75
1:D:269:VAL:HG21	1:D:336:LYS:HG2	1.68	0.75
1:C:28:TYR:HA	1:C:79:ALA:HB2	1.68	0.75
1:C:412:ASP:HB2	1:C:437:ARG:HD2	1.68	0.74
1:B:351:LYS:HD2	1:B:351:LYS:H	1.52	0.74
1:B:325:GLU:O	1:B:329:ILE:HG13	1.87	0.74
1:C:57:LEU:HD22	1:C:57:LEU:H	1.52	0.74
1:D:45:ALA:HB1	1:D:54:TYR:HB3	1.70	0.74
1:D:201:VAL:HG12	1:D:225:THR:HB	1.70	0.74
1:D:361:LEU:O	1:D:365:ILE:HG13	1.87	0.74
1:D:440:LYS:HE3	1:D:440:LYS:HA	1.67	0.74
1:D:290:LEU:HD22	1:D:290:LEU:H	1.53	0.73
1:D:70:SER:HA	1:D:292:ALA:HB2	1.68	0.73
1:C:267:ILE:HG21	1:C:339:LYS:HE2	1.70	0.73
1:B:303:PHE:O	1:B:307:VAL:HG23	1.89	0.73
1:C:392:THR:HG23	1:C:393:GLY:N	2.03	0.73
1:C:374:ILE:HA	1:C:378:THR:HG21	1.71	0.72
1:D:305:LYS:NZ	1:D:305:LYS:HB3	2.04	0.72
1:A:386:ILE:H	1:A:386:ILE:CD1	2.02	0.72
1:D:424:SER:OG	1:D:429:ILE:HD11	1.88	0.72
1:C:148:GLN:HG2	1:C:152:ARG:NH1	2.04	0.72
1:D:165:SER:HB2	4:D:2598:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:MET:HB2	1:B:38:GLY:HA2	1.71	0.72
1:B:24:ILE:HG22	1:B:24:ILE:O	1.89	0.72
1:C:71:ASN:O	1:C:73:ILE:HG13	1.89	0.72
1:A:66:GLU:HG3	1:A:297:LEU:HD13	1.71	0.72
1:A:285:VAL:HG23	1:A:286:TYR:N	2.04	0.71
1:C:383:ARG:HH22	1:C:402:GLN:HE21	1.38	0.71
1:D:34:ILE:HG12	1:D:58:ALA:HA	1.72	0.71
1:B:366:SER:HB2	1:B:373:ALA:HB2	1.72	0.71
1:C:185:ASN:O	1:C:189:LEU:HG	1.90	0.71
1:A:241:VAL:HG23	1:A:242:VAL:HG23	1.73	0.71
1:A:295:ILE:HD13	1:A:300:ALA:HB3	1.73	0.71
1:A:333:SER:HB3	1:A:336:LYS:CG	2.19	0.71
1:C:263:THR:CG2	1:C:446:VAL:HG22	2.19	0.71
1:A:295:ILE:HG13	1:A:295:ILE:O	1.90	0.71
1:C:389:GLY:CA	1:C:392:THR:HG22	2.20	0.71
1:D:388:GLU:HA	1:D:391:ARG:HG2	1.73	0.71
1:B:405:ASP:HB3	1:B:435:ILE:HD11	1.71	0.70
1:D:323:TRP:HA	1:D:326:ALA:HB3	1.72	0.70
1:D:60:ARG:HA	4:D:2516:HOH:O	1.91	0.70
1:B:375:THR:HG23	1:B:377:ARG:H	1.57	0.70
1:B:404:LEU:N	1:B:404:LEU:HD22	2.07	0.70
1:C:126:MET:CE	1:C:152:ARG:HB3	2.21	0.70
1:A:304:ASN:HA	1:A:307:VAL:HG22	1.73	0.70
1:C:230:ARG:HG3	1:C:235:HIS:HB3	1.74	0.70
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.56	0.70
1:B:143:LEU:O	1:B:147:GLU:HG3	1.92	0.70
1:B:320:LEU:O	1:B:324:GLU:HG3	1.92	0.70
1:B:37:LYS:HG2	1:B:53:THR:HG22	1.74	0.70
1:D:172:LYS:HB3	1:D:173:PRO:HD2	1.73	0.70
1:A:314:GLU:HG2	1:A:316:ALA:H	1.55	0.70
1:B:332:ASN:CG	1:B:333:SER:H	1.93	0.70
1:B:273:GLU:O	1:B:277:VAL:HG23	1.92	0.69
1:D:149:TRP:HE3	1:D:153:LEU:HD11	1.56	0.69
1:A:282:ARG:HH21	1:A:322:ALA:HA	1.57	0.69
1:B:286:TYR:HA	1:B:289:PHE:HB2	1.74	0.69
1:A:45:ALA:C	1:A:46:LYS:HD2	2.13	0.69
1:D:425:ALA:O	1:D:429:ILE:HG13	1.92	0.69
1:A:69:GLU:HG2	1:A:297:LEU:HG	1.75	0.69
1:D:305:LYS:HZ2	1:D:305:LYS:HB3	1.56	0.69
1:D:333:SER:O	1:D:337:ILE:HG12	1.92	0.69
1:C:109:LYS:HD3	1:C:132:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ILE:HD12	1:D:447:LEU:HD21	1.73	0.68
1:D:43:PRO:O	1:D:44:HIS:HB2	1.92	0.68
1:D:95:ARG:HB3	1:D:259:LEU:CD1	2.21	0.68
1:A:259:LEU:O	1:A:261:LYS:HG3	1.93	0.68
1:B:340:LEU:HD21	1:B:354:ILE:HD13	1.73	0.68
1:C:336:LYS:HE3	1:C:452:SER:HB3	1.74	0.68
1:D:283:GLU:HB3	1:D:286:TYR:CZ	2.28	0.68
1:B:358:HIS:CE1	1:B:360:GLU:HB3	2.29	0.68
1:B:332:ASN:CG	1:B:333:SER:N	2.46	0.68
1:C:332:ASN:HD22	1:C:364:ARG:HD2	1.59	0.68
1:C:439:SER:HB2	1:C:442:LYS:HD2	1.76	0.68
1:D:432:LEU:O	1:D:432:LEU:HD23	1.94	0.68
1:A:274:ASP:O	1:A:277:VAL:HG12	1.93	0.68
1:B:102:LEU:HG	1:B:106:LEU:HD22	1.75	0.68
1:B:34:ILE:HG12	1:B:58:ALA:HA	1.76	0.68
1:C:443:LYS:HG3	1:C:444:GLU:H	1.58	0.68
1:D:91:GLU:HB3	1:D:265:LYS:HD3	1.76	0.68
1:A:296:THR:O	1:A:297:LEU:HB2	1.92	0.68
1:B:321:ARG:HA	1:B:324:GLU:OE1	1.94	0.68
1:D:404:LEU:N	1:D:404:LEU:HD22	2.08	0.68
1:C:394:ARG:HE	1:C:394:ARG:HA	1.60	0.67
1:B:384:GLU:O	1:B:388:GLU:HG2	1.94	0.67
1:C:341:ARG:O	1:C:345:GLU:HG3	1.94	0.67
1:C:26:GLU:HG3	1:C:78:ASN:ND2	2.09	0.67
1:D:273:GLU:O	1:D:274:ASP:HB3	1.95	0.67
1:D:369:PHE:CE1	1:D:370:LEU:HD22	2.30	0.67
1:A:234:ARG:HH22	3:A:6002:IPA:H2	1.59	0.67
1:B:62:ARG:HB2	4:B:2009:HOH:O	1.95	0.67
1:D:362:VAL:HG13	1:D:399:VAL:HG22	1.77	0.67
1:A:110:ARG:HD2	1:A:221:ARG:HG3	1.78	0.66
1:A:402:GLN:O	1:A:404:LEU:HD22	1.96	0.66
1:C:418:ILE:HG12	1:C:425:ALA:HB2	1.75	0.66
1:C:339:LYS:O	1:C:343:ILE:HG13	1.95	0.66
1:D:260:ALA:HB2	4:D:2799:HOH:O	1.94	0.66
1:C:333:SER:HB3	1:C:336:LYS:HG2	1.77	0.66
1:B:37:LYS:HG2	1:B:53:THR:CG2	2.26	0.66
1:C:68:PHE:O	1:C:70:SER:N	2.28	0.66
1:A:100:LYS:NZ	1:A:104:ARG:NH2	2.43	0.66
1:A:359:ASN:HA	1:A:362:VAL:HB	1.78	0.66
1:B:364:ARG:O	1:B:368:VAL:HG23	1.96	0.66
1:B:50:ARG:HG2	1:B:50:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:PRO:HB2	1:D:398:ILE:HG22	1.77	0.66
1:D:365:ILE:HD12	1:D:399:VAL:HG21	1.77	0.66
1:C:263:THR:HG22	1:C:445:ALA:O	1.95	0.66
1:D:368:VAL:HG12	1:D:368:VAL:O	1.95	0.66
1:B:122:THR:HG21	1:B:152:ARG:HD3	1.77	0.65
1:A:444:GLU:HB3	4:A:2628:HOH:O	1.96	0.65
1:C:375:THR:HG23	1:C:377:ARG:H	1.61	0.65
1:C:24:ILE:H	1:C:24:ILE:CD1	1.98	0.65
1:A:305:LYS:HG2	1:A:323:TRP:CD2	2.32	0.65
1:B:273:GLU:O	1:B:276:ARG:HG2	1.97	0.65
1:B:279:TYR:CE1	1:B:330:ALA:HB2	2.32	0.65
1:D:134:THR:HB	1:D:194:MET:HB2	1.79	0.65
1:D:158:GLU:HB3	4:D:2667:HOH:O	1.97	0.65
1:C:356:THR:HB	1:C:419:MET:HG2	1.79	0.65
1:A:413:ALA:CB	1:A:436:LEU:HD23	2.27	0.65
1:A:442:LYS:HA	1:A:442:LYS:NZ	2.12	0.65
1:B:372:PRO:HG2	1:B:395:PHE:CG	2.31	0.65
1:C:134:THR:HG21	4:C:2617:HOH:O	1.96	0.64
1:D:340:LEU:HA	1:D:343:ILE:CD1	2.27	0.64
1:D:80:ALA:C	1:D:82:PRO:HD3	2.17	0.64
1:D:213:ALA:O	1:D:221:ARG:NH2	2.29	0.64
1:A:46:LYS:HA	1:A:46:LYS:HE3	1.79	0.64
1:A:66:GLU:HA	1:A:297:LEU:CD1	2.27	0.64
1:D:418:ILE:CD1	1:D:429:ILE:HA	2.27	0.64
1:B:387:LEU:HD23	1:B:387:LEU:O	1.97	0.64
1:C:126:MET:HE3	1:C:152:ARG:HB3	1.79	0.64
1:D:350:ASP:HB3	1:D:414:ASN:HB3	1.78	0.64
1:B:434:ARG:NH2	1:B:434:ARG:HB2	2.12	0.64
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.64
1:B:165:SER:O	1:B:169:LYS:HD2	1.98	0.64
1:D:149:TRP:O	1:D:153:LEU:HD13	1.98	0.64
1:D:33:THR:HG23	1:D:56:ALA:O	1.98	0.64
1:A:334:LYS:O	1:A:338:ARG:HG2	1.98	0.64
1:A:93:SER:HA	1:A:265:LYS:HG2	1.80	0.64
1:A:438:PRO:HB2	1:A:443:LYS:CA	2.25	0.63
1:D:340:LEU:O	1:D:343:ILE:HG12	1.97	0.63
1:A:357:ARG:HD3	1:A:428:TYR:OH	1.97	0.63
1:C:148:GLN:HG2	1:C:152:ARG:CZ	2.27	0.63
1:C:69:GLU:HG3	1:C:75:PHE:CZ	2.33	0.63
1:A:425:ALA:O	1:A:429:ILE:HG12	1.97	0.63
1:B:351:LYS:HB2	1:B:390:PHE:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:LEU:HG	1:D:343:ILE:HD11	1.79	0.63
1:D:45:ALA:CB	1:D:54:TYR:HB3	2.27	0.63
1:D:37:LYS:HA	1:D:53:THR:HG22	1.81	0.63
1:D:336:LYS:O	1:D:340:LEU:HB2	1.98	0.63
1:D:36:VAL:HG11	1:D:42:VAL:HG21	1.81	0.63
1:A:386:ILE:HD12	1:A:386:ILE:N	2.08	0.63
1:A:69:GLU:OE1	1:A:297:LEU:HD11	1.99	0.63
1:C:334:LYS:HG2	1:C:338:ARG:HE	1.62	0.63
1:D:369:PHE:CD1	1:D:371:ILE:HB	2.34	0.63
1:A:65:ILE:HG22	1:A:297:LEU:HD11	1.81	0.62
1:C:389:GLY:HA2	1:C:392:THR:CG2	2.28	0.62
1:B:234:ARG:O	1:B:237:ILE:HG23	1.99	0.62
1:A:285:VAL:HG21	1:A:322:ALA:HB1	1.81	0.62
1:C:148:GLN:NE2	1:C:152:ARG:HH12	1.94	0.62
1:C:257:LYS:HZ2	1:C:260:ALA:HB3	1.64	0.62
1:B:289:PHE:O	1:B:292:ALA:HB3	1.99	0.62
1:C:143:LEU:HD13	1:C:167:ARG:HD2	1.82	0.62
1:D:408:ILE:HG22	1:D:409:ASP:N	2.08	0.62
1:C:161:VAL:O	1:C:172:LYS:HG2	2.00	0.62
1:D:394:ARG:N	1:D:394:ARG:HD3	2.15	0.62
1:B:122:THR:HG21	1:B:152:ARG:CD	2.30	0.62
1:B:149:TRP:O	1:B:153:LEU:HD22	1.99	0.61
1:B:374:ILE:O	1:B:374:ILE:HG22	1.99	0.61
1:B:433:GLY:HA2	1:B:436:LEU:HD12	1.81	0.61
1:A:357:ARG:HD3	1:A:428:TYR:CZ	2.35	0.61
1:B:352:ILE:CG2	1:B:415:VAL:HB	2.29	0.61
1:C:408:ILE:HG23	1:C:409:ASP:N	2.10	0.61
1:D:289:PHE:C	1:D:291:ARG:H	2.04	0.61
1:C:254:LEU:O	1:C:255:ALA:HB2	2.00	0.61
1:C:148:GLN:O	1:C:152:ARG:HG3	2.00	0.61
1:C:378:THR:O	1:C:379:SER:O	2.19	0.61
1:A:408:ILE:O	1:A:408:ILE:HG22	2.01	0.61
1:A:413:ALA:HB3	1:A:436:LEU:HD23	1.82	0.61
1:A:382:GLU:O	1:A:383:ARG:HG2	2.01	0.61
1:C:100:LYS:HE2	1:C:104:ARG:HE	1.65	0.61
1:B:301:GLU:O	1:B:303:PHE:N	2.29	0.61
1:D:96:ASP:OD2	1:D:259:LEU:HD13	2.01	0.61
1:A:351:LYS:HD3	1:A:412:ASP:O	1.99	0.60
1:B:126:MET:HE3	1:B:152:ARG:HG2	1.83	0.60
1:A:109:LYS:HD3	1:A:132:LEU:HD21	1.82	0.60
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLU:HA	1:C:229:GLU:OE2	2.02	0.60
1:A:307:VAL:HG23	1:A:308:MET:H	1.66	0.60
1:C:205:PRO:HB2	1:C:230:ARG:NH1	2.15	0.60
1:D:191:ASN:OD1	1:D:192:ARG:HD2	2.02	0.60
1:D:269:VAL:HG21	1:D:336:LYS:CG	2.30	0.60
1:A:125:ALA:O	1:A:129:ILE:HG13	2.01	0.60
1:A:377:ARG:NH1	1:A:378:THR:HA	2.16	0.60
1:B:333:SER:HB3	1:B:336:LYS:CG	2.29	0.60
1:A:393:GLY:C	1:A:395:PHE:H	2.03	0.60
1:C:418:ILE:HG12	1:C:425:ALA:CB	2.32	0.60
1:D:305:LYS:N	1:D:305:LYS:HZ3	1.97	0.60
1:A:387:LEU:O	1:A:411:PRO:HG2	2.02	0.60
1:D:210:VAL:HG21	1:D:237:ILE:HD12	1.82	0.60
1:D:37:LYS:HA	1:D:53:THR:CG2	2.32	0.60
1:A:191:ASN:HD22	1:A:191:ASN:H	1.50	0.60
1:B:110:ARG:HH12	1:B:219:PRO:HA	1.67	0.60
1:D:160:TYR:O	1:D:172:LYS:HB3	2.01	0.59
1:D:368:VAL:O	1:D:369:PHE:HB2	2.01	0.59
1:A:391:ARG:HB2	1:A:411:PRO:CG	2.26	0.59
1:B:415:VAL:HG12	1:B:416:GLY:N	2.17	0.59
1:C:116:PRO:HG2	1:C:251:PRO:HA	1.84	0.59
1:C:379:SER:OG	1:C:382:GLU:HG3	2.02	0.59
1:B:23:MET:C	1:B:25:ALA:H	2.06	0.59
1:B:283:GLU:C	1:B:285:VAL:H	2.05	0.59
1:A:295:ILE:HB	1:A:299:ARG:N	2.16	0.59
1:C:322:ALA:HA	1:C:324:GLU:HG2	1.82	0.59
1:B:450:LEU:N	1:B:450:LEU:HD22	2.17	0.59
1:D:109:LYS:HD3	1:D:132:LEU:HD21	1.85	0.59
1:D:366:SER:O	1:D:369:PHE:O	2.20	0.59
1:C:69:GLU:HG3	1:C:75:PHE:HZ	1.67	0.59
1:D:418:ILE:HD11	1:D:429:ILE:HA	1.85	0.59
1:A:269:VAL:HG21	1:A:336:LYS:HG2	1.84	0.59
1:C:393:GLY:O	1:C:394:ARG:O	2.21	0.59
1:D:325:GLU:C	1:D:327:ARG:H	2.05	0.59
1:A:372:PRO:HG3	1:A:395:PHE:HE2	1.68	0.59
1:B:442:LYS:HE3	4:B:3002:HOH:O	2.01	0.59
1:C:87:TYR:HE2	4:C:2561:HOH:O	1.85	0.59
1:B:115:LEU:HB3	1:B:119:SER:OG	2.02	0.58
1:C:231:GLU:HB2	4:C:2883:HOH:O	2.02	0.58
1:C:110:ARG:HG3	1:C:242:VAL:O	2.03	0.58
1:A:122:THR:HG22	1:A:126:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ILE:CG2	1:C:339:LYS:HE2	2.33	0.58
1:C:340:LEU:HD11	1:C:354:ILE:HD13	1.85	0.58
1:A:432:LEU:O	1:A:432:LEU:HD13	2.03	0.58
1:A:361:LEU:O	1:A:361:LEU:HD23	2.04	0.58
1:B:290:LEU:HB3	1:B:296:THR:CA	2.27	0.58
1:C:194:MET:HA	1:C:219:PRO:HD2	1.85	0.58
1:D:84:PRO:HG2	4:D:2119:HOH:O	2.03	0.58
1:C:134:THR:HB	1:C:194:MET:HB2	1.85	0.58
1:C:323:TRP:CE2	1:C:327:ARG:HB2	2.38	0.58
1:D:149:TRP:CE3	1:D:153:LEU:HD11	2.38	0.58
1:D:346:ARG:HG3	1:D:347:HIS:CD2	2.38	0.58
1:C:160:TYR:O	1:C:172:LYS:HB3	2.03	0.58
1:A:143:LEU:O	1:A:147:GLU:HG3	2.03	0.58
1:B:273:GLU:HA	1:B:276:ARG:HG2	1.85	0.58
1:D:305:LYS:HD2	1:D:305:LYS:N	2.18	0.58
1:A:295:ILE:CB	1:A:299:ARG:HB3	2.34	0.58
1:A:404:LEU:HB3	1:A:410:VAL:HG11	1.86	0.58
1:B:103:GLU:HG3	1:B:426:ARG:NH1	2.19	0.58
1:C:375:THR:HG23	1:C:377:ARG:N	2.17	0.58
1:D:77:ASP:OD2	1:D:80:ALA:HB3	2.03	0.58
1:A:278:GLU:O	1:A:282:ARG:HG2	2.03	0.58
1:B:122:THR:CG2	1:B:152:ARG:HD3	2.34	0.58
1:A:230:ARG:NH2	3:A:6001:IPA:H2	2.18	0.58
1:C:211:GLN:HG2	1:C:215:MET:SD	2.44	0.58
1:C:432:LEU:O	1:C:436:LEU:HG	2.04	0.58
1:A:375:THR:OG1	1:A:376:HIS:N	2.35	0.57
1:D:239:LYS:O	1:D:243:GLY:HA2	2.04	0.57
1:D:404:LEU:H	1:D:404:LEU:HD22	1.69	0.57
1:B:372:PRO:HB2	1:B:398:ILE:HG22	1.86	0.57
1:C:68:PHE:HB3	1:C:75:PHE:CD2	2.39	0.57
1:A:115:LEU:HD12	1:A:121:LYS:HG2	1.87	0.57
1:A:31:ARG:HB2	1:A:31:ARG:HH11	1.68	0.57
1:B:62:ARG:O	1:B:66:GLU:HG3	2.04	0.57
1:D:132:LEU:CD2	1:D:458:VAL:HG11	2.35	0.57
1:A:259:LEU:HD21	1:A:262:TYR:HD2	1.69	0.57
1:D:238:LEU:O	1:D:243:GLY:N	2.37	0.57
1:A:318:GLU:HA	1:A:318:GLU:OE1	2.04	0.57
1:A:374:ILE:HD11	1:A:386:ILE:HG21	1.85	0.57
1:D:306:ILE:HG23	1:D:307:VAL:N	2.12	0.57
1:D:376:HIS:CD2	1:D:377:ARG:HG2	2.40	0.57
1:D:45:ALA:HB3	1:D:54:TYR:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:HIS:O	1:B:230:ARG:HD2	2.05	0.57
1:A:114:VAL:HA	1:A:225:THR:O	2.05	0.57
1:A:301:GLU:O	1:A:302:ASP:HB2	2.05	0.57
1:B:340:LEU:HD21	1:B:354:ILE:CD1	2.35	0.57
1:C:126:MET:HE1	1:C:152:ARG:HB3	1.87	0.57
1:A:393:GLY:C	1:A:395:PHE:N	2.59	0.57
1:B:414:ASN:O	1:B:445:ALA:HB1	2.05	0.57
1:C:352:ILE:O	1:C:397:ALA:HA	2.04	0.57
1:A:295:ILE:HG22	1:A:299:ARG:HB3	1.87	0.56
1:B:362:VAL:HG23	1:B:363:TYR:H	1.69	0.56
1:C:263:THR:HG21	1:C:446:VAL:HG22	1.86	0.56
1:D:278:GLU:O	1:D:282:ARG:HG2	2.05	0.56
1:B:103:GLU:HG3	1:B:426:ARG:CZ	2.34	0.56
1:C:49:SER:HB3	1:C:53:THR:OG1	2.05	0.56
1:B:432:LEU:HD12	1:B:436:LEU:HG	1.87	0.56
1:C:333:SER:HB3	1:C:336:LYS:CG	2.34	0.56
1:C:418:ILE:HD12	1:C:419:MET:N	2.21	0.56
1:B:354:ILE:HG22	1:B:355:PHE:N	2.19	0.56
1:C:24:ILE:N	1:C:24:ILE:HD12	2.05	0.56
1:C:93:SER:HA	1:C:265:LYS:HG2	1.86	0.56
1:D:369:PHE:HD1	1:D:371:ILE:HB	1.71	0.56
1:B:450:LEU:H	1:B:450:LEU:HD22	1.71	0.56
1:D:172:LYS:HE2	4:D:2211:HOH:O	2.04	0.56
1:A:285:VAL:O	1:A:290:LEU:HD23	2.04	0.56
1:A:393:GLY:O	1:A:395:PHE:N	2.39	0.56
1:B:23:MET:HB2	1:B:38:GLY:CA	2.35	0.56
1:A:283:GLU:O	1:A:287:LYS:HG2	2.05	0.56
1:B:268:PHE:HA	1:B:451:ILE:O	2.05	0.56
1:B:322:ALA:C	1:B:324:GLU:H	2.09	0.56
1:B:400:SER:HB3	1:B:404:LEU:HD21	1.87	0.56
1:C:361:LEU:O	1:C:361:LEU:HD22	2.05	0.56
1:C:425:ALA:O	1:C:427:GLU:N	2.37	0.56
1:D:234:ARG:NH1	1:D:234:ARG:HG2	2.21	0.56
1:D:24:ILE:HG22	1:D:24:ILE:O	2.06	0.56
1:D:256:GLY:C	1:D:258:HIS:H	2.09	0.56
1:A:113:ILE:HG22	1:A:113:ILE:O	2.06	0.56
1:A:205:PRO:HB2	1:A:230:ARG:NH1	2.21	0.56
1:A:320:LEU:HD23	1:A:320:LEU:C	2.26	0.56
1:A:330:ALA:O	1:A:331:PHE:C	2.44	0.56
1:C:103:GLU:HB3	1:C:426:ARG:NH2	2.21	0.56
1:C:250:PHE:HD1	1:C:251:PRO:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:HIS:HD2	1:C:361:LEU:H	1.52	0.56
1:D:95:ARG:HB2	1:D:98:GLN:HG3	1.88	0.56
1:C:42:VAL:HB	1:C:45:ALA:HB2	1.88	0.55
1:D:379:SER:HB3	1:D:382:GLU:CB	2.35	0.55
1:D:93:SER:HA	1:D:264:ILE:O	2.06	0.55
1:C:148:GLN:NE2	1:C:152:ARG:HH22	2.04	0.55
1:C:257:LYS:HZ3	1:C:260:ALA:HB3	1.69	0.55
1:A:282:ARG:HG3	1:A:329:ILE:HD11	1.86	0.55
1:D:180:ASP:O	1:D:184:VAL:HG23	2.06	0.55
1:D:306:ILE:HG13	1:D:307:VAL:N	2.20	0.55
1:A:391:ARG:NH1	1:A:391:ARG:HG3	2.21	0.55
1:B:290:LEU:CB	1:B:296:THR:HA	2.33	0.55
1:B:374:ILE:HG12	1:B:386:ILE:HD12	1.88	0.55
1:C:263:THR:HG22	1:C:446:VAL:HA	1.87	0.55
1:C:332:ASN:O	1:C:333:SER:C	2.44	0.55
1:C:261:LYS:O	1:C:444:GLU:HB3	2.06	0.55
1:A:442:LYS:HZ3	1:A:442:LYS:HA	1.70	0.55
1:B:126:MET:CE	1:B:152:ARG:HG2	2.36	0.55
1:C:136:THR:HB	1:C:174:LEU:HD23	1.88	0.55
1:C:406:GLU:HG2	1:C:406:GLU:O	2.06	0.55
1:D:372:PRO:HD3	1:D:395:PHE:CE1	2.41	0.55
1:A:334:LYS:O	1:A:338:ARG:CG	2.54	0.55
1:C:361:LEU:O	1:C:365:ILE:HG13	2.07	0.55
1:B:291:ARG:N	1:B:296:THR:HG22	2.22	0.55
1:A:350:ASP:HB3	1:A:414:ASN:HB3	1.89	0.55
1:C:395:PHE:CD1	1:C:395:PHE:O	2.60	0.55
1:C:36:VAL:O	1:C:54:TYR:HB2	2.07	0.55
1:C:85:THR:HG23	1:C:86:PRO:HD2	1.88	0.55
1:B:120:GLY:HA2	4:B:2256:HOH:O	2.07	0.55
1:B:69:GLU:HG2	1:B:291:ARG:HH11	1.71	0.55
1:D:360:GLU:O	1:D:363:TYR:HB3	2.06	0.55
1:B:382:GLU:O	1:B:386:ILE:HG13	2.07	0.54
1:B:264:ILE:N	1:B:264:ILE:HD12	2.22	0.54
1:B:88:PHE:HB3	1:B:156:PHE:CD1	2.43	0.54
1:C:50:ARG:O	1:C:51:SER:HB2	2.06	0.54
1:C:96:ASP:OD2	1:C:96:ASP:N	2.40	0.54
1:D:62:ARG:NH1	1:D:219:PRO:O	2.37	0.54
1:D:373:ALA:O	1:D:374:ILE:HG13	2.07	0.54
1:C:228:PHE:CD1	1:C:245:LYS:HE2	2.43	0.54
1:D:378:THR:HG22	1:D:379:SER:N	2.22	0.54
1:A:321:ARG:O	1:A:321:ARG:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:HH22	3:A:6001:IPA:H2	1.72	0.54
1:D:336:LYS:HZ1	1:D:420:SER:CB	2.21	0.54
1:A:122:THR:HG21	1:A:152:ARG:HD3	1.89	0.54
1:A:314:GLU:HG2	1:A:315:ARG:N	2.23	0.54
1:A:338:ARG:O	1:A:341:ARG:HB3	2.07	0.54
1:A:356:THR:HG23	1:A:362:VAL:HG22	1.89	0.54
1:B:351:LYS:HB2	1:B:390:PHE:CE1	2.43	0.54
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.73	0.54
1:C:63:ASP:HA	1:C:66:GLU:OE2	2.08	0.54
1:D:227:THR:HG23	4:D:2756:HOH:O	2.08	0.54
1:A:295:ILE:HB	1:A:299:ARG:HB3	1.90	0.54
1:B:110:ARG:NH1	1:B:219:PRO:HA	2.22	0.54
1:C:451:ILE:HG22	1:C:452:SER:N	2.22	0.54
1:C:272:ALA:HB3	1:C:275:GLU:CG	2.35	0.54
1:D:328:ARG:HG3	1:D:328:ARG:HH11	1.73	0.54
1:A:74:GLU:HA	1:A:74:GLU:OE2	2.08	0.54
1:B:122:THR:HG21	1:B:152:ARG:CZ	2.38	0.54
1:B:31:ARG:CG	1:B:187:GLU:HB3	2.38	0.54
1:B:334:LYS:O	1:B:338:ARG:HG3	2.08	0.54
1:B:344:LEU:CD2	1:B:352:ILE:HD11	2.38	0.54
1:B:62:ARG:N	4:B:2009:HOH:O	2.21	0.54
1:D:261:LYS:HE3	1:D:438:PRO:HG3	1.89	0.54
1:D:418:ILE:HG12	1:D:432:LEU:HD13	1.89	0.54
1:A:24:ILE:HG22	1:A:25:ALA:N	2.22	0.54
1:A:283:GLU:C	1:A:285:VAL:N	2.61	0.54
1:A:99:GLU:HG3	1:A:426:ARG:NH2	2.23	0.54
1:D:409:ASP:O	1:D:410:VAL:O	2.25	0.54
1:A:44:HIS:CG	1:A:60:ARG:HD2	2.43	0.53
1:B:441:GLY:O	1:B:442:LYS:C	2.45	0.53
1:A:180:ASP:OD2	4:A:2475:HOH:O	2.19	0.53
1:C:381:GLU:HG3	1:C:382:GLU:H	1.73	0.53
1:D:105:TRP:CD1	1:D:222:LEU:HD13	2.44	0.53
1:D:388:GLU:OE2	1:D:391:ARG:NE	2.42	0.53
1:B:50:ARG:HG2	1:B:50:ARG:NH2	2.23	0.53
1:C:149:TRP:O	1:C:153:LEU:HD22	2.08	0.53
1:C:325:GLU:OE2	1:C:328:ARG:HD3	2.09	0.53
1:D:351:LYS:HB2	1:D:413:ALA:HA	1.91	0.53
1:C:140:VAL:O	1:C:178:THR:HA	2.08	0.53
1:D:162:GLY:O	1:D:175:THR:HA	2.09	0.53
1:A:205:PRO:O	1:A:206:ALA:C	2.46	0.53
1:A:323:TRP:O	1:A:327:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLU:HB2	1:A:431:ARG:HH21	1.74	0.53
1:A:46:LYS:HD2	1:A:46:LYS:N	2.24	0.53
1:A:62:ARG:HH11	1:A:110:ARG:HD3	1.73	0.53
1:D:389:GLY:O	1:D:395:PHE:HB2	2.08	0.53
1:A:309:ALA:O	1:A:310:SER:CB	2.55	0.53
1:A:409:ASP:O	1:A:410:VAL:HB	2.09	0.53
1:A:426:ARG:HH11	1:A:426:ARG:HG3	1.74	0.53
1:D:340:LEU:CG	1:D:343:ILE:HD11	2.39	0.53
1:D:387:LEU:O	1:D:391:ARG:HG2	2.10	0.52
1:D:356:THR:O	1:D:401:SER:HA	2.09	0.52
1:A:122:THR:HG22	1:A:126:MET:HE2	1.90	0.52
1:B:254:LEU:HD22	1:B:254:LEU:N	2.24	0.52
1:C:259:LEU:O	1:C:261:LYS:N	2.36	0.52
1:D:33:THR:HG21	1:D:55:ARG:HG2	1.92	0.52
1:B:24:ILE:CG2	1:B:24:ILE:O	2.58	0.52
1:C:201:VAL:O	1:C:205:PRO:HD3	2.09	0.52
1:C:263:THR:HG22	1:C:446:VAL:HG22	1.90	0.52
1:D:336:LYS:NZ	1:D:420:SER:HB2	2.24	0.52
1:D:163:GLU:O	1:D:170:GLU:HB2	2.10	0.52
1:C:389:GLY:O	1:C:392:THR:HG22	2.08	0.52
1:A:172:LYS:HD3	1:B:50:ARG:NE	2.25	0.52
1:A:30:GLU:OE2	1:A:31:ARG:NH1	2.42	0.52
1:A:344:LEU:HD12	1:A:369:PHE:CD2	2.45	0.52
1:B:187:GLU:H	1:B:187:GLU:CD	2.13	0.52
1:B:449:GLU:O	1:B:451:ILE:HG13	2.10	0.52
1:C:259:LEU:C	1:C:261:LYS:H	2.13	0.52
1:D:95:ARG:CB	1:D:259:LEU:HD11	2.27	0.52
1:B:248:GLU:HG3	1:B:249:LEU:N	2.24	0.52
1:C:35:VAL:HA	1:C:54:TYR:O	2.09	0.52
1:D:150:LYS:HD3	1:D:163:GLU:HB2	1.91	0.52
1:D:441:GLY:O	1:D:442:LYS:HB2	2.09	0.52
1:A:102:LEU:O	1:A:106:LEU:HD22	2.09	0.52
1:C:356:THR:HG23	1:C:362:VAL:HG22	1.91	0.52
1:D:378:THR:HG22	1:D:382:GLU:HB3	1.92	0.52
1:D:81:ASP:N	1:D:82:PRO:HD3	2.25	0.52
1:A:359:ASN:HA	1:A:362:VAL:CG2	2.40	0.52
1:A:416:GLY:HA3	1:A:436:LEU:HD11	1.91	0.52
1:B:122:THR:HG21	1:B:152:ARG:NH2	2.24	0.52
1:C:426:ARG:HH11	1:C:426:ARG:HG3	1.75	0.52
1:C:329:ILE:HD11	4:C:2804:HOH:O	2.10	0.52
1:C:334:LYS:CG	1:C:338:ARG:HE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:HB3	4:A:2835:HOH:O	2.11	0.51
1:A:269:VAL:HG22	1:A:336:LYS:HE3	1.91	0.51
1:C:356:THR:CG2	1:C:362:VAL:HG22	2.40	0.51
1:D:194:MET:HA	1:D:219:PRO:HD2	1.91	0.51
1:A:45:ALA:HB3	4:A:2010:HOH:O	2.10	0.51
1:B:248:GLU:HG3	1:B:249:LEU:H	1.74	0.51
1:C:232:ASP:HB2	4:C:2589:HOH:O	2.11	0.51
1:C:347:HIS:O	1:C:349:LYS:N	2.44	0.51
1:A:290:LEU:O	1:A:291:ARG:CB	2.58	0.51
1:B:378:THR:HB	1:B:382:GLU:HB2	1.92	0.51
1:A:280:GLU:C	1:A:282:ARG:H	2.13	0.51
1:C:394:ARG:HA	1:C:394:ARG:NE	2.24	0.51
1:C:69:GLU:H	1:C:75:PHE:HE2	1.58	0.51
1:B:350:ASP:O	1:B:352:ILE:HG23	2.10	0.51
1:B:366:SER:CB	1:B:373:ALA:HB2	2.40	0.51
1:D:230:ARG:HH21	1:D:234:ARG:HD3	1.75	0.51
1:A:388:GLU:O	1:A:392:THR:HG23	2.10	0.51
1:A:42:VAL:HG22	1:A:67:TYR:CE1	2.46	0.51
1:C:33:THR:HG21	1:C:55:ARG:HE	1.76	0.51
1:D:318:GLU:O	1:D:319:ALA:HB2	2.11	0.51
1:A:295:ILE:CG2	1:A:299:ARG:HB3	2.41	0.51
1:B:391:ARG:HG3	4:B:2869:HOH:O	2.10	0.51
1:C:57:LEU:HD22	1:C:57:LEU:N	2.23	0.51
1:D:249:LEU:HB3	1:D:254:LEU:HD21	1.93	0.51
1:D:450:LEU:HD23	1:D:450:LEU:N	2.24	0.51
1:D:67:TYR:HA	1:D:70:SER:OG	2.09	0.51
1:A:172:LYS:HD3	1:B:50:ARG:HE	1.76	0.51
1:A:34:ILE:HG12	1:A:58:ALA:HA	1.92	0.51
1:A:62:ARG:HB3	4:A:2002:HOH:O	2.10	0.51
1:C:286:TYR:C	1:C:288:GLN:H	2.14	0.51
1:C:349:LYS:O	1:C:349:LYS:HG2	2.11	0.51
1:D:361:LEU:CD1	1:D:365:ILE:HD11	2.40	0.51
1:A:110:ARG:HG3	1:A:242:VAL:O	2.11	0.51
1:A:327:ARG:HH21	1:A:422:SER:HB3	1.76	0.51
1:B:130:ASN:ND2	1:B:268:PHE:HE1	2.09	0.51
1:B:434:ARG:NH2	1:B:434:ARG:CB	2.73	0.51
1:B:438:PRO:HA	1:B:445:ALA:HB2	1.93	0.51
1:A:234:ARG:C	1:A:236:GLU:H	2.15	0.50
1:C:371:ILE:CG2	1:C:399:VAL:HG12	2.41	0.50
1:D:59:PHE:HA	1:D:216:SER:O	2.11	0.50
1:A:283:GLU:C	1:A:285:VAL:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HB	1:A:450:LEU:HD22	1.92	0.50
1:B:369:PHE:HB2	1:B:371:ILE:CD1	2.41	0.50
1:C:57:LEU:O	1:C:60:ARG:HG2	2.12	0.50
1:D:136:THR:N	1:D:173:PRO:O	2.42	0.50
1:D:259:LEU:C	1:D:261:LYS:H	2.13	0.50
1:B:63:ASP:OD1	4:B:2110:HOH:O	2.18	0.50
1:C:259:LEU:HD23	1:C:259:LEU:O	2.11	0.50
1:D:152:ARG:CG	1:D:152:ARG:HH11	2.25	0.50
1:D:44:HIS:ND1	1:D:60:ARG:HD2	2.26	0.50
1:A:42:VAL:CG1	1:A:43:PRO:HD2	2.37	0.50
1:C:343:ILE:HD11	1:C:450:LEU:HD21	1.93	0.50
1:A:327:ARG:O	1:A:330:ALA:HB3	2.12	0.50
1:C:331:PHE:CE2	1:C:421:GLY:HA2	2.47	0.50
1:C:426:ARG:HA	1:C:429:ILE:HD12	1.94	0.50
1:C:57:LEU:CD2	1:C:57:LEU:H	2.22	0.50
1:D:257:LYS:HG2	4:D:2604:HOH:O	2.11	0.50
1:D:305:LYS:CB	1:D:305:LYS:NZ	2.73	0.50
1:A:351:LYS:NZ	1:A:351:LYS:HB3	2.27	0.50
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.76	0.50
1:C:418:ILE:CG1	1:C:425:ALA:HB2	2.40	0.50
1:A:364:ARG:O	1:A:368:VAL:HG23	2.12	0.50
1:B:301:GLU:C	1:B:303:PHE:H	2.14	0.50
1:C:221:ARG:NH2	1:C:241:VAL:O	2.45	0.50
1:D:340:LEU:O	1:D:344:LEU:HG	2.11	0.50
1:D:336:LYS:NZ	1:D:452:SER:HB2	2.27	0.50
1:A:430:GLN:O	1:A:433:GLY:N	2.43	0.50
1:A:140:VAL:O	1:A:178:THR:HA	2.12	0.49
1:A:400:SER:OG	1:A:401:SER:N	2.45	0.49
1:C:126:MET:SD	1:C:153:LEU:HD13	2.52	0.49
1:C:237:ILE:HG13	1:C:238:LEU:N	2.27	0.49
1:C:390:PHE:CE2	1:C:398:ILE:HG12	2.48	0.49
1:D:112:CYS:O	1:D:246:VAL:HG22	2.12	0.49
1:A:414:ASN:OD1	1:A:439:SER:HB2	2.12	0.49
1:A:357:ARG:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:115:LEU:O	1:A:121:LYS:HE3	2.12	0.49
1:A:259:LEU:HD21	1:A:262:TYR:CD2	2.47	0.49
1:B:134:THR:HB	1:B:194:MET:HB2	1.95	0.49
1:B:110:ARG:HD2	1:B:221:ARG:HG3	1.94	0.49
1:B:88:PHE:CD2	1:B:133:SER:HA	2.47	0.49
1:C:229:GLU:OE2	1:C:235:HIS:NE2	2.45	0.49
1:A:141:PRO:HD2	1:A:145:LEU:HD12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:PRO:O	1:B:254:LEU:HD23	2.11	0.49
1:B:290:LEU:C	1:B:296:THR:HG22	2.33	0.49
1:B:99:GLU:HA	1:B:99:GLU:OE1	2.12	0.49
1:A:39:ASP:HB3	1:A:42:VAL:HG23	1.94	0.49
1:B:336:LYS:HE3	1:B:452:SER:OG	2.13	0.49
1:B:450:LEU:H	1:B:450:LEU:CD2	2.25	0.49
1:A:180:ASP:OD1	1:D:143:LEU:HB2	2.13	0.49
1:A:330:ALA:O	1:A:332:ASN:N	2.45	0.49
1:B:253:SER:C	1:B:254:LEU:HD22	2.33	0.49
1:C:364:ARG:O	1:C:368:VAL:HG23	2.13	0.49
1:C:262:TYR:CE2	1:C:433:GLY:HA3	2.48	0.49
1:D:441:GLY:O	1:D:442:LYS:CB	2.61	0.49
1:A:256:GLY:O	1:A:258:HIS:N	2.42	0.49
1:B:247:PHE:C	1:B:247:PHE:CD1	2.86	0.49
1:C:348:ARG:HG3	1:C:349:LYS:H	1.77	0.49
1:A:191:ASN:ND2	1:A:191:ASN:H	2.11	0.49
1:A:379:SER:HB2	1:A:382:GLU:HB2	1.94	0.49
1:B:433:GLY:O	1:B:436:LEU:HB2	2.12	0.49
1:C:196:LEU:HG	1:C:218:ALA:HB3	1.94	0.49
1:C:61:TYR:O	1:C:65:ILE:HG12	2.13	0.49
1:D:27:ILE:HG13	1:D:27:ILE:O	2.13	0.49
1:C:291:ARG:O	1:C:292:ALA:HB3	2.13	0.49
1:A:304:ASN:HD22	1:A:307:VAL:CG2	2.26	0.49
1:B:382:GLU:HA	1:B:385:GLU:HB3	1.94	0.49
1:C:375:THR:OG1	1:C:376:HIS:N	2.43	0.49
1:C:28:TYR:CA	1:C:79:ALA:HB2	2.40	0.49
1:A:389:GLY:O	1:A:395:PHE:HB2	2.12	0.48
1:B:210:VAL:HG21	1:B:237:ILE:HD12	1.94	0.48
1:B:350:ASP:HB3	1:B:414:ASN:OD1	2.13	0.48
1:B:434:ARG:CB	1:B:434:ARG:HH21	2.25	0.48
1:C:431:ARG:O	1:C:435:ILE:HG13	2.13	0.48
1:C:42:VAL:HG12	1:C:45:ALA:H	1.77	0.48
1:D:383:ARG:O	1:D:387:LEU:HG	2.13	0.48
1:C:333:SER:O	1:C:337:ILE:HG12	2.13	0.48
1:D:340:LEU:CD2	1:D:343:ILE:HD11	2.43	0.48
1:D:352:ILE:HD12	1:D:353:ILE:H	1.78	0.48
1:C:152:ARG:C	1:C:154:GLY:H	2.15	0.48
1:C:34:ILE:HG12	1:C:58:ALA:HA	1.95	0.48
1:D:96:ASP:H	1:D:259:LEU:CD1	2.26	0.48
1:D:259:LEU:C	1:D:261:LYS:N	2.67	0.48
1:D:267:ILE:O	1:D:451:ILE:N	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HG	1:C:218:ALA:CB	2.44	0.48
1:A:136:THR:N	1:A:173:PRO:O	2.32	0.48
1:A:259:LEU:HD22	1:A:261:LYS:HG3	1.95	0.48
1:B:105:TRP:HE3	1:B:106:LEU:HD13	1.78	0.48
1:C:159:GLU:OE2	1:C:159:GLU:N	2.39	0.48
1:C:204:LEU:N	1:C:205:PRO:CD	2.77	0.48
1:D:449:GLU:HG2	1:D:451:ILE:CG1	2.43	0.48
1:C:418:ILE:CD1	1:C:425:ALA:HB2	2.44	0.48
1:A:259:LEU:HD22	1:A:259:LEU:C	2.34	0.48
1:C:115:LEU:HB3	1:C:119:SER:HB2	1.94	0.48
1:D:369:PHE:O	1:D:371:ILE:N	2.41	0.48
1:D:391:ARG:HG3	1:D:392:THR:H	1.79	0.48
1:B:304:ASN:HA	1:B:307:VAL:HB	1.96	0.48
1:C:217:ILE:O	1:C:218:ALA:C	2.51	0.48
1:C:361:LEU:HD22	1:C:365:ILE:HG13	1.96	0.48
1:C:440:LYS:HG2	1:C:441:GLY:N	2.27	0.48
1:D:352:ILE:HA	1:D:415:VAL:O	2.14	0.48
1:D:65:ILE:O	1:D:68:PHE:HB2	2.13	0.48
1:A:102:LEU:HG	1:A:106:LEU:CD2	2.44	0.48
1:A:439:SER:O	1:A:441:GLY:N	2.46	0.48
1:C:132:LEU:O	1:C:133:SER:HB2	2.14	0.48
1:C:338:ARG:O	1:C:341:ARG:HB3	2.14	0.48
1:C:356:THR:HB	1:C:419:MET:CG	2.44	0.48
1:D:339:LYS:O	1:D:343:ILE:HG23	2.14	0.48
1:A:295:ILE:HB	1:A:299:ARG:CB	2.44	0.47
1:C:272:ALA:O	1:C:274:ASP:N	2.45	0.47
1:D:116:PRO:CG	1:D:251:PRO:HG3	2.44	0.47
1:A:277:VAL:HG13	1:A:278:GLU:N	2.29	0.47
1:A:304:ASN:C	1:A:306:ILE:H	2.18	0.47
1:A:234:ARG:NH2	3:A:6002:IPA:H2	2.29	0.47
1:B:110:ARG:NH1	1:B:219:PRO:O	2.44	0.47
1:B:282:ARG:O	1:B:322:ALA:HB1	2.14	0.47
1:D:27:ILE:HD12	1:D:27:ILE:C	2.34	0.47
1:A:259:LEU:HD22	1:A:261:LYS:H	1.79	0.47
1:B:105:TRP:CE3	1:B:106:LEU:HD13	2.49	0.47
1:C:254:LEU:O	1:C:255:ALA:CB	2.62	0.47
1:C:361:LEU:CD1	1:C:419:MET:HG3	2.40	0.47
1:C:71:ASN:O	1:C:73:ILE:N	2.42	0.47
1:D:266:ARG:HB3	1:D:451:ILE:HD12	1.95	0.47
1:A:261:LYS:NZ	1:A:261:LYS:HB3	2.29	0.47
1:A:426:ARG:NH2	4:A:2471:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:CD1	1:B:106:LEU:HD22	2.44	0.47
1:D:140:VAL:O	1:D:178:THR:HA	2.14	0.47
1:D:149:TRP:HE3	1:D:153:LEU:CD1	2.24	0.47
1:D:361:LEU:HD13	1:D:365:ILE:HG13	1.95	0.47
1:D:84:PRO:HB3	4:D:2177:HOH:O	2.14	0.47
1:A:355:PHE:CD2	1:A:356:THR:N	2.83	0.47
1:B:333:SER:CB	1:B:336:LYS:HG2	2.40	0.47
1:B:412:ASP:OD2	1:B:437:ARG:HG2	2.15	0.47
1:C:68:PHE:O	1:C:69:GLU:C	2.53	0.47
1:D:460:THR:O	1:D:461:ALA:HB2	2.15	0.47
1:D:74:GLU:HA	1:D:74:GLU:OE1	2.14	0.47
1:B:350:ASP:HB2	1:B:414:ASN:HB3	1.95	0.47
1:B:67:TYR:C	1:B:67:TYR:CD1	2.87	0.47
1:C:105:TRP:O	1:C:109:LYS:N	2.46	0.47
1:C:125:ALA:O	1:C:129:ILE:HG13	2.13	0.47
1:C:426:ARG:HA	1:C:429:ILE:CD1	2.44	0.47
1:D:344:LEU:O	1:D:346:ARG:N	2.48	0.47
1:A:352:ILE:HD11	1:A:354:ILE:HD11	1.97	0.47
1:B:28:TYR:HE1	1:B:37:LYS:HD2	1.79	0.47
1:D:250:PHE:O	1:D:253:SER:HB2	2.15	0.47
1:A:389:GLY:HA2	1:A:392:THR:OG1	2.14	0.47
1:A:390:PHE:HA	1:A:395:PHE:CB	2.44	0.47
1:B:405:ASP:CB	1:B:435:ILE:HD11	2.41	0.47
1:C:348:ARG:HG3	1:C:349:LYS:N	2.29	0.47
1:C:363:TYR:O	1:C:367:LYS:HG2	2.15	0.47
1:A:122:THR:O	1:A:126:MET:HE2	2.15	0.47
1:A:295:ILE:HD13	1:A:300:ALA:CB	2.43	0.47
1:A:404:LEU:O	1:A:410:VAL:HG11	2.15	0.47
1:B:31:ARG:HG2	1:B:187:GLU:HB3	1.95	0.47
1:C:26:GLU:HG2	1:C:27:ILE:N	2.29	0.47
1:D:132:LEU:HD23	1:D:458:VAL:CG2	2.32	0.47
1:A:307:VAL:HG23	1:A:308:MET:N	2.29	0.47
1:B:279:TYR:OH	1:B:422:SER:HB3	2.15	0.47
1:D:327:ARG:NH2	1:D:358:HIS:NE2	2.63	0.47
1:D:418:ILE:CG1	1:D:432:LEU:HD13	2.45	0.47
1:B:81:ASP:O	1:B:192:ARG:HA	2.14	0.47
1:B:283:GLU:C	1:B:285:VAL:N	2.68	0.47
1:B:405:ASP:HB3	1:B:435:ILE:CD1	2.43	0.47
1:B:60:ARG:NH1	4:B:2110:HOH:O	2.43	0.47
1:C:290:LEU:HD23	1:C:290:LEU:H	1.80	0.47
1:D:115:LEU:O	1:D:121:LYS:NZ	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:HA	1:A:362:VAL:CB	2.44	0.46
1:A:403:VAL:HG23	1:A:403:VAL:O	2.15	0.46
1:B:375:THR:HG23	1:B:377:ARG:N	2.28	0.46
1:A:121:LYS:HE2	1:A:225:THR:C	2.36	0.46
1:A:122:THR:HG21	1:A:152:ARG:NE	2.30	0.46
1:B:205:PRO:HA	1:B:237:ILE:HD11	1.97	0.46
1:B:403:VAL:HG21	1:B:431:ARG:HE	1.80	0.46
1:C:168:ILE:HG12	1:C:170:GLU:HG3	1.97	0.46
1:D:32:GLY:HA3	1:D:215:MET:HE2	1.97	0.46
1:A:374:ILE:HD11	1:A:386:ILE:CG2	2.45	0.46
1:B:369:PHE:HB2	1:B:371:ILE:HG13	1.98	0.46
1:C:152:ARG:C	1:C:154:GLY:N	2.69	0.46
1:C:267:ILE:HD11	1:C:448:TYR:HD2	1.79	0.46
1:A:191:ASN:ND2	4:A:2501:HOH:O	2.47	0.46
1:A:365:ILE:O	1:A:369:PHE:HD1	1.99	0.46
1:D:100:LYS:HD3	1:D:426:ARG:NH2	2.25	0.46
1:D:403:VAL:HG11	1:D:431:ARG:HD3	1.96	0.46
1:D:43:PRO:HG3	1:D:67:TYR:CD2	2.50	0.46
1:A:205:PRO:HA	1:A:237:ILE:HD11	1.96	0.46
1:A:259:LEU:CD1	1:A:260:ALA:N	2.77	0.46
1:B:102:LEU:CG	1:B:106:LEU:HD22	2.43	0.46
1:B:299:ARG:C	1:B:301:GLU:H	2.17	0.46
1:C:27:ILE:HG22	1:C:36:VAL:HG13	1.96	0.46
1:D:376:HIS:HB3	1:D:402:GLN:HE22	1.80	0.46
1:D:66:GLU:O	1:D:68:PHE:N	2.48	0.46
1:B:367:LYS:C	1:B:369:PHE:N	2.67	0.46
1:D:198:PHE:CE1	1:D:204:LEU:HD13	2.50	0.46
1:D:333:SER:HB3	1:D:336:LYS:HG3	1.97	0.46
1:D:404:LEU:O	1:D:411:PRO:HD2	2.15	0.46
1:B:45:ALA:HB1	1:B:54:TYR:HB3	1.97	0.46
1:C:164:PHE:HE1	1:C:185:ASN:CG	2.18	0.46
1:C:423:GLY:O	1:C:424:SER:HB2	2.16	0.46
1:D:420:SER:OG	1:D:421:GLY:N	2.47	0.46
1:D:443:LYS:O	1:D:444:GLU:HG3	2.15	0.46
1:A:191:ASN:N	1:A:191:ASN:HD22	2.10	0.46
1:B:371:ILE:HA	1:B:372:PRO:HD3	1.68	0.46
1:C:259:LEU:C	1:C:261:LYS:N	2.69	0.46
1:B:434:ARG:HB2	1:B:434:ARG:CZ	2.44	0.46
1:C:284:LYS:C	1:C:286:TYR:N	2.66	0.46
1:D:274:ASP:HA	1:D:277:VAL:CG2	2.46	0.46
1:D:424:SER:HA	1:D:449:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HD12	1:A:254:LEU:N	2.31	0.46
1:A:304:ASN:HA	1:A:307:VAL:CG2	2.44	0.46
1:A:377:ARG:O	1:A:378:THR:C	2.53	0.46
1:A:451:ILE:HG22	1:A:452:SER:N	2.31	0.46
1:C:162:GLY:HA3	1:C:172:LYS:HB2	1.98	0.46
1:C:347:HIS:O	1:C:348:ARG:C	2.55	0.46
1:D:268:PHE:HA	1:D:451:ILE:O	2.16	0.46
1:A:282:ARG:HG3	1:A:329:ILE:CD1	2.46	0.45
1:A:340:LEU:O	1:A:344:LEU:HG	2.16	0.45
1:C:149:TRP:O	1:C:152:ARG:N	2.50	0.45
1:A:390:PHE:HA	1:A:395:PHE:HB3	1.98	0.45
1:B:344:LEU:O	1:B:348:ARG:HG3	2.15	0.45
1:D:110:ARG:HE	1:D:221:ARG:HG3	1.81	0.45
1:A:149:TRP:HA	1:A:152:ARG:HH11	1.81	0.45
1:A:388:GLU:O	1:A:392:THR:N	2.48	0.45
1:B:378:THR:O	1:B:379:SER:HB2	2.17	0.45
1:C:116:PRO:HD2	1:C:119:SER:OG	2.16	0.45
1:C:407:GLY:O	1:C:408:ILE:HB	2.17	0.45
1:C:263:THR:HG23	1:C:446:VAL:HG13	1.99	0.45
1:D:172:LYS:HB3	1:D:173:PRO:CD	2.44	0.45
1:D:256:GLY:O	1:D:258:HIS:N	2.40	0.45
1:D:258:HIS:C	1:D:260:ALA:H	2.20	0.45
1:D:336:LYS:HZ1	1:D:420:SER:HB2	1.82	0.45
1:A:271:LEU:HD21	1:A:452:SER:HB3	1.99	0.45
1:C:239:LYS:HA	1:C:243:GLY:C	2.36	0.45
1:C:94:LEU:N	1:C:264:ILE:O	2.39	0.45
1:C:60:ARG:O	1:C:61:TYR:C	2.54	0.45
1:D:357:ARG:HE	1:D:428:TYR:HE2	1.65	0.45
1:B:199:ASP:O	1:B:200:GLU:C	2.53	0.45
1:B:276:ARG:HG3	1:B:277:VAL:N	2.32	0.45
1:B:390:PHE:CE2	1:B:398:ILE:HG12	2.51	0.45
1:B:415:VAL:CG1	1:B:416:GLY:N	2.79	0.45
1:C:322:ALA:C	1:C:324:GLU:N	2.70	0.45
1:C:412:ASP:HB2	1:C:437:ARG:NH1	2.32	0.45
1:D:457:GLU:O	1:D:458:VAL:HB	2.16	0.45
1:A:62:ARG:NH1	1:A:110:ARG:HD3	2.31	0.45
1:A:372:PRO:HG3	1:A:395:PHE:CE2	2.49	0.45
1:A:443:LYS:O	1:A:444:GLU:HG3	2.17	0.45
1:B:26:GLU:HG2	1:B:27:ILE:N	2.31	0.45
1:B:427:GLU:HG2	1:B:428:TYR:CD2	2.52	0.45
1:D:43:PRO:O	1:D:44:HIS:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HG	1:A:218:ALA:CB	2.47	0.45
1:B:31:ARG:HG2	1:B:187:GLU:CG	2.46	0.45
1:B:375:THR:O	1:B:383:ARG:NH2	2.49	0.45
1:C:101:ALA:HB2	1:C:247:PHE:CE1	2.52	0.45
1:C:358:HIS:HB3	1:C:361:LEU:HB3	1.99	0.45
1:D:195:LEU:HD23	1:D:220:PHE:HB2	1.99	0.45
1:A:431:ARG:N	1:A:431:ARG:HD3	2.32	0.45
1:B:347:HIS:ND1	1:B:415:VAL:HG21	2.32	0.45
1:C:271:LEU:HA	1:C:271:LEU:HD12	1.81	0.45
1:C:389:GLY:C	1:C:392:THR:HG22	2.36	0.45
1:D:261:LYS:HA	1:D:444:GLU:HG2	1.99	0.45
1:A:241:VAL:HG23	1:A:242:VAL:N	2.32	0.45
1:A:398:ILE:CD1	1:A:399:VAL:N	2.66	0.45
1:B:339:LYS:O	1:B:342:GLU:HB2	2.17	0.45
1:C:232:ASP:OD1	1:C:234:ARG:HB2	2.16	0.45
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.81	0.45
1:D:116:PRO:HG3	1:D:251:PRO:HG3	1.99	0.45
1:A:266:ARG:HH21	1:A:266:ARG:HG2	1.82	0.45
1:A:339:LYS:O	1:A:343:ILE:HG13	2.17	0.45
1:B:329:ILE:O	1:B:332:ASN:OD1	2.35	0.45
1:B:430:GLN:HB2	1:B:430:GLN:HE21	1.53	0.45
1:D:394:ARG:HG2	1:D:394:ARG:O	2.17	0.45
1:D:42:VAL:HB	1:D:54:TYR:CD2	2.51	0.45
1:C:325:GLU:HG3	1:C:329:ILE:CD1	2.36	0.44
1:D:29:TYR:H	1:D:79:ALA:HA	1.82	0.44
1:D:328:ARG:HG3	1:D:328:ARG:NH1	2.32	0.44
1:D:352:ILE:HD11	1:D:354:ILE:HG12	1.99	0.44
1:B:322:ALA:C	1:B:324:GLU:N	2.71	0.44
1:C:103:GLU:HA	1:C:103:GLU:OE2	2.16	0.44
1:D:172:LYS:CB	1:D:173:PRO:HD2	2.43	0.44
1:D:26:GLU:HG2	1:D:27:ILE:N	2.32	0.44
1:A:81:ASP:O	1:A:192:ARG:HA	2.17	0.44
1:A:85:THR:HG23	1:A:86:PRO:HD2	1.99	0.44
1:B:429:ILE:HD11	1:B:449:GLU:OE2	2.18	0.44
1:C:190:GLY:O	1:C:217:ILE:HG23	2.17	0.44
1:D:109:LYS:O	1:D:220:PHE:HA	2.17	0.44
4:A:2006:HOH:O	1:D:142:THR:HG22	2.16	0.44
1:A:432:LEU:C	1:A:432:LEU:HD13	2.38	0.44
1:B:404:LEU:N	1:B:404:LEU:CD2	2.77	0.44
1:C:327:ARG:O	1:C:331:PHE:HB2	2.16	0.44
1:D:372:PRO:CB	1:D:398:ILE:HG22	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.98	0.44
1:A:259:LEU:HD13	1:A:261:LYS:H	1.83	0.44
1:A:288:GLN:HB2	1:A:290:LEU:HD22	1.99	0.44
1:A:320:LEU:HD23	1:A:320:LEU:O	2.17	0.44
1:A:377:ARG:NH1	1:A:377:ARG:HG3	2.32	0.44
1:B:31:ARG:HG2	1:B:187:GLU:HG2	1.99	0.44
1:C:202:HIS:O	1:C:205:PRO:HD2	2.17	0.44
1:C:250:PHE:CD1	1:C:251:PRO:HD2	2.50	0.44
1:C:266:ARG:HB2	4:C:2247:HOH:O	2.17	0.44
1:A:201:VAL:HG22	1:A:201:VAL:O	2.17	0.44
1:A:288:GLN:C	1:A:290:LEU:H	2.21	0.44
1:B:399:VAL:HG13	1:B:399:VAL:O	2.18	0.44
1:C:247:PHE:CE1	1:C:249:LEU:HB2	2.53	0.44
1:A:269:VAL:HG23	4:A:2285:HOH:O	2.17	0.44
1:A:326:ALA:O	1:A:329:ILE:HB	2.17	0.44
1:A:359:ASN:O	1:A:362:VAL:N	2.51	0.44
1:B:207:GLU:HG2	1:B:234:ARG:NH1	2.32	0.44
1:B:248:GLU:CG	1:B:249:LEU:N	2.80	0.44
1:C:356:THR:O	1:C:401:SER:HA	2.18	0.44
1:D:305:LYS:N	1:D:305:LYS:CD	2.81	0.44
1:D:361:LEU:HD22	1:D:364:ARG:HD2	1.99	0.44
1:A:116:PRO:O	1:A:119:SER:OG	2.33	0.44
1:A:431:ARG:H	1:A:431:ARG:HD3	1.81	0.44
1:C:96:ASP:CG	1:C:259:LEU:HD22	2.38	0.44
1:A:134:THR:HB	1:A:135:PRO:HD2	2.00	0.44
1:A:66:GLU:CG	1:A:297:LEU:HD13	2.44	0.44
1:A:300:ALA:HB1	1:A:304:ASN:HB2	1.99	0.44
1:B:354:ILE:HG22	1:B:355:PHE:H	1.81	0.44
1:B:366:SER:HA	1:B:371:ILE:HB	2.00	0.44
1:D:290:LEU:HD13	1:D:290:LEU:N	2.33	0.44
1:D:325:GLU:C	1:D:327:ARG:N	2.71	0.44
1:D:449:GLU:O	1:D:451:ILE:HG13	2.17	0.44
1:D:83:ILE:HD13	1:D:171:LEU:O	2.18	0.44
1:A:205:PRO:HB2	1:A:230:ARG:HH11	1.81	0.43
1:B:22:GLN:O	1:B:24:ILE:HG13	2.17	0.43
1:B:425:ALA:O	1:B:429:ILE:HG13	2.18	0.43
1:C:92:ILE:HG21	1:C:127:ALA:HB2	1.99	0.43
1:C:405:ASP:HA	1:C:410:VAL:HG22	1.99	0.43
1:C:426:ARG:NH1	1:C:426:ARG:HG3	2.33	0.43
1:C:95:ARG:O	1:C:98:GLN:N	2.51	0.43
1:A:29:TYR:H	1:A:79:ALA:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HH11	1:B:110:ARG:HD3	1.83	0.43
1:C:340:LEU:HD11	1:C:354:ILE:CD1	2.48	0.43
1:D:280:GLU:O	1:D:282:ARG:N	2.37	0.43
1:D:405:ASP:HB3	1:D:435:ILE:CD1	2.39	0.43
1:D:456:GLY:O	1:D:457:GLU:HB2	2.18	0.43
1:A:103:GLU:HG3	1:A:426:ARG:HD3	2.00	0.43
1:A:180:ASP:OD1	1:A:209:TYR:OH	2.28	0.43
1:A:286:TYR:CE2	1:A:323:TRP:HA	2.53	0.43
1:A:418:ILE:HD12	1:A:429:ILE:HD13	1.99	0.43
1:A:430:GLN:HG3	4:A:2471:HOH:O	2.18	0.43
1:A:85:THR:HG22	1:A:86:PRO:O	2.18	0.43
1:B:391:ARG:HD2	1:B:391:ARG:O	2.18	0.43
1:C:283:GLU:O	1:C:284:LYS:CB	2.66	0.43
1:C:361:LEU:O	1:C:365:ILE:CG1	2.67	0.43
1:C:392:THR:HG23	1:C:393:GLY:H	1.82	0.43
1:D:404:LEU:N	1:D:404:LEU:CD2	2.78	0.43
1:A:270:PRO:O	1:A:335:ASN:ND2	2.52	0.43
1:A:385:GLU:O	1:A:388:GLU:N	2.47	0.43
1:A:425:ALA:HB1	1:A:428:TYR:HD2	1.83	0.43
1:C:323:TRP:CZ2	1:C:327:ARG:HB2	2.53	0.43
1:C:331:PHE:CE1	1:C:358:HIS:HB2	2.54	0.43
1:C:403:VAL:HG21	1:C:431:ARG:CZ	2.48	0.43
1:D:417:VAL:HG12	1:D:419:MET:CE	2.49	0.43
1:D:458:VAL:HG12	1:D:459:ASN:N	2.33	0.43
1:A:305:LYS:C	1:A:306:ILE:HG13	2.39	0.43
1:A:351:LYS:NZ	1:A:390:PHE:CE1	2.87	0.43
1:A:425:ALA:HB1	1:A:428:TYR:CD2	2.53	0.43
1:B:299:ARG:C	1:B:301:GLU:N	2.72	0.43
1:D:261:LYS:CA	1:D:444:GLU:HG2	2.49	0.43
1:D:269:VAL:O	1:D:269:VAL:HG23	2.17	0.43
1:D:289:PHE:C	1:D:291:ARG:N	2.71	0.43
1:D:376:HIS:HB3	1:D:402:GLN:NE2	2.34	0.43
1:D:73:ILE:HG22	1:D:74:GLU:N	2.33	0.43
1:A:285:VAL:CG2	1:A:286:TYR:H	2.12	0.43
1:B:357:ARG:HG3	1:B:357:ARG:O	2.18	0.43
1:C:421:GLY:O	1:C:422:SER:CB	2.66	0.43
1:D:110:ARG:NE	1:D:221:ARG:HG3	2.33	0.43
1:D:356:THR:HB	1:D:419:MET:CG	2.49	0.43
1:D:132:LEU:HD23	1:D:458:VAL:HG11	2.00	0.43
1:A:169:LYS:NZ	1:A:185:ASN:HD21	2.16	0.43
1:A:228:PHE:CD1	1:A:245:LYS:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:TYR:O	1:A:432:LEU:HB3	2.19	0.43
1:B:103:GLU:OE1	1:B:426:ARG:HD2	2.19	0.43
1:C:229:GLU:HG3	4:C:2633:HOH:O	2.18	0.43
1:B:201:VAL:O	1:B:201:VAL:HG22	2.18	0.43
1:B:357:ARG:HD3	1:B:428:TYR:OH	2.18	0.43
1:B:437:ARG:O	1:B:438:PRO:O	2.36	0.43
1:C:361:LEU:HD13	1:C:361:LEU:O	2.18	0.43
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.92	0.43
1:D:388:GLU:OE2	1:D:391:ARG:CZ	2.67	0.43
1:A:103:GLU:HA	1:A:106:LEU:HD23	2.01	0.43
1:A:122:THR:HG22	1:A:126:MET:HE1	2.00	0.43
1:A:141:PRO:HD2	1:A:145:LEU:CD1	2.49	0.43
1:A:336:LYS:O	1:A:340:LEU:HB2	2.19	0.43
1:B:187:GLU:HG3	1:B:215:MET:CE	2.49	0.43
1:B:273:GLU:HG3	1:B:276:ARG:HD3	2.00	0.43
1:B:400:SER:CB	1:B:404:LEU:HD11	2.49	0.43
1:C:171:LEU:C	1:C:172:LYS:HE2	2.39	0.43
1:C:96:ASP:OD1	1:C:259:LEU:HB2	2.19	0.43
1:A:202:HIS:O	1:A:205:PRO:HD2	2.19	0.43
1:B:231:GLU:OE2	1:B:232:ASP:N	2.52	0.43
1:B:332:ASN:O	1:B:333:SER:O	2.36	0.43
1:C:354:ILE:HD11	1:C:419:MET:SD	2.58	0.43
1:C:72:GLY:O	1:C:73:ILE:C	2.56	0.43
1:D:329:ILE:CD1	1:D:330:ALA:N	2.72	0.43
1:D:340:LEU:HD23	1:D:343:ILE:HD11	1.99	0.43
1:D:68:PHE:C	1:D:70:SER:H	2.22	0.43
1:C:269:VAL:HG21	1:C:336:LYS:HD3	2.01	0.42
1:D:62:ARG:HD3	1:D:110:ARG:NH1	2.33	0.42
1:D:34:ILE:HD13	1:D:34:ILE:HA	1.85	0.42
1:D:421:GLY:C	1:D:423:GLY:N	2.72	0.42
1:D:52:GLY:O	1:D:53:THR:HG23	2.18	0.42
1:A:231:GLU:HG3	1:D:118:GLY:HA2	2.00	0.42
1:A:46:LYS:HE2	4:A:2260:HOH:O	2.18	0.42
1:B:209:TYR:OH	1:C:142:THR:HB	2.18	0.42
1:B:329:ILE:HG22	1:B:329:ILE:O	2.18	0.42
1:B:48:ASP:OD1	1:B:50:ARG:HB3	2.19	0.42
1:C:375:THR:CG2	1:C:378:THR:HG23	2.31	0.42
1:D:115:LEU:HD12	1:D:121:LYS:HG2	2.00	0.42
1:B:295:ILE:HG23	1:B:295:ILE:O	2.19	0.42
1:B:435:ILE:O	1:B:437:ARG:HD2	2.18	0.42
1:B:80:ALA:C	1:B:82:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:NH1	4:C:2340:HOH:O	2.52	0.42
1:D:26:GLU:CG	1:D:27:ILE:N	2.82	0.42
1:D:413:ALA:HB3	1:D:436:LEU:HD23	2.01	0.42
1:B:102:LEU:HG	1:B:106:LEU:CD2	2.46	0.42
1:B:122:THR:HG22	1:B:122:THR:O	2.18	0.42
1:C:148:GLN:HE21	1:C:152:ARG:NH1	1.97	0.42
1:C:196:LEU:HD13	1:C:198:PHE:CZ	2.54	0.42
1:C:358:HIS:O	1:C:362:VAL:HG23	2.19	0.42
1:C:269:VAL:HG22	1:C:452:SER:HB3	2.01	0.42
1:D:191:ASN:OD1	1:D:192:ARG:CD	2.65	0.42
1:D:453:ARG:HB2	1:D:454:GLY:H	1.69	0.42
1:A:258:HIS:O	1:A:259:LEU:C	2.58	0.42
1:A:325:GLU:O	1:A:326:ALA:C	2.56	0.42
1:A:335:ASN:O	1:A:339:LYS:HB2	2.19	0.42
1:A:65:ILE:HG22	1:A:297:LEU:CD1	2.47	0.42
1:B:290:LEU:HD22	1:B:296:THR:C	2.40	0.42
1:B:372:PRO:HG2	1:B:395:PHE:CD1	2.54	0.42
1:B:68:PHE:HB3	1:B:75:PHE:CE2	2.54	0.42
1:B:93:SER:HA	1:B:264:ILE:O	2.20	0.42
1:C:100:LYS:HD2	1:C:247:PHE:HE2	1.84	0.42
1:D:309:ALA:O	1:D:311:GLY:N	2.52	0.42
1:D:336:LYS:NZ	1:D:420:SER:CB	2.82	0.42
1:A:269:VAL:CG2	1:A:336:LYS:HE3	2.50	0.42
1:A:59:PHE:HA	1:A:216:SER:O	2.20	0.42
1:A:92:ILE:HD12	1:A:92:ILE:N	2.34	0.42
1:D:44:HIS:HE1	1:D:63:ASP:OD1	2.01	0.42
1:D:33:THR:HG21	1:D:55:ARG:CG	2.50	0.42
1:D:68:PHE:CD1	1:D:75:PHE:CD2	3.06	0.42
1:A:239:LYS:HA	1:A:243:GLY:C	2.39	0.42
1:B:163:GLU:OE1	1:B:168:ILE:HG22	2.19	0.42
1:B:196:LEU:HG	1:B:218:ALA:HB3	2.01	0.42
1:B:356:THR:OG1	1:B:361:LEU:HD13	2.20	0.42
1:C:24:ILE:HG13	4:C:2709:HOH:O	2.18	0.42
1:C:254:LEU:C	1:C:254:LEU:HD23	2.40	0.42
1:C:267:ILE:CD1	1:C:448:TYR:HD2	2.32	0.42
1:C:372:PRO:HD2	1:C:398:ILE:HG22	2.01	0.42
1:D:138:ILE:HD12	1:D:138:ILE:N	2.35	0.42
1:D:152:ARG:HH11	1:D:152:ARG:HB2	1.85	0.42
1:D:167:ARG:C	1:D:168:ILE:CG1	2.88	0.42
1:D:109:LYS:HE2	1:D:458:VAL:CG1	2.50	0.42
1:A:301:GLU:O	1:A:302:ASP:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HG13	4:B:2122:HOH:O	2.18	0.42
1:B:382:GLU:O	1:B:385:GLU:HB3	2.20	0.42
1:C:418:ILE:HD12	1:C:419:MET:H	1.85	0.42
1:C:65:ILE:O	1:C:69:GLU:HB2	2.20	0.42
1:D:337:ILE:HD11	1:D:361:LEU:HD21	2.01	0.42
1:A:81:ASP:N	1:A:82:PRO:HD3	2.35	0.42
1:B:263:THR:HG23	1:B:444:GLU:HB3	2.02	0.42
1:B:367:LYS:O	1:B:369:PHE:N	2.53	0.42
1:C:62:ARG:NH1	1:C:219:PRO:O	2.51	0.42
1:C:325:GLU:HA	1:C:328:ARG:HB3	2.02	0.42
1:C:340:LEU:HD22	1:C:344:LEU:HG	2.02	0.42
1:C:396:ARG:HH11	1:C:396:ARG:HG2	1.83	0.42
1:C:50:ARG:HG2	1:C:50:ARG:NH1	2.34	0.42
1:D:276:ARG:O	1:D:279:TYR:HB3	2.20	0.42
1:D:403:VAL:HG21	1:D:431:ARG:NH1	2.34	0.42
1:B:115:LEU:HD21	1:B:247:PHE:HE1	1.85	0.42
1:B:338:ARG:O	1:B:342:GLU:HG3	2.20	0.42
1:B:43:PRO:C	1:B:45:ALA:H	2.24	0.42
1:B:99:GLU:CA	1:B:99:GLU:OE1	2.68	0.42
1:C:355:PHE:CD2	1:C:418:ILE:HD13	2.54	0.42
1:C:415:VAL:CG1	1:C:416:GLY:N	2.83	0.42
1:D:152:ARG:HH11	1:D:152:ARG:CB	2.33	0.42
1:D:164:PHE:O	1:D:164:PHE:HD1	2.03	0.42
1:D:395:PHE:O	1:D:397:ALA:N	2.53	0.42
1:D:57:LEU:HD22	4:D:2560:HOH:O	2.19	0.42
1:A:340:LEU:HD22	1:A:344:LEU:HD11	2.02	0.41
1:B:360:GLU:N	1:B:362:VAL:HG22	2.35	0.41
1:B:436:LEU:HD11	1:B:447:LEU:HB2	2.02	0.41
1:C:399:VAL:O	1:C:399:VAL:HG13	2.20	0.41
1:D:312:TYR:O	1:D:317:TYR:HB2	2.19	0.41
1:D:368:VAL:CG1	1:D:368:VAL:O	2.67	0.41
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.85	0.41
1:A:303:PHE:O	1:A:303:PHE:CD1	2.73	0.41
1:A:52:GLY:HA3	4:A:2818:HOH:O	2.19	0.41
1:B:405:ASP:HA	1:B:410:VAL:HG12	2.01	0.41
1:B:450:LEU:N	1:B:450:LEU:CD2	2.81	0.41
1:C:220:PHE:C	1:C:221:ARG:HG3	2.40	0.41
1:C:415:VAL:HG12	1:C:416:GLY:N	2.34	0.41
1:D:105:TRP:HE3	1:D:106:LEU:HD12	1.85	0.41
1:D:364:ARG:HG3	1:D:368:VAL:HG21	2.01	0.41
1:D:390:PHE:CE2	1:D:398:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:GLU:HG2	1:D:451:ILE:HD11	2.02	0.41
1:A:220:PHE:C	1:A:221:ARG:HG2	2.39	0.41
1:A:230:ARG:HH22	3:A:6001:IPA:C3	2.33	0.41
1:A:267:ILE:HG21	1:A:339:LYS:HE2	2.03	0.41
1:A:373:ALA:O	1:A:374:ILE:HG13	2.20	0.41
1:A:266:ARG:HD3	1:A:451:ILE:HD12	2.02	0.41
1:B:31:ARG:HG3	1:B:187:GLU:HB3	2.03	0.41
1:B:137:LEU:HB2	1:B:193:PHE:CD2	2.56	0.41
1:D:261:LYS:C	1:D:444:GLU:HB3	2.41	0.41
1:B:101:ALA:HA	1:B:247:PHE:CD2	2.55	0.41
1:B:205:PRO:O	1:B:206:ALA:C	2.57	0.41
1:B:207:GLU:HG3	4:B:2032:HOH:O	2.20	0.41
1:B:327:ARG:NH1	1:B:423:GLY:H	2.17	0.41
1:C:153:LEU:O	1:C:156:PHE:HB2	2.19	0.41
1:D:283:GLU:HB3	1:D:286:TYR:CE1	2.56	0.41
1:D:418:ILE:CD1	1:D:447:LEU:HD21	2.47	0.41
1:A:60:ARG:HG3	1:A:60:ARG:HH21	1.85	0.41
1:B:232:ASP:OD1	1:B:234:ARG:HB2	2.20	0.41
1:B:257:LYS:HA	1:B:257:LYS:HD3	1.82	0.41
1:B:67:TYR:CD1	1:B:68:PHE:N	2.89	0.41
1:B:88:PHE:HB3	1:B:156:PHE:CE1	2.55	0.41
1:C:141:PRO:HD2	1:C:145:LEU:HD13	2.02	0.41
1:D:28:TYR:N	1:D:28:TYR:CD1	2.88	0.41
1:D:305:LYS:HE3	1:D:320:LEU:HD11	2.02	0.41
1:D:355:PHE:CG	1:D:356:THR:N	2.89	0.41
1:A:434:ARG:HG2	1:A:434:ARG:H	1.75	0.41
1:C:102:LEU:O	1:C:106:LEU:HB2	2.20	0.41
1:A:24:ILE:HG22	1:A:25:ALA:H	1.86	0.41
1:B:152:ARG:NH1	4:B:2621:HOH:O	2.53	0.41
1:C:194:MET:CE	1:C:219:PRO:HG3	2.50	0.41
1:C:24:ILE:HB	1:C:25:ALA:H	1.66	0.41
1:D:432:LEU:C	1:D:432:LEU:HD23	2.41	0.41
1:D:27:ILE:HD12	1:D:79:ALA:HB2	2.03	0.41
1:A:305:LYS:HG2	1:A:323:TRP:CE3	2.56	0.41
1:A:305:LYS:HE2	1:A:320:LEU:HG	2.02	0.41
1:C:337:ILE:HG21	1:C:364:ARG:HH12	1.85	0.41
1:C:405:ASP:N	1:C:405:ASP:OD1	2.54	0.41
1:C:421:GLY:O	1:C:422:SER:HB2	2.21	0.41
1:D:438:PRO:HB3	1:D:444:GLU:CA	2.22	0.41
1:A:426:ARG:HA	1:A:429:ILE:CG1	2.51	0.41
1:A:59:PHE:CD2	1:A:214:GLN:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:HA	1:C:225:THR:O	2.21	0.41
1:C:358:HIS:CD2	1:C:361:LEU:H	2.36	0.41
1:C:337:ILE:HG21	1:C:364:ARG:NH1	2.36	0.41
1:D:217:ILE:O	1:D:218:ALA:C	2.59	0.41
1:A:100:LYS:HZ1	1:A:104:ARG:NH2	2.16	0.41
1:A:259:LEU:HD11	1:A:262:TYR:CD2	2.56	0.41
1:A:358:HIS:C	1:A:362:VAL:HG23	2.39	0.41
1:B:102:LEU:O	1:B:106:LEU:HD22	2.20	0.41
1:B:344:LEU:HD23	1:B:352:ILE:HD11	2.03	0.41
1:B:414:ASN:HA	1:B:437:ARG:O	2.20	0.41
1:C:143:LEU:CD1	1:C:167:ARG:HD2	2.48	0.41
1:C:224:LEU:O	1:C:225:THR:HB	2.21	0.41
1:C:284:LYS:HG2	4:C:2887:HOH:O	2.20	0.41
1:C:361:LEU:HD13	1:C:365:ILE:HD12	2.02	0.41
1:D:282:ARG:NH1	1:D:322:ALA:HA	2.35	0.41
1:D:46:LYS:HE3	1:D:55:ARG:O	2.20	0.41
1:D:68:PHE:HD2	1:D:68:PHE:HA	1.72	0.41
1:A:204:LEU:HD23	1:A:242:VAL:HG21	2.03	0.41
1:A:74:GLU:OE2	1:A:74:GLU:CA	2.66	0.41
1:B:427:GLU:HG2	1:B:428:TYR:N	2.36	0.41
1:C:165:SER:HB2	4:C:2529:HOH:O	2.21	0.41
1:C:331:PHE:CD1	1:C:358:HIS:HB2	2.56	0.41
1:C:340:LEU:HD22	1:C:344:LEU:HD11	2.03	0.41
1:C:409:ASP:O	1:C:410:VAL:HB	2.21	0.41
1:D:167:ARG:O	1:D:168:ILE:HG12	2.21	0.41
1:D:264:ILE:HG22	1:D:265:LYS:N	2.35	0.41
1:D:29:TYR:HB2	1:D:79:ALA:HB1	2.01	0.41
1:D:67:TYR:O	1:D:67:TYR:CD1	2.74	0.41
1:A:344:LEU:HD12	1:A:369:PHE:CE2	2.56	0.40
1:A:29:TYR:N	1:A:79:ALA:HA	2.36	0.40
1:B:285:VAL:HG11	1:B:322:ALA:HB2	2.03	0.40
1:B:71:ASN:O	1:B:72:GLY:C	2.59	0.40
1:C:354:ILE:HG23	1:C:399:VAL:HA	2.03	0.40
1:C:412:ASP:HB2	1:C:437:ARG:CD	2.47	0.40
1:D:226:ALA:HB2	4:D:2283:HOH:O	2.20	0.40
1:A:140:VAL:HG21	1:A:146:ALA:HB2	2.03	0.40
1:C:258:HIS:C	1:C:260:ALA:H	2.24	0.40
1:C:340:LEU:HD22	1:C:344:LEU:CD1	2.51	0.40
1:C:389:GLY:HA3	1:C:395:PHE:CZ	2.57	0.40
1:D:227:THR:CG2	4:D:2756:HOH:O	2.69	0.40
1:B:92:ILE:N	1:B:92:ILE:HD12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:PHE:HB3	1:C:75:PHE:CE2	2.56	0.40
1:C:95:ARG:O	1:C:96:ASP:C	2.60	0.40
1:D:340:LEU:HA	1:D:343:ILE:HD11	2.01	0.40
1:D:361:LEU:HD13	1:D:365:ILE:CG1	2.51	0.40
1:D:264:ILE:HG23	1:D:447:LEU:HD22	2.03	0.40
1:D:66:GLU:C	1:D:68:PHE:N	2.75	0.40
1:A:303:PHE:O	1:A:303:PHE:HD1	2.04	0.40
1:B:122:THR:HG21	1:B:152:ARG:NE	2.36	0.40
1:C:441:GLY:HA3	4:C:3007:HOH:O	2.22	0.40
1:D:250:PHE:HA	1:D:251:PRO:HD3	1.91	0.40
1:D:372:PRO:CG	1:D:398:ILE:HG22	2.51	0.40
1:A:312:TYR:O	1:A:313:ASP:C	2.60	0.40
1:A:430:GLN:O	1:A:431:ARG:C	2.60	0.40
1:A:65:ILE:HA	1:A:65:ILE:HD13	1.93	0.40
1:C:262:TYR:HE1	1:C:264:ILE:HD11	1.86	0.40
1:D:140:VAL:HG22	1:D:177:SER:O	2.22	0.40
1:D:97:TYR:HE1	1:D:259:LEU:HD21	1.86	0.40
1:D:371:ILE:HA	1:D:372:PRO:HD3	1.94	0.40
1:D:430:GLN:O	1:D:431:ARG:C	2.60	0.40
1:D:35:VAL:HG22	1:D:55:ARG:HG3	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2319:HOH:O	4:B:2932:HOH:O[1_455]	1.98	0.22
4:B:2454:HOH:O	4:B:2522:HOH:O[1_655]	2.16	0.04
4:B:2433:HOH:O	4:B:2745:HOH:O[1_455]	2.18	0.02
4:D:2465:HOH:O	4:D:2580:HOH:O[1_655]	2.18	0.02

## 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	432/472 (92%)	343 (79%)	67 (16%)	22 (5%)	2	2
1	B	415/472 (88%)	341 (82%)	57 (14%)	17 (4%)	3	3
1	C	410/472 (87%)	304 (74%)	64 (16%)	42 (10%)	0	0
1	D	422/472 (89%)	313 (74%)	77 (18%)	32 (8%)	1	1
All	All	1679/1888 (89%)	1301 (78%)	265 (16%)	113 (7%)	1	1

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	297	LEU
1	A	307	VAL
1	A	313	ASP
1	A	331	PHE
1	A	440	LYS
1	A	455	THR
1	B	23	MET
1	B	302	ASP
1	B	333	SER
1	B	375	THR
1	B	438	PRO
1	B	443	LYS
1	C	24	ILE
1	C	47	PHE
1	C	61	TYR
1	C	69	GLU
1	C	73	ILE
1	C	255	ALA
1	C	258	HIS
1	C	274	ASP
1	C	284	LYS
1	C	295	ILE
1	C	348	ARG
1	C	379	SER
1	C	394	ARG
1	C	395	PHE
1	C	406	GLU
1	C	408	ILE
1	D	39	ASP
1	D	48	ASP
1	D	346	ARG
1	D	372	PRO

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Mol	Chain	Res	Type
1	D	396	ARG
1	D	410	VAL
1	D	442	LYS
1	A	291	ARG
1	A	294	GLY
1	A	314	GLU
1	A	374	ILE
1	A	378	THR
1	A	379	SER
1	A	394	ARG
1	A	411	PRO
1	B	25	ALA
1	B	360	GLU
1	B	409	ASP
1	B	412	ASP
1	C	25	ALA
1	C	51	SER
1	C	68	PHE
1	C	273	GLU
1	C	282	ARG
1	C	368	VAL
1	C	393	GLY
1	C	419	MET
1	C	420	SER
1	C	426	ARG
1	D	52	GLY
1	D	67	TYR
1	D	72	GLY
1	D	281	LYS
1	D	293	ARG
1	D	310	SER
1	D	319	ALA
1	D	374	ILE
1	D	408	ILE
1	D	458	VAL
1	A	290	LEU
1	A	330	ALA
1	A	444	GLU
1	B	380	ARG
1	C	96	ASP
1	C	131	GLU
1	C	291	ARG

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Mol	Chain	Res	Type
1	C	367	LYS
1	C	443	LYS
1	D	86	PRO
1	D	257	LYS
1	D	426	ARG
1	A	273	GLU
1	A	410	VAL
1	B	397	ALA
1	C	42	VAL
1	C	45	ALA
1	C	53	THR
1	C	333	SER
1	C	371	ILE
1	C	410	VAL
1	D	41	HIS
1	D	46	LYS
1	D	49	SER
1	B	379	SER
1	B	442	LYS
1	C	440	LYS
1	D	259	LEU
1	D	307	VAL
1	D	369	PHE
1	D	407	GLY
1	D	457	GLU
1	A	383	ARG
1	B	374	ILE
1	C	287	LYS
1	C	370	LEU
1	C	403	VAL
1	B	24	ILE
1	D	242	VAL
1	D	306	ILE
1	B	362	VAL
1	A	306	ILE
1	C	417	VAL
1	D	251	PRO
1	D	368	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	366/398 (92%)	333 (91%)	33 (9%)	9	18
1	B	357/398 (90%)	332 (93%)	25 (7%)	15	30
1	C	343/398 (86%)	323 (94%)	20 (6%)	20	40
1	D	349/398 (88%)	314 (90%)	35 (10%)	7	14
All	All	1415/1592 (89%)	1302 (92%)	113 (8%)	12	24

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	69	GLU
1	A	74	GLU
1	A	87	TYR
1	A	106	LEU
1	A	113	ILE
1	A	133	SER
1	A	137	LEU
1	A	153	LEU
1	A	191	ASN
1	A	195	LEU
1	A	221	ARG
1	A	227	THR
1	A	229	GLU
1	A	231	GLU
1	A	293	ARG
1	A	296	THR
1	A	302	ASP
1	A	304	ASN
1	A	308	MET
1	A	314	GLU
1	A	321	ARG
1	A	340	LEU
1	A	346	ARG

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Mol	Chain	Res	Type
1	A	351	LYS
1	A	352	ILE
1	A	358	HIS
1	A	367	LYS
1	A	398	ILE
1	A	411	PRO
1	A	414	ASN
1	A	431	ARG
1	A	442	LYS
1	B	31	ARG
1	B	67	TYR
1	B	106	LEU
1	B	134	THR
1	B	153	LEU
1	B	195	LEU
1	B	227	THR
1	B	232	ASP
1	B	237	ILE
1	B	249	LEU
1	B	252	ASP
1	B	273	GLU
1	B	286	TYR
1	B	289	PHE
1	B	318	GLU
1	B	331	PHE
1	B	345	GLU
1	B	350	ASP
1	B	351	LYS
1	B	362	VAL
1	B	391	ARG
1	B	414	ASN
1	B	430	GLN
1	B	432	LEU
1	B	437	ARG
1	C	24	ILE
1	C	54	TYR
1	C	87	TYR
1	C	93	SER
1	C	106	LEU
1	C	134	THR
1	C	195	LEU
1	C	234	ARG

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Mol	Chain	Res	Type
1	C	259	LEU
1	C	323	TRP
1	C	331	PHE
1	C	338	ARG
1	C	340	LEU
1	C	354	ILE
1	C	356	THR
1	C	369	PHE
1	C	381	GLU
1	C	418	ILE
1	C	426	ARG
1	C	432	LEU
1	D	27	ILE
1	D	57	LEU
1	D	68	PHE
1	D	96	ASP
1	D	114	VAL
1	D	152	ARG
1	D	155	ILE
1	D	195	LEU
1	D	221	ARG
1	D	229	GLU
1	D	232	ASP
1	D	258	HIS
1	D	274	ASP
1	D	284	LYS
1	D	290	LEU
1	D	305	LYS
1	D	306	ILE
1	D	328	ARG
1	D	331	PHE
1	D	346	ARG
1	D	352	ILE
1	D	356	THR
1	D	357	ARG
1	D	358	HIS
1	D	367	LYS
1	D	370	LEU
1	D	392	THR
1	D	394	ARG
1	D	395	PHE
1	D	403	VAL

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Mol	Chain	Res	Type
1	D	404	LEU
1	D	405	ASP
1	D	409	ASP
1	D	440	LYS
1	D	453	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	78	ASN
1	A	185	ASN
1	A	191	ASN
1	A	304	ASN
1	A	335	ASN
1	B	44	HIS
1	B	71	ASN
1	B	130	ASN
1	B	203	HIS
1	B	214	GLN
1	B	359	ASN
1	B	430	GLN
1	C	71	ASN
1	C	78	ASN
1	C	148	GLN
1	C	185	ASN
1	C	332	ASN
1	C	402	GLN
1	D	44	HIS
1	D	78	ASN
1	D	98	GLN
1	D	211	GLN
1	D	359	ASN
1	D	402	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 ⓘ

11 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	$\# Z  > 2$
2	PO4	A	4001	-	4,4,4	1.66	1 (25%)	6,6,6	0.43	0
3	IPA	A	6002	-	3,3,3	0.42	0	3,3,3	0.37	0
2	PO4	B	4002	-	4,4,4	1.68	0	6,6,6	0.42	0
2	PO4	B	4008	-	4,4,4	1.65	1 (25%)	6,6,6	0.40	0
2	PO4	D	4005	-	4,4,4	1.64	0	6,6,6	0.43	0
2	PO4	C	4003	-	4,4,4	1.75	0	6,6,6	0.42	0
2	PO4	D	4006	-	4,4,4	1.61	0	6,6,6	0.48	0
3	IPA	A	6003	-	3,3,3	0.38	0	3,3,3	0.33	0
2	PO4	B	4007	-	4,4,4	1.71	0	6,6,6	0.42	0
2	PO4	D	4004	-	4,4,4	1.81	2 (50%)	6,6,6	0.43	0
3	IPA	A	6001	-	3,3,3	0.42	0	3,3,3	0.38	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4004	PO4	P-O4	-2.07	1.48	1.54
2	B	4008	PO4	P-O3	-2.05	1.48	1.54
2	A	4001	PO4	P-O2	-2.05	1.48	1.54
2	D	4004	PO4	P-O2	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6002	IPA	3	0
2	B	4002	PO4	1	0
3	A	6001	IPA	3	0

## 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	434/472 (91%)	0.06	31 (7%) 16 11	12, 46, 121, 131	0
1	B	423/472 (89%)	-0.03	23 (5%) 25 20	11, 47, 122, 129	0
1	C	414/472 (87%)	0.19	17 (4%) 37 30	19, 68, 120, 132	0
1	D	428/472 (90%)	0.27	37 (8%) 10 7	18, 70, 123, 131	0
All	All	1699/1888 (89%)	0.12	108 (6%) 19 14	11, 58, 122, 132	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	7.2
1	A	291	ARG	6.4
1	C	285	VAL	5.4
1	C	279	TYR	5.4
1	D	52	GLY	5.3
1	D	307	VAL	4.9
1	D	51	SER	4.8
1	D	260	ALA	4.6
1	D	323	TRP	4.6
1	D	308	MET	4.5
1	B	308	MET	4.4
1	C	288	GLN	4.0
1	D	309	ALA	4.0
1	C	286	TYR	3.9
1	A	320	LEU	3.9
1	D	293	ARG	3.9
1	B	287	LYS	3.9
1	B	23	MET	3.8
1	D	288	GLN	3.7
1	A	303	PHE	3.5
1	A	313	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	ALA	3.4
1	D	316	ALA	3.4
1	C	320	LEU	3.4
1	A	390	PHE	3.4
1	B	286	TYR	3.4
1	B	302	ASP	3.3
1	D	296	THR	3.3
1	D	50	ARG	3.2
1	A	323	TRP	3.2
1	D	320	LEU	3.2
1	B	306	ILE	3.2
1	D	294	GLY	3.1
1	D	441	GLY	3.1
1	B	307	VAL	3.1
1	D	281	LYS	3.1
1	B	285	VAL	3.1
1	B	441	GLY	3.1
1	D	256	GLY	3.0
1	B	303	PHE	3.0
1	B	277	VAL	3.0
1	D	319	ALA	3.0
1	B	443	LYS	3.0
1	B	284	LYS	2.9
1	A	298	ARG	2.9
1	D	38	GLY	2.9
1	D	322	ALA	2.9
1	D	279	TYR	2.9
1	A	441	GLY	2.9
1	A	456	GLY	2.9
1	A	317	TYR	2.8
1	D	285	VAL	2.8
1	A	406	GLU	2.8
1	A	301	GLU	2.8
1	A	405	ASP	2.7
1	D	310	SER	2.7
1	D	295	ILE	2.7
1	D	329	ILE	2.7
1	C	23	MET	2.7
1	A	286	TYR	2.7
1	D	286	TYR	2.7
1	C	283	GLU	2.6
1	C	395	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	2.6
1	A	443	LYS	2.6
1	A	396	ARG	2.6
1	D	326	ALA	2.5
1	A	282	ARG	2.5
1	B	439	SER	2.5
1	D	461	ALA	2.5
1	B	390	PHE	2.5
1	A	277	VAL	2.4
1	D	53	THR	2.4
1	A	287	LYS	2.4
1	A	304	ASN	2.4
1	C	281	LYS	2.4
1	B	258	HIS	2.4
1	D	257	LYS	2.4
1	C	408	ILE	2.4
1	D	278	GLU	2.4
1	B	301	GLU	2.3
1	A	297	LEU	2.3
1	C	330	ALA	2.3
1	A	309	ALA	2.3
1	C	325	GLU	2.3
1	A	314	GLU	2.2
1	C	321	ARG	2.2
1	A	279	TYR	2.2
1	A	274	ASP	2.2
1	D	459	ASN	2.2
1	C	318	GLU	2.2
1	D	458	VAL	2.2
1	B	319	ALA	2.2
1	D	395	PHE	2.2
1	B	317	TYR	2.1
1	C	284	LYS	2.1
1	C	254	LEU	2.1
1	A	305	LYS	2.1
1	A	316	ALA	2.1
1	B	395	PHE	2.1
1	D	261	LYS	2.0
1	B	304	ASN	2.0
1	D	284	LYS	2.0
1	A	407	GLY	2.0
1	D	49	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	21	MET	2.0
1	B	289	PHE	2.0
1	C	289	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
2	PO4	A	4001	5/5	0.89	0.16	85,86,87,87	0
2	PO4	D	4005	5/5	0.89	0.23	113,114,114,114	0
2	PO4	B	4007	5/5	0.90	0.20	88,89,90,90	0
2	PO4	D	4006	5/5	0.91	0.16	75,75,76,77	0
2	PO4	B	4008	5/5	0.92	0.17	82,83,84,84	0
3	IPA	A	6003	4/4	0.94	0.19	58,59,59,60	0
3	IPA	A	6001	4/4	0.95	0.15	44,44,45,45	0
3	IPA	A	6002	4/4	0.96	0.10	40,41,41,41	0
2	PO4	D	4004	5/5	0.96	0.15	65,65,66,67	0
2	PO4	B	4002	5/5	0.96	0.12	64,67,67,68	0
2	PO4	C	4003	5/5	0.97	0.12	89,89,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.