



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 AM GMT

PDB ID : 2GK9  
Title : Human Phosphatidylinositol-4-phosphate 5-kinase, type II, gamma  
Authors : Uppenberg, J.; Hogbom, M.; Ogg, D.; Arrowsmith, C.; Berglund, H.; Collins, R.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Holmberg-Schiavone, L.; Edwards, A.; Hammarstrom, M.; Kotenyova, T.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Hallberg, B.M.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-03-31  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

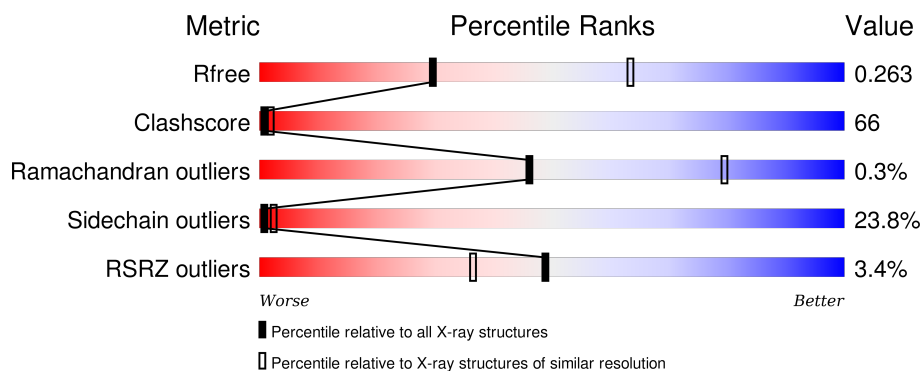
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>14%</div> <div>36%</div> <div>12%</div> <div>38%</div> </div>
1	B	392	<div> <div>3%</div> <div>15%</div> <div>39%</div> <div>10%</div> <div>36%</div> </div>
1	C	392	<div> <div>3%</div> <div>14%</div> <div>39%</div> <div>10%</div> <div>38%</div> </div>
1	D	392	<div> <div>2%</div> <div>15%</div> <div>36%</div> <div>13%</div> <div>36%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8233 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 phosphatidylinositol-4-phosphate 5-kinase, type II, gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			2023	1307	343	362	11			
1	B	250	Total	C	N	O	S	0	0	0
			2084	1345	353	375	11			
1	C	245	Total	C	N	O	S	0	0	0
			2042	1317	347	367	11			
1	D	250	Total	C	N	O	S	0	0	0
			2084	1345	353	375	11			

There are 8 discrepancies between the modelled and reference sequences:

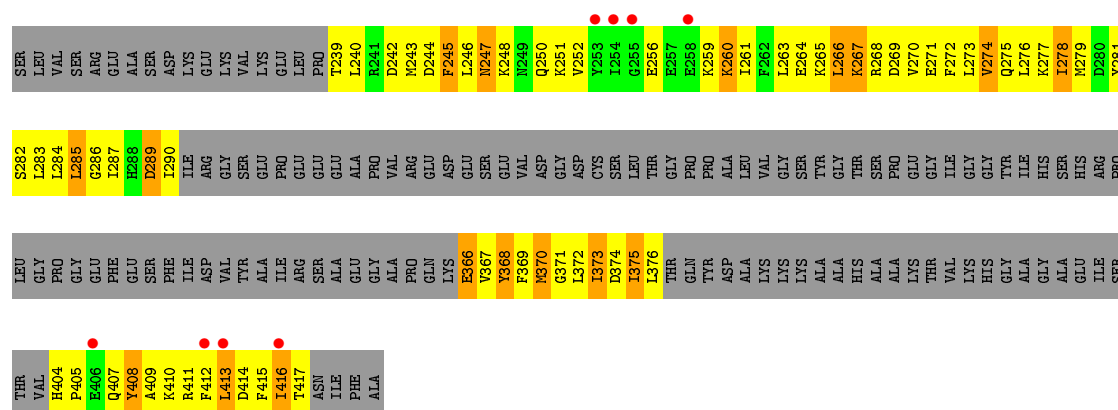
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	cloning artifact	UNP Q8TBX8
A	31	MET	-	cloning artifact	UNP Q8TBX8
B	30	SER	-	cloning artifact	UNP Q8TBX8
B	31	MET	-	cloning artifact	UNP Q8TBX8
C	30	SER	-	cloning artifact	UNP Q8TBX8
C	31	MET	-	cloning artifact	UNP Q8TBX8
D	30	SER	-	cloning artifact	UNP Q8TBX8
D	31	MET	-	cloning artifact	UNP Q8TBX8

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

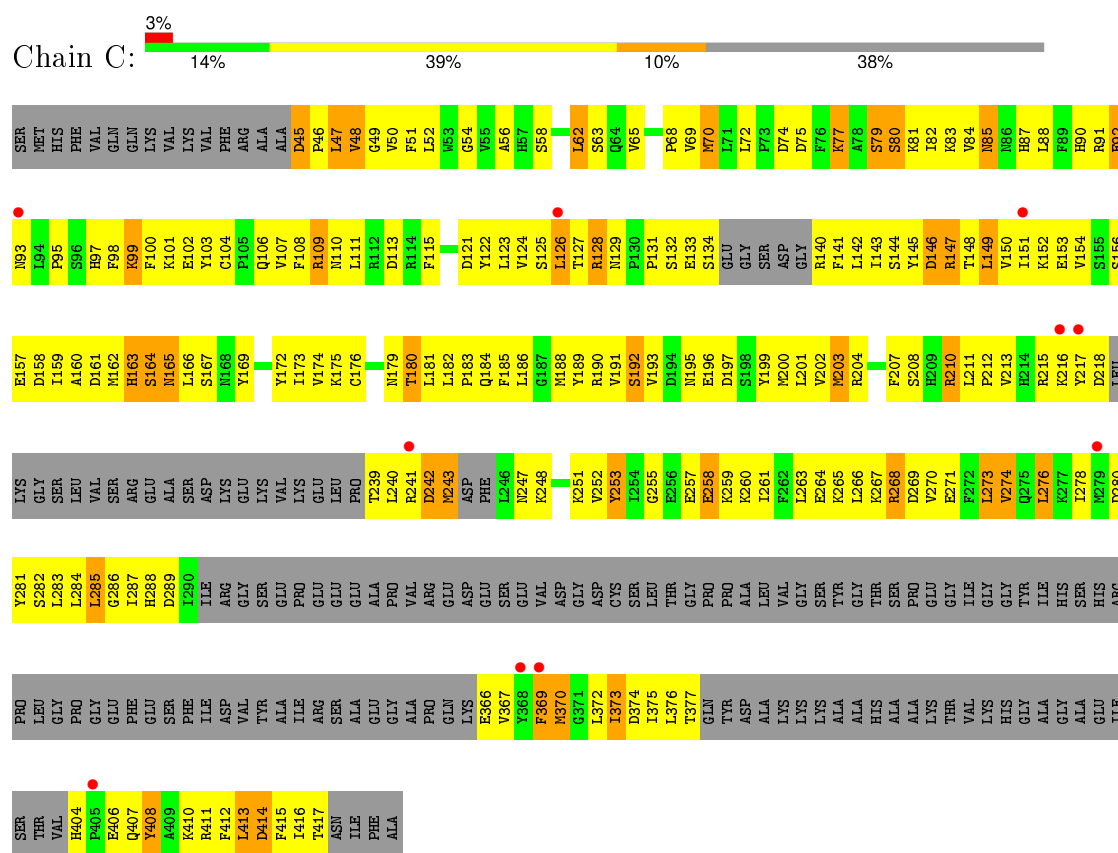
- Chain A: ■ 14% ■ 36% ■ 12% ■ 38%

THR	LEU	S282	L219	S156	N93	SER
VAL	GLY	L283	K220	E157	L94	NET
H404	PRO	L284	G221	D158	P95	HIS
P405	GLY	L285	SER	I159	S96	PHE
E406	GLY	G286	LEU	A160	H97	VAL
Q407	PHE	L287	VAL	D161	F98	GLN
Y408	GLY	H288	SER	H162	K99	GLN
A409	SER	D289	ARG	M163	F100	LYS
K410	PHE	L290	GLU	S164		LYS
R411	ILE	L291	ALA	N165	Y103	VAL
R412	ASP	ARG	SER	L166	G104	VAL
L413	VAL	GLY	ASP	S167	P105	PHE
D414	TYR	SER	LYS	H168	Q106	ARG
F415	ALA	GLU	GLU	H169	V107	ALA
I416	ILE	PRO	LYS	H170	F108	ALA
T417	ILE	PRO	VAL	Q171	R109	
ASN	SER	GLY	LYS	Y172	N110	
ILE	ALA	GLU	GLU	I173	L111	D45
ALA	GLY	ALA	LEU	V174	R112	P46
	GLY	ALA	PRO	K175	D113	L47
	ALA	VAL	T239	G176	R114	V48
	PRO	ARG	L240	H177	F115	V50
	GLN	GLY	R241	G178	G116	F51
	LYS	ASP	D242	H179	I117	L52
	E366	GLU	M243	T180	D118	M53
	V367	SER	D244	L181	D119	G54
	Y368	GLU	PHE	L182	Q120	V55
	F369	VAL	LEU	P183	D121	A56
	M370	ASP	M247	Q184	Y122	H57
	G371	GLY	K248	F185	L123	S58
	L372	ASP		L186	V124	I59
	L373	CYS	Y253	G187	S125	B60
	D374	SER	L254	M188	L126	E61
	I375	LEU	GLY	Y189	T127	L62
	L376	THR	GLU	R190	R128	S63
	THR	GLY	GLU	V191	N129	Q64
	GLN	PRO	GLU	S192		V65
	TYR	PRO	K259	V193	S132	M70
	ASP	ALA	K260	D194	E133	L71
	ALA	LEU	L261	N195	S134	L72
	LYS	VAL	F262	E196	F135	P73
	LYS	GLY	L263	D197	GLY	D74
	LYS	SER	L264	S198	SER	D75
	ALA	TYR	K265	Y199	ASP	F76
	ALA	GLY	L266	M200	GLY	K77
	HIS	THR	K267	L201	ARG	A78
	ALA	SER	R268	V202	F141	S79
	ALA	PRO	D269	K283	L142	S80
	LYS	GLU	V270	R204	L143	R81
	THR	GLY	E271		S144	I82
	VAL	ILE	F272		Y145	K83
	LYS	GLY	L273	H209	D146	V84
	LYS	GLY	V274	R210	R147	M85
	GLY	TYR	Q275	L211	T148	N86
	ALA	ILE	L276	F212		H87
	ALA	ILE	L277	V213		L88
	ALA	SER	K278	H214	I151	F89
	GLU	ALA	I278	R215	K152	H90
	GLU	GLY	R279	R216	E153	R91
	ILE	ARG	D280	Y217	V154	P92
	SER	PRO	Y281	V218	S155	

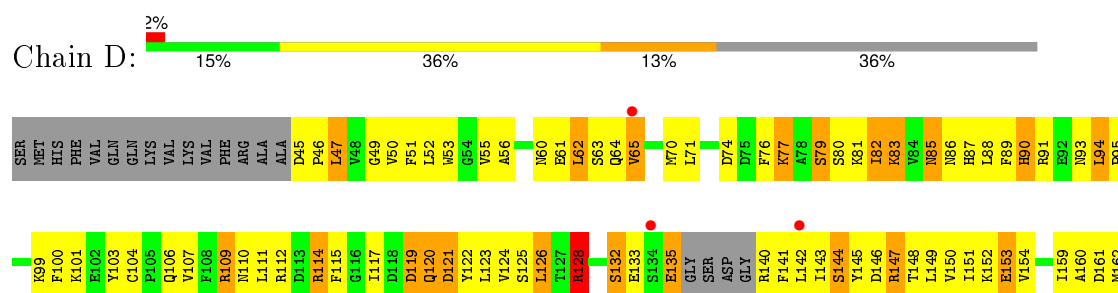
- Chain B:
- 
- | Amino Acid | Frequency (%) |
|------------|---------------|
| SER        | 3%            |
| MET        |               |
| HIS        |               |
| PHE        |               |
| VAL        |               |
| GLN        |               |
| GLY        |               |
| LYS        |               |
| VAL        |               |
| LVS        |               |
| VAL        |               |
| VAL        |               |
| PHE        |               |
| ARG        |               |
| ALA        |               |
| ALA        |               |
| D45        |               |
| P46        |               |
| L47        |               |
| V48        |               |
| G49        |               |
| V50        |               |
| F51        |               |
| L52        |               |
| L53        |               |
| G54        |               |
| V55        |               |
| A56        |               |
| H57        |               |
| S58        |               |
| I59        |               |
| L62        |               |
| S63        |               |
| Q64        |               |
| V65        |               |
| P66        |               |
| P67        |               |
| P68        |               |
| V69        |               |
| M70        |               |
| L71        |               |
| L72        |               |
| P73        |               |
| D74        |               |
| D75        |               |
| F76        |               |
| K77        |               |
| A78        |               |
| S79        |               |
| S80        |               |
| K81        |               |
| I82        |               |
| K83        |               |
| N86        |               |
| H87        |               |
| L88        |               |
| F89        |               |
| R90        |               |
| E92        |               |
| N93        |               |
| L94        |               |
| P95        |               |
| F98        |               |
| R99        |               |
| F100       |               |
| K101       |               |
| M102       |               |
| Y103       |               |
| C104       |               |
| P105       |               |
| Q106       |               |
| V107       |               |
| I108       |               |
| R109       |               |
| H110       |               |
| L111       |               |
| R112       |               |
| N117       |               |
| D113       |               |
| R114       |               |
| I117       |               |
| Q120       |               |
| D121       |               |
| L122       |               |
| L123       |               |
| V124       |               |
| S125       |               |
| L126       |               |
| R127       |               |
| R128       |               |
| S132       |               |
| E133       |               |
| S134       |               |
| E135       |               |
| GLY        |               |
| SER        |               |
| ASP        |               |
| GLY        |               |
| R140       |               |
| F141       |               |
| L142       |               |
| L143       |               |
| S144       |               |
| Y145       |               |
| D146       |               |
| R147       |               |
| T148       |               |
| L149       |               |
| V150       |               |
| I151       |               |
| K152       |               |
| D153       |               |
| V154       |               |
| F157       |               |



• Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma



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H163	L163	H288	GLU	K409
S164	VAL	D289	SER	K410
N165	SER	I290	PHE	R411
L166	ARG	ILE	ILE	F412
S167	GLU	ARG	ASP	L413
N168	ALA	GLY	VAL	D414
Y169	SER	SER	TYR	F415
H170	ASP	GLU	ALA	I416
Q171	LYS	PRO	ILE	T417
Y172	GLU	GLU	ARG	ASN
I173	GLU	GLU	SER	ILE
V174	VAL	ALA	ALA	PHE
K175	LYS	GLU	GLU	ALA
C176	GLU	PRO	GLY	
H177	LEU	VAL	ALA	
G178	PRO	ARG	PRO	
N179	T239	GLN	GLN	
T180	ASP	LYS	LYS	
L181	GLU	E366	E366	
L182	L181	Y367	Y367	
P183	F245	Y368	Y368	
Q184	L246	F369	F369	
F185	VAL	M370	M370	
L186	GLY	G371	G371	
G187	ASP	L372	L372	
M188	Y252	I373	I373	
Y189	G255	D374	D374	
R190	E256	I375	I375	
V191	THR	L376	L376	
S192	GLY	THR	THR	
V193	E257	GLN	GLN	
D194	E258	TYR	TYR	
N195	K259	ASP	ASP	
E196	K260	ALA	ALA	
D197	I281	LYS	LYS	
S198	F262	LYS	LYS	
Y199	L263	LYS	LYS	
M200	E264	ALA	ALA	
L201	K265	ALA	ALA	
V202	L266	HIS	HIS	
M203	K267	ALA	ALA	
R204	D269	ALA	ALA	
N205	V270	LYS	LYS	
M206	E271	THR	THR	
F207	F272	VAL	VAL	
S208	L273	LYS	LYS	
H209	V274	HIS	HIS	
R210	Q275	GLY	GLY	
L211	L276	ALA	ALA	
P212	K277	GLY	GLY	
V213	I278	SER	ALA	
H214	M279	HIS	GLU	
R215	D280	ARG	ILE	
K216	Y281	PRO	SER	
Y217	S282	LEU	THR	
D218	L283	GLY	VAL	
L219	L284	PRO	H404	
K220	L285	GLY	Q407	
G221	G286	GLU	Y408	
SER	I287	PHE		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.39Å 95.39Å 189.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.80) 95.5 (29.74-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.254 , 0.297 0.256 , 0.263	Depositor DCC
$R_{free}$ test set	1894 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 85.7	EDS
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 40811 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.47	0/2068	0.58	4/2784 (0.1%)
1	B	0.47	0/2132	0.52	2/2872 (0.1%)
1	C	0.50	0/2088	0.58	5/2813 (0.2%)
1	D	0.45	0/2132	0.55	1/2872 (0.0%)
All	All	0.47	0/8420	0.56	12/11341 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	253	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	244	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	242	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	414	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	280	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	161	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	45	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	218	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	414	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	414	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	253	TYR	CB-CG-CD1	5.03	124.02	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	MET	Peptide
1	B	91	ARG	Peptide
1	D	128	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2023	0	2012	301	0
1	B	2084	0	2068	279	0
1	C	2042	0	2028	277	0
1	D	2084	0	2068	265	0
All	All	8233	0	8176	1077	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 66.

All (1077) 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:C:266:LEU:CD2	1:C:413:LEU:HD23	1.52	1.39
1:C:176:CYS:SG	1:C:180:THR:HG22	1.65	1.34
1:A:72:LEU:HD21	1:B:95:PRO:CA	1.64	1.25
1:A:72:LEU:CD2	1:B:95:PRO:HA	1.67	1.24
1:D:285:LEU:CD2	1:D:370:MET:HG2	1.66	1.24
1:C:266:LEU:HD23	1:C:413:LEU:CD2	1.68	1.24
1:D:285:LEU:HD23	1:D:370:MET:CG	1.69	1.21
1:D:215:ARG:HG2	1:D:215:ARG:HH11	1.13	1.12
1:B:266:LEU:HD22	1:B:413:LEU:HD23	1.24	1.12
1:D:220:LYS:HD2	1:D:282:SER:HB3	1.30	1.12
1:A:372:LEU:HD21	1:A:412:PHE:CZ	1.85	1.11
1:A:83:LYS:HD2	1:A:99:LYS:HD3	1.20	1.09
1:D:111:LEU:HD21	1:D:173:ILE:HG13	1.28	1.08
1:C:81:LYS:HD3	1:C:190:ARG:HH22	1.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD21	1:B:416:ILE:HD11	1.34	1.07
1:A:72:LEU:HG	1:A:73:PRO:HD2	1.33	1.06
1:C:266:LEU:HD23	1:C:413:LEU:HD23	1.07	1.05
1:D:141:PHE:CE1	1:D:152:LYS:HD2	1.89	1.05
1:B:140:ARG:HG3	1:B:153:GLU:HB3	1.39	1.04
1:D:285:LEU:HD23	1:D:370:MET:HG2	1.10	1.04
1:C:176:CYS:SG	1:C:180:THR:CG2	2.45	1.03
1:B:206:MET:CE	1:B:373:ILE:HG22	1.88	1.03
1:A:103:TYR:HB2	1:A:188:MET:HG2	1.40	1.02
1:C:266:LEU:HD22	1:C:413:LEU:HD23	1.42	1.01
1:D:285:LEU:HD23	1:D:370:MET:CB	1.89	1.01
1:D:111:LEU:CD2	1:D:173:ILE:HG13	1.90	1.01
1:B:126:LEU:HD12	1:B:151:ILE:HD11	1.39	1.01
1:A:266:LEU:CD2	1:A:413:LEU:HD23	1.90	1.01
1:A:47:LEU:HD12	1:A:191:VAL:HG22	1.41	1.01
1:B:283:LEU:HD21	1:B:370:MET:HE2	1.41	1.00
1:C:126:LEU:HD23	1:C:144:SER:HB2	1.45	0.99
1:C:270:VAL:HG11	1:C:413:LEU:HD11	1.45	0.97
1:A:417:THR:CG2	1:A:417:THR:O	2.10	0.97
1:B:83:LYS:HB3	1:C:83:LYS:HB3	1.46	0.97
1:A:417:THR:HG22	1:A:417:THR:O	1.63	0.96
1:B:206:MET:HE3	1:B:373:ILE:HG22	1.47	0.96
1:B:90:HIS:CE1	1:B:92:GLU:H	1.84	0.96
1:B:55:VAL:O	1:B:59:ILE:HG12	1.67	0.94
1:A:90:HIS:NE2	1:A:92:GLU:HB3	1.83	0.94
1:D:289:ASP:HB2	1:D:366:GLU:OE1	1.66	0.94
1:A:124:VAL:O	1:A:128:ARG:HB2	1.68	0.93
1:B:411:ARG:O	1:B:415:PHE:HB2	1.67	0.92
1:D:141:PHE:HE1	1:D:152:LYS:HD2	1.24	0.92
1:A:266:LEU:HD22	1:A:413:LEU:HD23	1.50	0.92
1:C:103:TYR:HB3	1:C:163:HIS:NE2	1.85	0.92
1:D:107:VAL:HG11	1:D:166:LEU:HD11	1.51	0.92
1:D:372:LEU:HD12	1:D:372:LEU:H	1.33	0.91
1:C:70:MET:HE3	1:D:46:PRO:HG3	1.49	0.91
1:C:404:HIS:HB2	1:C:407:GLN:HG3	1.49	0.91
1:D:124:VAL:HG23	1:D:128:ARG:HG3	1.53	0.91
1:C:140:ARG:HG2	1:C:153:GLU:HB3	1.50	0.90
1:A:372:LEU:HD21	1:A:412:PHE:CE2	2.06	0.90
1:B:90:HIS:HE1	1:B:92:GLU:HB3	1.34	0.90
1:D:192:SER:HA	1:D:196:GLU:O	1.69	0.90
1:A:52:LEU:HB3	1:A:127:THR:HG22	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HB3	1:B:190:ARG:HB3	1.50	0.90
1:C:52:LEU:HD23	1:C:127:THR:HA	1.55	0.89
1:B:412:PHE:CZ	1:B:416:ILE:HD13	2.08	0.88
1:B:285:LEU:HD22	1:B:286:GLY:H	1.40	0.86
1:A:281:TYR:HD1	1:A:372:LEU:HD11	1.38	0.86
1:C:80:SER:O	1:C:101:LYS:HA	1.73	0.86
1:D:285:LEU:HD23	1:D:370:MET:HB3	1.56	0.86
1:C:215:ARG:HD3	1:C:217:TYR:OH	1.75	0.86
1:D:258:GLU:HA	1:D:261:ILE:HD13	1.58	0.86
1:B:281:TYR:HA	1:B:374:ASP:HB3	1.59	0.85
1:D:169:TYR:CZ	1:D:173:ILE:HD11	2.11	0.85
1:C:257:GLU:O	1:C:261:ILE:HD12	1.76	0.85
1:A:213:VAL:HG23	1:A:287:ILE:H	1.42	0.84
1:C:267:LYS:HA	1:C:413:LEU:CD2	2.07	0.84
1:B:271:GLU:O	1:B:275:GLN:HG3	1.77	0.84
1:A:47:LEU:CD1	1:A:191:VAL:HG22	2.06	0.84
1:A:372:LEU:CD2	1:A:412:PHE:CZ	2.60	0.83
1:A:288:HIS:HB3	1:A:367:VAL:HB	1.59	0.83
1:D:257:GLU:O	1:D:261:ILE:HD12	1.78	0.83
1:D:273:LEU:HG	1:D:278:ILE:HD12	1.60	0.83
1:B:266:LEU:CD2	1:B:413:LEU:HD23	2.06	0.83
1:C:266:LEU:CD2	1:C:413:LEU:CD2	2.37	0.83
1:A:126:LEU:HD11	1:A:202:VAL:HG11	1.61	0.83
1:D:143:ILE:HG23	1:D:147:ARG:HA	1.60	0.82
1:B:283:LEU:HD21	1:B:370:MET:CE	2.09	0.82
1:A:407:GLN:OE1	1:A:407:GLN:HA	1.80	0.82
1:A:281:TYR:CD1	1:A:372:LEU:HD11	2.15	0.82
1:A:83:LYS:HD2	1:A:99:LYS:CD	2.08	0.82
1:A:217:TYR:H	1:A:285:LEU:HB3	1.44	0.82
1:A:74:ASP:HA	1:A:77:LYS:HE3	1.60	0.82
1:A:366:GLU:HB3	1:A:368:TYR:HE1	1.42	0.81
1:A:274:VAL:HG13	1:A:405:PRO:HB3	1.62	0.81
1:C:99:LYS:HB2	1:C:192:SER:HB2	1.62	0.81
1:B:412:PHE:CZ	1:B:416:ILE:CD1	2.63	0.81
1:A:46:PRO:O	1:A:50:VAL:HG23	1.80	0.81
1:B:273:LEU:HD12	1:B:278:ILE:HG21	1.63	0.81
1:D:218:ASP:OD1	1:D:282:SER:HB2	1.81	0.80
1:D:124:VAL:CG2	1:D:128:ARG:HG3	2.10	0.80
1:D:285:LEU:HD21	1:D:370:MET:HG2	1.62	0.80
1:C:373:ILE:HD13	1:C:374:ASP:N	1.97	0.80
1:D:74:ASP:HA	1:D:77:LYS:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CE1	1:A:184:GLN:HG2	2.17	0.80
1:D:220:LYS:HD2	1:D:282:SER:CB	2.10	0.79
1:A:134:SER:HB2	1:A:143:ILE:HD12	1.62	0.79
1:B:173:ILE:HG23	1:B:178:GLY:HA2	1.63	0.79
1:D:260:LYS:HE3	1:D:264:GLU:OE2	1.82	0.79
1:A:133:GLU:HA	1:A:142:LEU:HA	1.63	0.79
1:C:267:LYS:HA	1:C:413:LEU:HD22	1.62	0.79
1:C:103:TYR:HD1	1:C:188:MET:O	1.66	0.78
1:D:180:THR:OG1	1:D:182:LEU:HB2	1.82	0.78
1:A:279:MET:N	1:A:279:MET:SD	2.51	0.78
1:D:190:ARG:HD3	1:D:199:TYR:CE2	2.18	0.78
1:D:220:LYS:CD	1:D:282:SER:HB3	2.12	0.78
1:C:270:VAL:CG1	1:C:413:LEU:HD11	2.12	0.78
1:A:215:ARG:HB2	1:A:287:ILE:HD12	1.63	0.78
1:B:62:LEU:HD11	1:B:105:PRO:HB3	1.65	0.78
1:D:265:LYS:HG2	1:D:268:ARG:NH2	1.99	0.78
1:C:284:LEU:HB2	1:C:373:ILE:HG21	1.65	0.78
1:B:266:LEU:HD11	1:B:416:ILE:HG13	1.66	0.78
1:C:111:LEU:HD22	1:C:173:ILE:HD13	1.65	0.78
1:B:267:LYS:HG2	1:B:268:ARG:N	1.98	0.78
1:C:81:LYS:HD3	1:C:190:ARG:NH2	1.99	0.78
1:D:255:GLY:O	1:D:259:LYS:HB2	1.84	0.77
1:B:165:ASN:OD1	1:B:169:TYR:HB2	1.84	0.77
1:C:74:ASP:HA	1:C:77:LYS:HG3	1.67	0.77
1:A:72:LEU:HD11	1:B:95:PRO:HG3	1.66	0.77
1:B:286:GLY:O	1:B:368:TYR:HA	1.85	0.77
1:D:170:HIS:O	1:D:174:VAL:HG23	1.84	0.77
1:D:215:ARG:HG2	1:D:215:ARG:NH1	1.91	0.77
1:C:140:ARG:HG3	1:C:140:ARG:HH11	1.48	0.77
1:C:270:VAL:HG11	1:C:413:LEU:CD1	2.15	0.77
1:B:285:LEU:HD23	1:B:370:MET:HB3	1.65	0.76
1:C:255:GLY:HA3	1:C:258:GLU:OE2	1.84	0.76
1:C:288:HIS:O	1:C:366:GLU:HA	1.85	0.76
1:C:83:LYS:HD2	1:C:99:LYS:NZ	2.00	0.76
1:D:417:THR:O	1:D:417:THR:HG22	1.84	0.76
1:A:90:HIS:CD2	1:A:92:GLU:H	2.03	0.76
1:C:285:LEU:HD12	1:C:370:MET:HG2	1.67	0.76
1:D:81:LYS:HD3	1:D:101:LYS:HE3	1.66	0.76
1:B:215:ARG:HB2	1:B:287:ILE:HB	1.68	0.76
1:B:417:THR:O	1:B:417:THR:HG22	1.85	0.76
1:A:72:LEU:HG	1:A:73:PRO:CD	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:MET:O	1:C:166:LEU:HB2	1.85	0.76
1:A:217:TYR:HB3	1:A:219:LEU:HD21	1.68	0.76
1:D:261:ILE:HA	1:D:264:GLU:OE1	1.85	0.76
1:C:126:LEU:CD2	1:C:144:SER:HB2	2.15	0.75
1:B:259:LYS:O	1:B:263:LEU:HG	1.86	0.75
1:C:126:LEU:HD11	1:C:151:ILE:HD11	1.68	0.75
1:D:80:SER:O	1:D:101:LYS:HA	1.86	0.75
1:A:276:LEU:HD12	1:A:278:ILE:HD11	1.68	0.75
1:D:261:ILE:H	1:D:261:ILE:HD12	1.52	0.75
1:A:259:LYS:O	1:A:263:LEU:HD12	1.85	0.75
1:C:287:ILE:HA	1:C:367:VAL:O	1.85	0.75
1:A:62:LEU:HD12	1:D:89:PHE:HZ	1.51	0.75
1:D:266:LEU:HD22	1:D:413:LEU:HD23	1.67	0.75
1:D:372:LEU:HD12	1:D:372:LEU:N	2.02	0.74
1:B:80:SER:O	1:B:101:LYS:HA	1.87	0.74
1:A:154:VAL:O	1:A:199:TYR:HB2	1.86	0.74
1:D:133:GLU:HA	1:D:142:LEU:HD23	1.68	0.74
1:C:411:ARG:O	1:C:415:PHE:HB2	1.87	0.74
1:B:90:HIS:CE1	1:B:92:GLU:HB3	2.18	0.74
1:A:151:ILE:HG23	1:A:202:VAL:HG22	1.69	0.74
1:B:217:TYR:CE2	1:B:240:LEU:HD12	2.22	0.74
1:A:62:LEU:HD23	1:A:109:ARG:NE	2.03	0.74
1:D:65:VAL:HG12	1:D:109:ARG:HH22	1.53	0.74
1:B:94:LEU:HD12	1:B:98:PHE:CE1	2.22	0.74
1:A:404:HIS:HD2	1:A:407:GLN:HG2	1.50	0.74
1:C:45:ASP:HB3	1:C:48:VAL:HG12	1.68	0.74
1:B:83:LYS:HD2	1:C:83:LYS:HD3	1.70	0.73
1:B:107:VAL:HG12	1:B:111:LEU:HD12	1.70	0.73
1:D:122:TYR:O	1:D:126:LEU:HB2	1.88	0.73
1:B:90:HIS:HE1	1:B:92:GLU:CB	2.02	0.73
1:A:165:ASN:O	1:A:169:TYR:CB	2.37	0.73
1:C:270:VAL:HG21	1:C:413:LEU:HG	1.70	0.73
1:A:72:LEU:O	1:A:75:ASP:HB2	1.89	0.73
1:C:70:MET:CE	1:D:46:PRO:HG3	2.17	0.73
1:C:184:GLN:OE1	1:C:204:ARG:HD2	1.89	0.73
1:A:180:THR:HB	1:A:269:ASP:OD1	1.89	0.73
1:B:90:HIS:ND1	1:B:91:ARG:N	2.36	0.72
1:A:59:ILE:HG21	1:A:123:LEU:HB2	1.70	0.72
1:B:171:GLN:O	1:B:174:VAL:HB	1.89	0.72
1:A:412:PHE:CE1	1:A:416:ILE:HG21	2.23	0.72
1:B:412:PHE:CE1	1:B:416:ILE:HD13	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:O	1:B:51:PHE:HB3	1.89	0.72
1:C:108:PHE:HB3	1:C:186:LEU:O	1.90	0.72
1:B:372:LEU:H	1:B:372:LEU:HD12	1.53	0.72
1:C:70:MET:HE2	1:D:93:ASN:O	1.90	0.72
1:B:99:LYS:HB2	1:B:192:SER:HB2	1.72	0.72
1:C:273:LEU:HD11	1:C:281:TYR:CE2	2.24	0.72
1:A:48:VAL:O	1:A:51:PHE:HB3	1.90	0.72
1:A:165:ASN:O	1:A:169:TYR:HB3	1.90	0.72
1:C:273:LEU:HA	1:C:278:ILE:HD12	1.71	0.71
1:A:272:PHE:HA	1:A:275:GLN:OE1	1.89	0.71
1:B:412:PHE:O	1:B:415:PHE:N	2.24	0.71
1:D:89:PHE:O	1:D:91:ARG:HG3	1.90	0.71
1:A:270:VAL:O	1:A:274:VAL:HG23	1.91	0.71
1:B:117:ILE:HD12	1:B:186:LEU:HD22	1.72	0.71
1:D:372:LEU:CD1	1:D:372:LEU:H	2.02	0.71
1:A:215:ARG:CB	1:A:287:ILE:HD12	2.20	0.71
1:D:65:VAL:HG12	1:D:109:ARG:NH2	2.06	0.71
1:A:266:LEU:HD23	1:A:413:LEU:HD23	1.72	0.71
1:C:124:VAL:HG23	1:C:128:ARG:HD3	1.73	0.70
1:C:85:ASN:HB3	1:C:97:HIS:NE2	2.06	0.70
1:C:273:LEU:HD12	1:C:278:ILE:CG2	2.21	0.70
1:B:52:LEU:HD22	1:B:126:LEU:O	1.92	0.70
1:A:90:HIS:NE2	1:A:92:GLU:CB	2.54	0.70
1:D:283:LEU:CD1	1:D:412:PHE:HZ	2.04	0.70
1:B:372:LEU:N	1:B:372:LEU:HD12	2.07	0.70
1:A:53:TRP:HB2	1:A:94:LEU:HD11	1.74	0.70
1:D:212:PRO:HD2	1:D:288:HIS:CE1	2.27	0.69
1:B:265:LYS:HG2	1:B:268:ARG:HH21	1.57	0.69
1:C:412:PHE:CE1	1:C:416:ILE:HD12	2.27	0.69
1:C:126:LEU:HD23	1:C:144:SER:CB	2.22	0.69
1:A:240:LEU:N	1:A:240:LEU:HD23	2.07	0.69
1:A:375:ILE:O	1:A:376:LEU:HD12	1.91	0.69
1:D:210:ARG:HG3	1:D:211:LEU:HD23	1.72	0.69
1:B:269:ASP:O	1:B:272:PHE:HB3	1.91	0.69
1:A:49:GLY:HA2	1:A:52:LEU:HD12	1.74	0.69
1:B:284:LEU:O	1:B:370:MET:HA	1.91	0.69
1:A:281:TYR:CB	1:A:374:ASP:O	2.40	0.69
1:A:134:SER:CB	1:A:143:ILE:HD12	2.23	0.69
1:A:173:ILE:HG23	1:A:178:GLY:HA2	1.74	0.69
1:A:51:PHE:HE2	1:A:151:ILE:HD13	1.57	0.69
1:A:273:LEU:HD23	1:A:278:ILE:HB	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:HD2	1:D:166:LEU:HD21	1.56	0.68
1:A:413:LEU:HA	1:A:416:ILE:CD1	2.23	0.68
1:D:259:LYS:O	1:D:263:LEU:HD12	1.93	0.68
1:B:59:ILE:CB	1:B:123:LEU:HD13	2.24	0.68
1:A:240:LEU:H	1:A:240:LEU:HD23	1.58	0.68
1:A:281:TYR:HB3	1:A:374:ASP:O	1.94	0.68
1:C:81:LYS:CD	1:C:190:ARG:HH22	2.01	0.68
1:C:266:LEU:HD23	1:C:413:LEU:HD21	1.74	0.68
1:B:273:LEU:HB2	1:B:278:ILE:HD12	1.76	0.68
1:D:110:ASN:O	1:D:114:ARG:HD3	1.94	0.68
1:A:220:LYS:HD2	1:A:280:ASP:OD1	1.94	0.68
1:D:47:LEU:HD12	1:D:191:VAL:HG12	1.74	0.68
1:A:107:VAL:HG11	1:A:166:LEU:HD21	1.76	0.67
1:B:141:PHE:CE1	1:B:152:LYS:HB2	2.29	0.67
1:C:284:LEU:O	1:C:370:MET:HA	1.93	0.67
1:A:62:LEU:HD23	1:A:109:ARG:HE	1.57	0.67
1:A:372:LEU:CD2	1:A:412:PHE:HZ	2.05	0.67
1:C:257:GLU:O	1:C:261:ILE:CD1	2.42	0.67
1:D:188:MET:HG3	1:D:201:LEU:HD12	1.74	0.67
1:A:288:HIS:ND1	1:A:367:VAL:HG21	2.10	0.67
1:B:217:TYR:HE2	1:B:240:LEU:HD12	1.59	0.67
1:A:404:HIS:CD2	1:A:407:GLN:HG2	2.29	0.67
1:D:215:ARG:CG	1:D:215:ARG:HH11	1.96	0.67
1:D:55:VAL:HG11	1:D:126:LEU:HD12	1.75	0.67
1:C:273:LEU:HD12	1:C:278:ILE:HG22	1.76	0.67
1:C:140:ARG:HG3	1:C:140:ARG:NH1	2.08	0.67
1:C:404:HIS:HB2	1:C:407:GLN:CG	2.23	0.67
1:A:59:ILE:HD13	1:A:123:LEU:HB2	1.77	0.67
1:B:103:TYR:HB2	1:B:188:MET:HG2	1.75	0.67
1:C:102:GLU:HG3	1:C:189:TYR:CD2	2.30	0.67
1:A:412:PHE:CZ	1:A:416:ILE:HD12	2.30	0.66
1:A:62:LEU:HD21	1:A:109:ARG:HB2	1.76	0.66
1:B:144:SER:HB3	1:B:149:LEU:O	1.96	0.66
1:C:266:LEU:O	1:C:270:VAL:N	2.24	0.66
1:A:373:ILE:HG12	1:A:374:ASP:N	2.11	0.66
1:A:106:GLN:O	1:A:109:ARG:HB3	1.95	0.66
1:C:165:ASN:HB2	1:C:276:LEU:HD22	1.77	0.66
1:B:154:VAL:HB	1:B:158:ASP:OD2	1.95	0.66
1:C:265:LYS:HG2	1:C:268:ARG:NH2	2.10	0.66
1:A:85:ASN:OD1	1:A:97:HIS:HA	1.95	0.66
1:B:103:TYR:CD1	1:B:188:MET:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:O	1:A:82:ILE:HD13	1.94	0.66
1:C:213:VAL:HG22	1:C:369:PHE:CE2	2.31	0.66
1:B:59:ILE:HB	1:B:123:LEU:HD13	1.78	0.65
1:C:416:ILE:O	1:C:416:ILE:HG22	1.96	0.65
1:A:109:ARG:HA	1:A:112:ARG:NH2	2.12	0.65
1:B:244:ASP:HA	1:B:247:ASN:HD21	1.61	0.65
1:A:86:ASN:OD1	1:D:80:SER:HA	1.95	0.65
1:A:172:TYR:OH	1:A:269:ASP:HA	1.96	0.65
1:B:366:GLU:OE1	1:B:368:TYR:HE2	1.78	0.65
1:A:191:VAL:O	1:A:191:VAL:HG22	1.95	0.65
1:A:115:PHE:CD1	1:A:184:GLN:OE1	2.48	0.65
1:A:124:VAL:HG23	1:A:128:ARG:HG3	1.78	0.65
1:D:413:LEU:HA	1:D:416:ILE:HD11	1.78	0.65
1:B:77:LYS:O	1:C:87:HIS:CD2	2.49	0.65
1:B:172:TYR:OH	1:B:268:ARG:NH1	2.30	0.65
1:C:242:ASP:OD2	1:C:243:MET:HG3	1.97	0.65
1:B:184:GLN:OE1	1:B:204:ARG:HD2	1.96	0.65
1:C:265:LYS:HG2	1:C:268:ARG:HH22	1.62	0.64
1:A:88:LEU:HD13	1:D:74:ASP:HB3	1.79	0.64
1:D:265:LYS:HG2	1:D:268:ARG:HH21	1.61	0.64
1:C:45:ASP:OD1	1:C:46:PRO:N	2.30	0.64
1:A:65:VAL:HG23	1:D:90:HIS:CE1	2.32	0.64
1:A:71:LEU:CD1	1:A:107:VAL:HA	2.28	0.64
1:A:254:ILE:O	1:A:254:ILE:HG23	1.97	0.64
1:C:267:LYS:HA	1:C:413:LEU:HD21	1.78	0.64
1:B:162:MET:HG2	1:B:188:MET:SD	2.37	0.64
1:C:273:LEU:HB2	1:C:278:ILE:HD12	1.80	0.64
1:B:151:ILE:HG13	1:B:202:VAL:HG13	1.80	0.64
1:A:213:VAL:HA	1:A:287:ILE:O	1.97	0.64
1:D:410:LYS:HG2	1:D:410:LYS:O	1.97	0.64
1:C:70:MET:HE2	1:C:72:LEU:HG	1.80	0.64
1:D:257:GLU:O	1:D:261:ILE:CD1	2.45	0.64
1:A:211:LEU:HD13	1:A:367:VAL:HG11	1.79	0.64
1:C:216:LYS:HA	1:C:285:LEU:O	1.98	0.63
1:B:77:LYS:O	1:C:87:HIS:HD2	1.81	0.63
1:C:266:LEU:O	1:C:270:VAL:HG23	1.99	0.63
1:C:103:TYR:OH	1:C:190:ARG:HB2	1.98	0.63
1:A:279:MET:CE	1:A:279:MET:H	2.11	0.63
1:A:81:LYS:HB2	1:D:85:ASN:HD22	1.62	0.63
1:C:270:VAL:HB	1:C:413:LEU:HD21	1.79	0.63
1:D:183:PRO:HB2	1:D:185:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:O	1:B:264:GLU:HB2	1.99	0.63
1:B:54:GLY:HA3	1:B:100:PHE:CE1	2.34	0.63
1:A:194:ASP:O	1:A:195:ASN:ND2	2.32	0.63
1:A:62:LEU:HD12	1:D:89:PHE:CZ	2.33	0.63
1:D:191:VAL:HG12	1:D:191:VAL:O	1.98	0.63
1:D:120:GLN:OE1	1:D:120:GLN:HA	1.99	0.63
1:A:124:VAL:HG23	1:A:128:ARG:CG	2.29	0.63
1:C:56:ALA:HA	1:C:123:LEU:HD13	1.80	0.62
1:B:163:HIS:CD2	1:B:188:MET:HE1	2.33	0.62
1:C:266:LEU:HD23	1:C:270:VAL:CG2	2.29	0.62
1:B:206:MET:HE1	1:B:373:ILE:HG22	1.80	0.62
1:A:281:TYR:HA	1:A:374:ASP:HB3	1.79	0.62
1:A:287:ILE:HG12	1:A:368:TYR:CD2	2.34	0.62
1:B:273:LEU:O	1:B:278:ILE:HB	1.98	0.62
1:C:133:GLU:O	1:C:134:SER:CB	2.47	0.62
1:B:112:ARG:HG3	1:B:112:ARG:HH11	1.65	0.62
1:D:133:GLU:HA	1:D:142:LEU:CD2	2.29	0.62
1:C:270:VAL:CG2	1:C:413:LEU:HD21	2.30	0.62
1:A:117:ILE:HD11	1:A:204:ARG:HD2	1.81	0.62
1:B:185:PHE:CD1	1:B:201:LEU:HD21	2.33	0.62
1:B:45:ASP:OD1	1:B:48:VAL:HB	1.99	0.62
1:D:220:LYS:NZ	1:D:280:ASP:OD1	2.33	0.61
1:C:126:LEU:HD11	1:C:151:ILE:CD1	2.29	0.61
1:B:372:LEU:H	1:B:372:LEU:CD1	2.14	0.61
1:C:280:ASP:HA	1:C:408:TYR:CE2	2.35	0.61
1:A:261:ILE:O	1:A:264:GLU:HB2	2.01	0.61
1:D:261:ILE:O	1:D:264:GLU:HB2	2.01	0.61
1:C:70:MET:HE3	1:D:46:PRO:CG	2.27	0.61
1:B:159:ILE:HD12	1:B:188:MET:SD	2.39	0.61
1:B:180:THR:HB	1:B:269:ASP:OD1	2.00	0.61
1:A:120:GLN:O	1:A:124:VAL:HG12	2.01	0.61
1:D:132:SER:O	1:D:142:LEU:HD23	2.00	0.61
1:C:142:LEU:HD12	1:C:200:MET:HE3	1.82	0.61
1:B:63:SER:OG	1:B:64:GLN:OE1	2.18	0.61
1:B:250:GLN:HG3	1:B:251:LYS:H	1.65	0.61
1:B:90:HIS:CD2	1:C:65:VAL:HG22	2.36	0.61
1:C:207:PHE:HD1	1:C:369:PHE:HB2	1.66	0.60
1:A:195:ASN:O	1:A:195:ASN:OD1	2.19	0.60
1:C:179:ASN:O	1:C:265:LYS:HD3	2.00	0.60
1:A:413:LEU:HA	1:A:416:ILE:HD11	1.83	0.60
1:D:181:LEU:HB2	1:D:372:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:HE1	1:D:46:PRO:HA	1.82	0.60
1:D:215:ARG:CG	1:D:215:ARG:NH1	2.59	0.60
1:B:270:VAL:HA	1:B:273:LEU:HD21	1.84	0.60
1:A:141:PHE:N	1:A:152:LYS:HA	2.15	0.60
1:B:108:PHE:HA	1:B:111:LEU:HB2	1.82	0.60
1:B:219:LEU:HD21	1:B:245:PHE:CD2	2.36	0.60
1:B:273:LEU:HD11	1:B:281:TYR:CE1	2.37	0.60
1:B:206:MET:HE3	1:B:373:ILE:CG2	2.28	0.60
1:B:103:TYR:HB2	1:B:188:MET:O	2.02	0.60
1:C:146:ASP:HB3	1:C:148:THR:OG1	2.02	0.60
1:C:154:VAL:O	1:C:199:TYR:HB2	2.01	0.60
1:C:131:PRO:HB3	1:C:144:SER:HA	1.82	0.60
1:C:102:GLU:HG3	1:C:189:TYR:CE2	2.37	0.60
1:C:270:VAL:HA	1:C:273:LEU:CD2	2.32	0.60
1:A:47:LEU:HD11	1:A:198:SER:HB2	1.83	0.60
1:B:167:SER:O	1:B:170:HIS:HB3	2.02	0.60
1:D:283:LEU:HD12	1:D:412:PHE:HZ	1.66	0.60
1:B:216:LYS:HB2	1:B:285:LEU:O	2.02	0.60
1:A:276:LEU:HB2	1:A:278:ILE:HG13	1.83	0.59
1:A:266:LEU:HD21	1:A:412:PHE:CE2	2.36	0.59
1:C:201:LEU:HD23	1:C:202:VAL:N	2.17	0.59
1:A:286:GLY:O	1:A:368:TYR:HA	2.01	0.59
1:C:270:VAL:HG21	1:C:413:LEU:CG	2.32	0.59
1:D:104:CYS:CB	1:D:107:VAL:HB	2.32	0.59
1:D:274:VAL:HG12	1:D:275:GLN:N	2.16	0.59
1:A:286:GLY:N	1:A:369:PHE:O	2.35	0.59
1:D:176:CYS:SG	1:D:180:THR:HG22	2.42	0.59
1:B:193:VAL:O	1:B:196:GLU:HG3	2.01	0.59
1:B:112:ARG:HG3	1:B:112:ARG:NH1	2.18	0.59
1:C:287:ILE:HG21	1:C:366:GLU:OE2	2.03	0.59
1:B:82:ILE:HD12	1:C:84:VAL:HG22	1.84	0.59
1:A:410:LYS:HG2	1:A:410:LYS:O	2.01	0.59
1:A:103:TYR:HB2	1:A:188:MET:CG	2.26	0.59
1:C:72:LEU:O	1:C:75:ASP:HB2	2.02	0.59
1:C:207:PHE:CD1	1:C:213:VAL:HG21	2.38	0.59
1:B:260:LYS:O	1:B:263:LEU:HB2	2.02	0.59
1:B:285:LEU:HD22	1:B:286:GLY:N	2.13	0.59
1:B:50:VAL:HG21	1:B:98:PHE:HB2	1.85	0.59
1:C:210:ARG:O	1:C:212:PRO:HD3	2.03	0.59
1:A:59:ILE:HD13	1:A:123:LEU:CB	2.33	0.59
1:C:133:GLU:HG2	1:C:134:SER:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:HIS:O	1:B:88:LEU:HB2	2.02	0.59
1:B:103:TYR:CB	1:B:188:MET:HG2	2.32	0.59
1:A:182:LEU:HD22	1:A:375:ILE:HG21	1.84	0.58
1:B:59:ILE:HG13	1:B:123:LEU:CD1	2.32	0.58
1:A:155:SER:O	1:A:158:ASP:HB2	2.03	0.58
1:D:62:LEU:O	1:D:109:ARG:NH2	2.36	0.58
1:D:47:LEU:HD11	1:D:200:MET:HE1	1.84	0.58
1:B:273:LEU:HD23	1:B:273:LEU:H	1.68	0.58
1:B:51:PHE:HE2	1:B:151:ILE:HD13	1.68	0.58
1:B:281:TYR:HB3	1:B:375:ILE:HG22	1.85	0.58
1:A:266:LEU:HD23	1:A:413:LEU:CD2	2.33	0.58
1:B:143:ILE:HG23	1:B:147:ARG:HA	1.83	0.58
1:C:287:ILE:HG23	1:C:366:GLU:HB3	1.85	0.58
1:C:46:PRO:O	1:C:193:VAL:HG21	2.03	0.58
1:C:270:VAL:HG21	1:C:413:LEU:CD2	2.34	0.58
1:D:288:HIS:HB3	1:D:367:VAL:HB	1.85	0.58
1:A:87:HIS:O	1:A:88:LEU:HB2	2.02	0.58
1:B:99:LYS:HB2	1:B:192:SER:CB	2.33	0.58
1:A:146:ASP:HB3	1:A:148:THR:OG1	2.04	0.58
1:A:375:ILE:HG13	1:A:376:LEU:HD12	1.85	0.58
1:D:115:PHE:HZ	1:D:169:TYR:HH	1.52	0.58
1:B:206:MET:CE	1:B:373:ILE:CG2	2.74	0.58
1:A:156:SER:HB2	1:A:199:TYR:CZ	2.38	0.58
1:A:115:PHE:CZ	1:A:184:GLN:HG2	2.38	0.58
1:B:143:ILE:CG2	1:B:147:ARG:HA	2.34	0.58
1:A:274:VAL:HG13	1:A:405:PRO:CB	2.33	0.57
1:C:103:TYR:CD1	1:C:188:MET:HG2	2.39	0.57
1:A:417:THR:HG23	1:A:417:THR:O	2.00	0.57
1:D:276:LEU:HB2	1:D:278:ILE:HG13	1.85	0.57
1:C:124:VAL:HG23	1:C:128:ARG:HB2	1.86	0.57
1:A:76:PHE:CD2	1:A:166:LEU:HD23	2.39	0.57
1:B:56:ALA:HA	1:B:123:LEU:HD11	1.86	0.57
1:B:102:GLU:OE2	1:B:105:PRO:HA	2.04	0.57
1:C:265:LYS:HA	1:C:268:ARG:NH1	2.18	0.57
1:C:268:ARG:HG3	1:C:269:ASP:N	2.19	0.57
1:B:263:LEU:O	1:B:264:GLU:C	2.42	0.57
1:B:265:LYS:CG	1:B:268:ARG:HH21	2.17	0.57
1:B:270:VAL:HG11	1:B:413:LEU:HD11	1.86	0.57
1:C:169:TYR:CE2	1:C:173:ILE:HD11	2.40	0.57
1:B:74:ASP:HB3	1:C:88:LEU:HD13	1.87	0.57
1:C:266:LEU:HD23	1:C:270:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG21	1:B:123:LEU:HB2	1.86	0.57
1:C:121:ASP:O	1:C:125:SER:HB2	2.04	0.57
1:A:366:GLU:HB3	1:A:368:TYR:CE1	2.33	0.57
1:A:154:VAL:HB	1:A:158:ASP:CB	2.35	0.57
1:B:76:PHE:CE2	1:B:167:SER:HA	2.39	0.57
1:B:120:GLN:O	1:B:124:VAL:HG12	2.05	0.57
1:D:212:PRO:HD2	1:D:288:HIS:ND1	2.20	0.57
1:A:217:TYR:CD1	1:A:285:LEU:HD12	2.40	0.57
1:B:412:PHE:CE2	1:B:416:ILE:CD1	2.88	0.57
1:D:111:LEU:HD23	1:D:173:ILE:HG21	1.85	0.57
1:A:52:LEU:CD2	1:A:127:THR:HA	2.35	0.57
1:C:169:TYR:CZ	1:C:173:ILE:HD11	2.40	0.57
1:B:103:TYR:CG	1:B:188:MET:HG2	2.39	0.56
1:A:165:ASN:O	1:A:169:TYR:HB2	2.05	0.56
1:D:181:LEU:HB2	1:D:372:LEU:CD1	2.34	0.56
1:B:54:GLY:HA3	1:B:100:PHE:CZ	2.40	0.56
1:D:47:LEU:HD12	1:D:191:VAL:CG1	2.35	0.56
1:B:146:ASP:O	1:B:148:THR:HG23	2.04	0.56
1:B:59:ILE:HG13	1:B:123:LEU:HD12	1.87	0.56
1:C:70:MET:CE	1:C:72:LEU:HG	2.36	0.56
1:A:169:TYR:O	1:A:173:ILE:HG12	2.04	0.56
1:B:81:LYS:HA	1:B:100:PHE:O	2.05	0.56
1:B:146:ASP:HB3	1:B:148:THR:OG1	2.05	0.56
1:A:70:MET:CE	1:B:46:PRO:HA	2.35	0.56
1:D:169:TYR:CE1	1:D:173:ILE:HD11	2.41	0.56
1:D:271:GLU:O	1:D:274:VAL:HB	2.05	0.56
1:B:172:TYR:OH	1:B:269:ASP:OD1	2.20	0.56
1:B:90:HIS:ND1	1:B:92:GLU:N	2.48	0.56
1:B:71:LEU:HD22	1:B:75:ASP:OD2	2.06	0.56
1:A:268:ARG:HG3	1:A:269:ASP:N	2.20	0.56
1:D:83:LYS:HD2	1:D:99:LYS:CE	2.35	0.56
1:C:215:ARG:O	1:C:286:GLY:HA2	2.05	0.56
1:A:217:TYR:HB2	1:A:285:LEU:CB	2.35	0.56
1:A:217:TYR:HB3	1:A:219:LEU:CD2	2.35	0.56
1:A:276:LEU:HB2	1:A:278:ILE:CG1	2.35	0.56
1:B:56:ALA:HA	1:B:123:LEU:CD1	2.36	0.56
1:C:50:VAL:CG1	1:C:191:VAL:HG23	2.36	0.56
1:C:242:ASP:OD1	1:C:415:PHE:CZ	2.58	0.56
1:A:268:ARG:O	1:A:271:GLU:HB3	2.06	0.56
1:C:50:VAL:HG11	1:C:191:VAL:HG23	1.87	0.56
1:D:161:ASP:HA	1:D:164:SER:OG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:CG2	1:A:123:LEU:HD22	2.35	0.56
1:B:173:ILE:HG23	1:B:178:GLY:CA	2.35	0.56
1:B:50:VAL:HG22	1:B:98:PHE:CD2	2.41	0.56
1:A:49:GLY:HA2	1:A:52:LEU:CD1	2.35	0.55
1:A:216:LYS:HA	1:A:285:LEU:O	2.06	0.55
1:C:45:ASP:OD1	1:C:46:PRO:CD	2.54	0.55
1:A:54:GLY:HA3	1:A:100:PHE:CE1	2.40	0.55
1:D:209:HIS:CD2	1:D:209:HIS:H	2.24	0.55
1:A:47:LEU:HD12	1:A:191:VAL:CG2	2.27	0.55
1:D:81:LYS:HA	1:D:100:PHE:O	2.07	0.55
1:D:375:ILE:O	1:D:376:LEU:HD23	2.05	0.55
1:B:366:GLU:O	1:B:368:TYR:CZ	2.59	0.55
1:A:83:LYS:CD	1:A:99:LYS:HD3	2.15	0.55
1:B:141:PHE:CD1	1:B:152:LYS:HB2	2.41	0.55
1:C:123:LEU:HD12	1:C:127:THR:OG1	2.06	0.55
1:B:102:GLU:OE1	1:B:105:PRO:HG3	2.07	0.55
1:B:117:ILE:CD1	1:B:186:LEU:HD22	2.37	0.55
1:A:90:HIS:CD2	1:A:92:GLU:N	2.73	0.55
1:D:259:LYS:C	1:D:263:LEU:HD12	2.26	0.55
1:C:115:PHE:CD2	1:C:184:GLN:HB3	2.41	0.55
1:D:81:LYS:CD	1:D:101:LYS:HE3	2.35	0.55
1:B:271:GLU:HA	1:B:274:VAL:HB	1.89	0.55
1:B:189:TYR:CD1	1:B:189:TYR:N	2.74	0.55
1:D:276:LEU:O	1:D:277:LYS:HB2	2.07	0.55
1:B:106:GLN:OE1	1:B:106:GLN:HA	2.06	0.55
1:A:88:LEU:HD13	1:D:74:ASP:CB	2.37	0.54
1:C:208:SER:HB3	1:C:211:LEU:O	2.07	0.54
1:A:71:LEU:HD11	1:A:107:VAL:HA	1.89	0.54
1:D:115:PHE:HB3	1:D:117:ILE:HD12	1.88	0.54
1:C:104:CYS:HB3	1:C:107:VAL:CG2	2.38	0.54
1:C:70:MET:HE1	1:D:46:PRO:CA	2.37	0.54
1:A:117:ILE:HD12	1:A:186:LEU:CD2	2.37	0.54
1:D:245:PHE:CD1	1:D:250:GLN:HB2	2.42	0.54
1:D:51:PHE:CE2	1:D:151:ILE:HD13	2.41	0.54
1:C:267:LYS:O	1:C:271:GLU:OE1	2.25	0.54
1:B:281:TYR:CB	1:B:375:ILE:HG22	2.38	0.54
1:D:188:MET:HG3	1:D:201:LEU:CD1	2.37	0.54
1:D:183:PRO:HB2	1:D:185:PHE:CZ	2.43	0.54
1:C:103:TYR:CD1	1:C:188:MET:O	2.54	0.54
1:B:122:TYR:CE1	1:B:149:LEU:HD13	2.42	0.54
1:C:259:LYS:O	1:C:263:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HD22	1:D:204:ARG:HA	1.89	0.54
1:A:259:LYS:C	1:A:263:LEU:HD12	2.28	0.54
1:B:147:ARG:HH11	1:B:147:ARG:HG2	1.72	0.54
1:A:70:MET:HE3	1:B:46:PRO:HA	1.88	0.54
1:A:114:ARG:CZ	1:A:174:VAL:HG13	2.38	0.54
1:D:187:GLY:HA3	1:D:202:VAL:HB	1.89	0.54
1:A:78:ALA:HB2	1:D:88:LEU:HB2	1.90	0.54
1:A:70:MET:HG2	1:A:70:MET:O	2.07	0.54
1:D:287:ILE:HA	1:D:367:VAL:O	2.07	0.54
1:A:151:ILE:CG2	1:A:202:VAL:HG22	2.38	0.54
1:C:216:LYS:O	1:C:216:LYS:HG2	2.08	0.53
1:A:52:LEU:HD23	1:A:127:THR:HA	1.90	0.53
1:B:216:LYS:HA	1:B:285:LEU:O	2.07	0.53
1:B:82:ILE:CD1	1:C:84:VAL:HG22	2.38	0.53
1:C:412:PHE:CE1	1:C:416:ILE:CD1	2.91	0.53
1:B:90:HIS:CE1	1:B:92:GLU:N	2.66	0.53
1:D:143:ILE:CG2	1:D:147:ARG:HA	2.36	0.53
1:A:284:LEU:O	1:A:370:MET:HA	2.08	0.53
1:B:89:PHE:HE1	1:C:106:GLN:HG2	1.71	0.53
1:D:104:CYS:HB3	1:D:107:VAL:CG2	2.39	0.53
1:C:45:ASP:OD1	1:C:46:PRO:HD2	2.08	0.53
1:A:272:PHE:HA	1:A:275:GLN:CD	2.28	0.53
1:B:176:CYS:O	1:B:179:ASN:OD1	2.26	0.53
1:B:273:LEU:HB2	1:B:278:ILE:CB	2.39	0.53
1:A:74:ASP:HA	1:A:77:LYS:CG	2.38	0.53
1:B:185:PHE:CE1	1:B:201:LEU:HD21	2.43	0.53
1:A:59:ILE:HD11	1:A:122:TYR:CD2	2.44	0.53
1:A:215:ARG:HB2	1:A:287:ILE:HB	1.90	0.53
1:B:74:ASP:HA	1:B:77:LYS:HG3	1.90	0.53
1:C:195:ASN:OD1	1:C:195:ASN:O	2.27	0.53
1:C:270:VAL:CB	1:C:413:LEU:HD21	2.39	0.53
1:B:240:LEU:HB3	1:B:244:ASP:HB2	1.89	0.53
1:B:273:LEU:HD23	1:B:273:LEU:N	2.24	0.53
1:D:50:VAL:HA	1:D:94:LEU:HD22	1.88	0.53
1:C:172:TYR:CE2	1:C:176:CYS:HB2	2.43	0.53
1:D:242:ASP:HB2	1:D:415:PHE:HZ	1.74	0.53
1:A:74:ASP:O	1:D:88:LEU:HD13	2.08	0.53
1:D:182:LEU:HD11	1:D:272:PHE:CD2	2.43	0.53
1:D:220:LYS:NZ	1:D:280:ASP:OD2	2.42	0.53
1:A:117:ILE:HD12	1:A:186:LEU:HD21	1.89	0.53
1:D:104:CYS:HB2	1:D:107:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:THR:CG2	1:B:417:THR:O	2.57	0.53
1:C:115:PHE:CG	1:C:184:GLN:HB3	2.44	0.53
1:D:115:PHE:CE1	1:D:184:GLN:HG2	2.44	0.52
1:A:281:TYR:HA	1:A:374:ASP:O	2.09	0.52
1:C:51:PHE:CE2	1:C:151:ILE:HD13	2.43	0.52
1:C:70:MET:CE	1:D:46:PRO:CG	2.84	0.52
1:A:52:LEU:CB	1:A:127:THR:HG22	2.34	0.52
1:B:54:GLY:HA3	1:B:100:PHE:CD1	2.43	0.52
1:B:147:ARG:NH1	1:B:147:ARG:HG2	2.23	0.52
1:A:126:LEU:CD1	1:A:202:VAL:HG11	2.36	0.52
1:C:273:LEU:CA	1:C:278:ILE:HD12	2.37	0.52
1:A:72:LEU:HD11	1:B:95:PRO:CG	2.37	0.52
1:B:273:LEU:HD12	1:B:278:ILE:CG2	2.38	0.52
1:B:220:LYS:HG3	1:B:282:SER:OG	2.08	0.52
1:B:287:ILE:HA	1:B:367:VAL:O	2.10	0.52
1:A:273:LEU:O	1:A:273:LEU:HD23	2.09	0.52
1:B:169:TYR:CZ	1:B:185:PHE:HD2	2.28	0.52
1:C:84:VAL:O	1:C:97:HIS:HA	2.10	0.52
1:A:57:HIS:O	1:A:61:GLU:HB2	2.09	0.52
1:D:262:PHE:CE2	1:D:266:LEU:HD12	2.44	0.52
1:A:106:GLN:HA	1:A:106:GLN:OE1	2.10	0.52
1:D:65:VAL:HG12	1:D:109:ARG:CZ	2.39	0.52
1:B:103:TYR:HB3	1:B:188:MET:HE2	1.91	0.52
1:D:195:ASN:OD1	1:D:195:ASN:O	2.28	0.52
1:C:47:LEU:HG	1:C:48:VAL:N	2.23	0.52
1:D:150:VAL:HG23	1:D:205:ASN:HB2	1.90	0.52
1:A:72:LEU:HD21	1:B:95:PRO:HA	0.73	0.52
1:D:170:HIS:NE2	1:D:174:VAL:HG22	2.25	0.52
1:D:242:ASP:HB2	1:D:415:PHE:CZ	2.45	0.52
1:D:135:GLU:HA	1:D:135:GLU:OE1	2.09	0.52
1:C:92:GLU:HG3	1:C:92:GLU:O	2.10	0.52
1:C:266:LEU:HD21	1:C:412:PHE:CE2	2.45	0.52
1:C:143:ILE:CG2	1:C:147:ARG:HA	2.40	0.52
1:C:267:LYS:CA	1:C:413:LEU:HD22	2.36	0.51
1:A:107:VAL:HG11	1:A:166:LEU:CD2	2.40	0.51
1:C:142:LEU:HD12	1:C:200:MET:CE	2.40	0.51
1:C:70:MET:CE	1:D:93:ASN:O	2.57	0.51
1:D:180:THR:HG1	1:D:182:LEU:H	1.58	0.51
1:B:71:LEU:HD12	1:B:170:HIS:CE1	2.44	0.51
1:B:218:ASP:HB2	1:B:239:THR:CG2	2.40	0.51
1:A:162:MET:HE1	1:A:185:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:LYS:CG	1:C:99:LYS:HE3	2.41	0.51
1:D:104:CYS:HB3	1:D:107:VAL:HB	1.91	0.51
1:A:217:TYR:N	1:A:285:LEU:HB3	2.20	0.51
1:A:209:HIS:H	1:A:209:HIS:CD2	2.26	0.51
1:B:283:LEU:HD13	1:B:416:ILE:HD12	1.91	0.51
1:A:59:ILE:HD13	1:A:123:LEU:HA	1.92	0.51
1:A:54:GLY:HA3	1:A:100:PHE:CD1	2.46	0.51
1:C:285:LEU:HD12	1:C:370:MET:CG	2.38	0.51
1:C:267:LYS:CA	1:C:413:LEU:CD2	2.86	0.51
1:D:270:VAL:HG13	1:D:281:TYR:OH	2.10	0.51
1:B:149:LEU:HD22	1:B:186:LEU:CD1	2.40	0.51
1:D:268:ARG:HG3	1:D:269:ASP:N	2.26	0.51
1:A:173:ILE:HG23	1:A:178:GLY:CA	2.40	0.51
1:A:274:VAL:CG1	1:A:405:PRO:HB3	2.36	0.51
1:C:104:CYS:SG	1:C:163:HIS:CE1	3.04	0.51
1:D:283:LEU:HD13	1:D:412:PHE:HZ	1.73	0.51
1:B:54:GLY:O	1:B:57:HIS:HB3	2.11	0.51
1:B:220:LYS:HE3	1:B:282:SER:OG	2.11	0.51
1:A:133:GLU:HG3	1:A:142:LEU:HD23	1.93	0.51
1:C:414:ASP:O	1:C:417:THR:HG22	2.09	0.51
1:A:220:LYS:NZ	1:A:220:LYS:HB2	2.26	0.51
1:C:159:ILE:HD12	1:C:188:MET:SD	2.51	0.51
1:D:83:LYS:HD2	1:D:99:LYS:HE3	1.92	0.51
1:C:79:SER:HB2	1:C:101:LYS:HE2	1.92	0.51
1:D:283:LEU:HD12	1:D:372:LEU:HG	1.93	0.51
1:B:287:ILE:HG23	1:B:366:GLU:HB2	1.92	0.51
1:A:51:PHE:CE2	1:A:126:LEU:HD21	2.46	0.51
1:D:273:LEU:HA	1:D:278:ILE:HD12	1.93	0.51
1:D:150:VAL:HG23	1:D:205:ASN:CB	2.41	0.51
1:D:193:VAL:HG12	1:D:193:VAL:O	2.10	0.51
1:D:408:TYR:O	1:D:411:ARG:HB2	2.11	0.51
1:A:273:LEU:O	1:A:278:ILE:HB	2.11	0.51
1:C:83:LYS:HD2	1:C:99:LYS:HZ2	1.73	0.51
1:C:215:ARG:HG2	1:C:215:ARG:HH11	1.76	0.51
1:A:146:ASP:OD1	1:A:148:THR:HG23	2.11	0.51
1:C:161:ASP:HA	1:C:164:SER:OG	2.11	0.50
1:C:162:MET:HG3	1:C:188:MET:SD	2.51	0.50
1:A:74:ASP:CA	1:A:77:LYS:HE3	2.35	0.50
1:C:121:ASP:HA	1:C:124:VAL:HG12	1.93	0.50
1:C:122:TYR:OH	1:C:202:VAL:HG21	2.11	0.50
1:D:262:PHE:CZ	1:D:266:LEU:HD12	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:HG12	1:B:275:GLN:N	2.26	0.50
1:A:411:ARG:O	1:A:415:PHE:HB2	2.11	0.50
1:C:416:ILE:O	1:C:416:ILE:CG2	2.59	0.50
1:C:268:ARG:HH11	1:C:268:ARG:HG2	1.75	0.50
1:A:78:ALA:CB	1:D:88:LEU:HB2	2.41	0.50
1:A:93:ASN:OD1	1:A:94:LEU:HG	2.10	0.50
1:D:417:THR:O	1:D:417:THR:CG2	2.56	0.50
1:C:149:LEU:HD13	1:C:186:LEU:HD12	1.94	0.50
1:B:217:TYR:CD2	1:B:240:LEU:HD12	2.46	0.50
1:B:273:LEU:HD11	1:B:281:TYR:CD1	2.46	0.50
1:C:192:SER:HB3	1:C:197:ASP:OD1	2.11	0.50
1:B:71:LEU:HD11	1:B:107:VAL:HA	1.93	0.50
1:A:80:SER:OG	1:A:80:SER:O	2.26	0.50
1:C:172:TYR:OH	1:C:268:ARG:NE	2.45	0.50
1:B:176:CYS:SG	1:B:180:THR:HG22	2.51	0.50
1:A:288:HIS:HB3	1:A:367:VAL:CB	2.37	0.50
1:A:132:SER:O	1:A:143:ILE:N	2.45	0.50
1:A:176:CYS:SG	1:A:180:THR:HG22	2.52	0.50
1:C:58:SER:O	1:C:62:LEU:HB2	2.12	0.50
1:A:76:PHE:CE2	1:A:167:SER:HA	2.46	0.50
1:D:124:VAL:CG1	1:D:125:SER:N	2.75	0.50
1:D:121:ASP:HA	1:D:124:VAL:HG12	1.92	0.50
1:A:146:ASP:O	1:A:146:ASP:OD1	2.29	0.50
1:A:65:VAL:HG21	1:D:90:HIS:HA	1.92	0.49
1:D:56:ALA:O	1:D:60:ASN:OD1	2.30	0.49
1:C:90:HIS:O	1:C:91:ARG:HB2	2.12	0.49
1:B:141:PHE:HE1	1:B:152:LYS:HB2	1.73	0.49
1:D:87:HIS:CD2	1:D:88:LEU:HG	2.47	0.49
1:C:278:ILE:HG21	1:C:375:ILE:HG23	1.94	0.49
1:B:266:LEU:HD11	1:B:416:ILE:CG1	2.38	0.49
1:A:124:VAL:HG23	1:A:128:ARG:CD	2.43	0.49
1:D:266:LEU:HD11	1:D:416:ILE:HD12	1.94	0.49
1:B:70:MET:HE2	1:B:72:LEU:HG	1.93	0.49
1:C:273:LEU:O	1:C:278:ILE:HB	2.12	0.49
1:B:219:LEU:HD21	1:B:245:PHE:CE2	2.47	0.49
1:B:90:HIS:CD2	1:C:65:VAL:CG2	2.95	0.49
1:D:124:VAL:O	1:D:128:ARG:HB2	2.12	0.49
1:A:112:ARG:HH11	1:A:112:ARG:HG3	1.77	0.49
1:D:180:THR:HG1	1:D:182:LEU:HB2	1.76	0.49
1:A:57:HIS:CE1	1:A:82:ILE:HG13	2.46	0.49
1:C:107:VAL:O	1:C:110:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:CG2	1:C:128:ARG:HD3	2.40	0.49
1:D:168:ASN:O	1:D:171:GLN:HB2	2.12	0.49
1:C:270:VAL:HA	1:C:273:LEU:HD23	1.94	0.49
1:C:72:LEU:HD23	1:D:95:PRO:HA	1.94	0.49
1:A:126:LEU:HD23	1:A:126:LEU:O	2.12	0.49
1:A:217:TYR:HB2	1:A:285:LEU:HB3	1.94	0.49
1:B:273:LEU:CD2	1:B:273:LEU:H	2.25	0.49
1:A:117:ILE:CG2	1:A:122:TYR:HB2	2.43	0.49
1:C:133:GLU:O	1:C:134:SER:HB2	2.12	0.49
1:D:281:TYR:O	1:D:408:TYR:OH	2.29	0.49
1:A:266:LEU:CD2	1:A:416:ILE:HD11	2.43	0.49
1:C:162:MET:HB3	1:C:188:MET:HE1	1.94	0.49
1:D:148:THR:O	1:D:149:LEU:HD23	2.13	0.49
1:B:62:LEU:O	1:B:109:ARG:NH2	2.46	0.49
1:D:65:VAL:HG12	1:D:109:ARG:NH1	2.27	0.49
1:B:74:ASP:HA	1:B:77:LYS:CG	2.43	0.49
1:D:207:PHE:HE2	1:D:216:LYS:HE3	1.78	0.49
1:A:277:LYS:HG2	1:A:277:LYS:O	2.13	0.49
1:A:285:LEU:HD22	1:A:286:GLY:H	1.77	0.49
1:D:62:LEU:O	1:D:65:VAL:HB	2.13	0.49
1:C:90:HIS:O	1:C:91:ARG:CB	2.60	0.49
1:B:265:LYS:HG2	1:B:268:ARG:NH2	2.26	0.48
1:A:51:PHE:CE2	1:A:151:ILE:HD13	2.42	0.48
1:A:133:GLU:CG	1:A:142:LEU:HD23	2.43	0.48
1:B:412:PHE:O	1:B:415:PHE:HB3	2.12	0.48
1:A:278:ILE:HA	1:A:279:MET:CE	2.43	0.48
1:C:153:GLU:HG3	1:C:154:VAL:N	2.28	0.48
1:D:266:LEU:HD21	1:D:412:PHE:CE2	2.48	0.48
1:A:50:VAL:HG21	1:A:193:VAL:CG2	2.43	0.48
1:C:106:GLN:OE1	1:C:109:ARG:NH1	2.45	0.48
1:A:408:TYR:O	1:A:408:TYR:CG	2.66	0.48
1:C:266:LEU:CD2	1:C:270:VAL:HG21	2.42	0.48
1:D:47:LEU:HD11	1:D:198:SER:HB2	1.95	0.48
1:D:285:LEU:HD22	1:D:286:GLY:N	2.29	0.48
1:B:147:ARG:HB3	1:B:209:HIS:HA	1.94	0.48
1:A:80:SER:HB2	1:D:86:ASN:OD1	2.14	0.48
1:B:289:ASP:OD2	1:B:290:ILE:N	2.46	0.48
1:A:85:ASN:OD1	1:A:97:HIS:ND1	2.47	0.48
1:A:155:SER:HB3	1:A:158:ASP:OD1	2.14	0.48
1:D:74:ASP:CA	1:D:77:LYS:HG3	2.40	0.48
1:C:124:VAL:HG21	1:C:128:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:GLU:O	1:C:93:ASN:HB2	2.13	0.48
1:D:207:PHE:CZ	1:D:284:LEU:HD11	2.49	0.48
1:D:121:ASP:N	1:D:121:ASP:OD1	2.45	0.48
1:C:273:LEU:CB	1:C:278:ILE:HD12	2.42	0.48
1:B:51:PHE:CE2	1:B:151:ILE:HG21	2.49	0.48
1:C:45:ASP:O	1:C:49:GLY:HA3	2.13	0.48
1:A:180:THR:HB	1:A:269:ASP:CG	2.34	0.48
1:B:176:CYS:O	1:B:177:HIS:HB2	2.14	0.48
1:A:373:ILE:CG1	1:A:374:ASP:N	2.74	0.48
1:C:126:LEU:CD1	1:C:151:ILE:HD11	2.42	0.48
1:C:201:LEU:HD22	1:C:203:MET:HG2	1.95	0.48
1:A:170:HIS:O	1:A:174:VAL:HG23	2.14	0.48
1:B:239:THR:O	1:B:239:THR:HG22	2.14	0.48
1:C:151:ILE:HA	1:C:201:LEU:O	2.14	0.47
1:B:94:LEU:HD12	1:B:98:PHE:CZ	2.49	0.47
1:C:115:PHE:CE2	1:C:184:GLN:HB3	2.49	0.47
1:A:411:ARG:O	1:A:415:PHE:CB	2.62	0.47
1:C:182:LEU:HD23	1:C:375:ILE:HD11	1.95	0.47
1:B:215:ARG:HB3	1:B:287:ILE:HD12	1.96	0.47
1:B:244:ASP:O	1:B:248:LYS:HG2	2.14	0.47
1:D:190:ARG:HB2	1:D:199:TYR:CD2	2.49	0.47
1:B:412:PHE:CE2	1:B:416:ILE:HD13	2.44	0.47
1:A:159:ILE:O	1:A:162:MET:HB2	2.13	0.47
1:A:59:ILE:HD13	1:A:123:LEU:CA	2.44	0.47
1:D:79:SER:OG	1:D:101:LYS:HE2	2.15	0.47
1:D:119:ASP:HA	1:D:122:TYR:HB3	1.95	0.47
1:C:260:LYS:HA	1:C:263:LEU:HD12	1.95	0.47
1:D:115:PHE:HZ	1:D:169:TYR:OH	1.97	0.47
1:D:164:SER:HG	1:D:165:ASN:H	1.61	0.47
1:C:266:LEU:HD23	1:C:270:VAL:HG23	1.96	0.47
1:C:373:ILE:C	1:C:373:ILE:HD13	2.35	0.47
1:D:216:LYS:O	1:D:216:LYS:HG2	2.14	0.47
1:A:59:ILE:HG21	1:A:123:LEU:HD22	1.95	0.47
1:A:65:VAL:HG12	1:A:65:VAL:O	2.15	0.47
1:D:47:LEU:HD11	1:D:200:MET:CE	2.45	0.47
1:C:207:PHE:CD1	1:C:369:PHE:HB2	2.47	0.47
1:C:273:LEU:HG	1:C:274:VAL:N	2.29	0.47
1:D:283:LEU:HD13	1:D:412:PHE:CZ	2.49	0.47
1:D:215:ARG:HB2	1:D:287:ILE:HB	1.95	0.47
1:B:266:LEU:CD2	1:B:416:ILE:HD11	2.24	0.47
1:A:159:ILE:HG22	1:A:160:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:PHE:HE2	1:C:151:ILE:HD13	1.80	0.47
1:D:83:LYS:HD2	1:D:99:LYS:HE2	1.96	0.47
1:D:176:CYS:O	1:D:179:ASN:OD1	2.32	0.47
1:B:167:SER:O	1:B:170:HIS:N	2.47	0.47
1:B:167:SER:O	1:B:171:GLN:HG2	2.14	0.47
1:D:210:ARG:HG3	1:D:211:LEU:N	2.29	0.47
1:B:93:ASN:O	1:B:93:ASN:OD1	2.32	0.47
1:B:273:LEU:HB2	1:B:278:ILE:CD1	2.44	0.47
1:C:104:CYS:HB3	1:C:107:VAL:HG21	1.95	0.47
1:A:117:ILE:HG22	1:A:122:TYR:HB2	1.97	0.47
1:A:81:LYS:CB	1:D:85:ASN:HD22	2.28	0.47
1:A:110:ASN:OD1	1:A:170:HIS:NE2	2.47	0.47
1:A:283:LEU:HB2	1:A:412:PHE:CZ	2.49	0.47
1:C:140:ARG:O	1:C:141:PHE:C	2.53	0.47
1:D:184:GLN:O	1:D:203:MET:HB3	2.14	0.47
1:A:117:ILE:HD13	1:A:186:LEU:HD13	1.97	0.47
1:A:171:GLN:HA	1:A:174:VAL:HG23	1.97	0.47
1:A:408:TYR:O	1:A:408:TYR:CD1	2.68	0.47
1:A:118:ASP:O	1:A:121:ASP:N	2.48	0.47
1:B:54:GLY:HA3	1:B:100:PHE:CE2	2.51	0.46
1:A:273:LEU:HD11	1:A:375:ILE:HB	1.97	0.46
1:D:160:ALA:O	1:D:164:SER:N	2.47	0.46
1:A:154:VAL:HB	1:A:158:ASP:HB2	1.95	0.46
1:B:98:PHE:CB	1:B:193:VAL:HG22	2.45	0.46
1:D:140:ARG:HB2	1:D:153:GLU:HB2	1.97	0.46
1:B:47:LEU:HG	1:B:191:VAL:CG2	2.45	0.46
1:C:252:VAL:HG12	1:C:252:VAL:O	2.13	0.46
1:B:260:LYS:HB2	1:B:260:LYS:HE2	1.51	0.46
1:B:371:GLY:O	1:B:373:ILE:HG23	2.14	0.46
1:D:159:ILE:O	1:D:162:MET:HB3	2.15	0.46
1:A:62:LEU:HD11	1:A:105:PRO:HB3	1.97	0.46
1:C:62:LEU:O	1:C:109:ARG:NH2	2.48	0.46
1:B:218:ASP:HB2	1:B:239:THR:HG22	1.97	0.46
1:A:153:GLU:HG3	1:A:154:VAL:N	2.29	0.46
1:B:273:LEU:HD13	1:B:375:ILE:HG21	1.96	0.46
1:A:281:TYR:CD1	1:A:372:LEU:CD1	2.94	0.46
1:B:59:ILE:CG2	1:B:123:LEU:HD13	2.45	0.46
1:D:163:HIS:O	1:D:166:LEU:HB3	2.16	0.46
1:C:87:HIS:CE1	1:C:88:LEU:HG	2.51	0.46
1:C:266:LEU:CD2	1:C:270:VAL:CG2	2.94	0.46
1:D:213:VAL:HA	1:D:287:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:CG2	1:A:191:VAL:O	2.61	0.46
1:B:273:LEU:HB2	1:B:278:ILE:CG1	2.46	0.46
1:C:181:LEU:HD12	1:C:266:LEU:HA	1.98	0.46
1:D:103:TYR:HB3	1:D:163:HIS:NE2	2.31	0.46
1:A:151:ILE:HG23	1:A:202:VAL:HG13	1.98	0.46
1:A:62:LEU:O	1:A:109:ARG:NH2	2.49	0.46
1:D:90:HIS:HB3	1:D:91:ARG:H	1.49	0.46
1:D:143:ILE:HG22	1:D:144:SER:O	2.16	0.46
1:C:207:PHE:CE1	1:C:213:VAL:HG21	2.51	0.46
1:B:265:LYS:O	1:B:266:LEU:C	2.53	0.46
1:B:217:TYR:CE1	1:B:285:LEU:HD12	2.51	0.46
1:D:149:LEU:CD2	1:D:204:ARG:HA	2.45	0.46
1:C:255:GLY:HA3	1:C:258:GLU:CD	2.35	0.46
1:A:118:ASP:O	1:A:121:ASP:HB2	2.16	0.46
1:C:373:ILE:O	1:C:373:ILE:HG12	2.16	0.46
1:C:83:LYS:HD2	1:C:99:LYS:HZ1	1.76	0.46
1:D:160:ALA:O	1:D:163:HIS:N	2.49	0.46
1:A:212:PRO:HD2	1:A:288:HIS:CD2	2.50	0.46
1:B:99:LYS:N	1:B:192:SER:O	2.49	0.46
1:C:50:VAL:O	1:C:54:GLY:N	2.47	0.46
1:B:277:LYS:HD3	1:B:277:LYS:O	2.15	0.46
1:A:266:LEU:HD21	1:A:416:ILE:HD11	1.99	0.45
1:C:101:LYS:HB2	1:C:190:ARG:NH2	2.31	0.45
1:A:47:LEU:CD1	1:A:191:VAL:O	2.64	0.45
1:C:157:GLU:O	1:C:160:ALA:N	2.49	0.45
1:C:270:VAL:CG2	1:C:413:LEU:CD2	2.92	0.45
1:D:287:ILE:HG23	1:D:367:VAL:O	2.16	0.45
1:C:79:SER:HB2	1:C:101:LYS:CE	2.45	0.45
1:D:267:LYS:HA	1:D:413:LEU:CD2	2.47	0.45
1:A:367:VAL:HG12	1:A:369:PHE:CE2	2.51	0.45
1:A:114:ARG:NH2	1:A:174:VAL:HG13	2.30	0.45
1:B:207:PHE:CZ	1:B:284:LEU:HD21	2.51	0.45
1:A:103:TYR:HE1	1:A:190:ARG:HB2	1.81	0.45
1:A:220:LYS:HD2	1:A:280:ASP:OD2	2.16	0.45
1:B:153:GLU:HG3	1:B:200:MET:HE2	1.98	0.45
1:B:62:LEU:HA	1:B:65:VAL:HG23	1.98	0.45
1:A:266:LEU:CD2	1:A:413:LEU:CD2	2.76	0.45
1:D:174:VAL:O	1:D:177:HIS:ND1	2.50	0.45
1:B:89:PHE:CE1	1:C:106:GLN:HG2	2.52	0.45
1:C:270:VAL:CG2	1:C:412:PHE:HD2	2.30	0.45
1:A:90:HIS:O	1:A:91:ARG:CG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:VAL:HG21	1:D:159:ILE:HD11	1.98	0.45
1:A:215:ARG:HB2	1:A:287:ILE:CD1	2.40	0.45
1:D:112:ARG:HG2	1:D:186:LEU:HB3	1.99	0.45
1:B:166:LEU:O	1:B:170:HIS:N	2.50	0.45
1:C:213:VAL:HG22	1:C:369:PHE:CD2	2.51	0.45
1:C:266:LEU:HD21	1:C:412:PHE:CD2	2.52	0.45
1:B:215:ARG:O	1:B:287:ILE:N	2.46	0.45
1:A:62:LEU:CD1	1:D:89:PHE:CZ	3.00	0.45
1:D:146:ASP:HB3	1:D:148:THR:OG1	2.16	0.45
1:B:71:LEU:CD1	1:B:107:VAL:HG22	2.47	0.45
1:C:81:LYS:HA	1:C:100:PHE:O	2.17	0.45
1:D:63:SER:C	1:D:65:VAL:H	2.19	0.45
1:B:266:LEU:O	1:B:270:VAL:HG23	2.16	0.45
1:B:219:LEU:HD22	1:B:415:PHE:CE2	2.52	0.45
1:D:162:MET:HG2	1:D:188:MET:SD	2.56	0.45
1:D:179:ASN:N	1:D:179:ASN:OD1	2.50	0.45
1:C:121:ASP:O	1:C:125:SER:N	2.49	0.45
1:C:175:LYS:HB3	1:C:175:LYS:HE3	1.64	0.45
1:A:84:VAL:HG22	1:D:82:ILE:HG23	1.98	0.45
1:D:207:PHE:CE2	1:D:216:LYS:HE3	2.51	0.45
1:B:180:THR:OG1	1:B:182:LEU:HB2	2.16	0.45
1:B:245:PHE:CZ	1:B:415:PHE:CE2	3.05	0.45
1:D:220:LYS:NZ	1:D:280:ASP:CG	2.70	0.45
1:B:59:ILE:HG21	1:B:123:LEU:HD13	1.99	0.45
1:A:74:ASP:O	1:A:77:LYS:HG2	2.17	0.45
1:D:106:GLN:OE1	1:D:109:ARG:NH1	2.50	0.45
1:D:65:VAL:HG12	1:D:109:ARG:HH12	1.80	0.45
1:A:266:LEU:HD23	1:A:266:LEU:O	2.16	0.45
1:D:170:HIS:HA	1:D:173:ILE:HG12	1.98	0.45
1:D:290:ILE:HD12	1:D:366:GLU:HA	1.99	0.45
1:D:283:LEU:HA	1:D:372:LEU:HA	1.99	0.45
1:C:215:ARG:NH1	1:C:248:LYS:HZ3	2.15	0.45
1:C:261:ILE:O	1:C:264:GLU:HB2	2.17	0.45
1:A:74:ASP:HA	1:A:77:LYS:HG3	1.99	0.45
1:D:407:GLN:N	1:D:407:GLN:HE21	2.14	0.45
1:A:162:MET:HE1	1:A:185:PHE:CE2	2.52	0.44
1:A:50:VAL:HG21	1:A:193:VAL:HG21	1.98	0.44
1:C:182:LEU:HD23	1:C:375:ILE:CD1	2.47	0.44
1:A:181:LEU:O	1:A:372:LEU:N	2.50	0.44
1:A:279:MET:HB2	1:A:280:ASP:H	1.66	0.44
1:A:281:TYR:CA	1:A:374:ASP:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASN:O	1:C:113:ASP:HB3	2.16	0.44
1:D:146:ASP:O	1:D:147:ARG:HB2	2.17	0.44
1:C:45:ASP:CG	1:C:46:PRO:HD2	2.38	0.44
1:B:54:GLY:HA3	1:B:100:PHE:CG	2.52	0.44
1:B:81:LYS:O	1:B:82:ILE:HD13	2.17	0.44
1:D:239:THR:O	1:D:239:THR:HG22	2.16	0.44
1:B:375:ILE:CG1	1:B:375:ILE:O	2.65	0.44
1:B:141:PHE:HD1	1:B:141:PHE:HA	1.66	0.44
1:D:161:ASP:C	1:D:164:SER:HG	2.18	0.44
1:C:68:PRO:HD3	1:C:106:GLN:NE2	2.33	0.44
1:D:220:LYS:HE2	1:D:220:LYS:HB3	1.35	0.44
1:A:273:LEU:HD11	1:A:375:ILE:CB	2.48	0.44
1:B:133:GLU:HA	1:B:142:LEU:HD23	1.99	0.44
1:D:219:LEU:N	1:D:283:LEU:O	2.49	0.44
1:C:115:PHE:CD1	1:C:184:GLN:HB3	2.53	0.44
1:C:85:ASN:OD1	1:C:85:ASN:N	2.50	0.44
1:A:56:ALA:O	1:A:60:ASN:ND2	2.50	0.44
1:C:273:LEU:HD12	1:C:278:ILE:HB	1.99	0.44
1:B:273:LEU:HA	1:B:276:LEU:HB2	2.00	0.44
1:C:140:ARG:O	1:C:142:LEU:HG	2.17	0.44
1:A:86:ASN:CG	1:D:80:SER:HA	2.37	0.44
1:A:261:ILE:HD12	1:A:261:ILE:N	2.33	0.44
1:D:140:ARG:NE	1:D:153:GLU:OE1	2.50	0.44
1:C:95:PRO:O	1:C:98:PHE:HD1	2.00	0.44
1:D:220:LYS:HE3	1:D:281:TYR:O	2.18	0.44
1:B:45:ASP:CG	1:B:48:VAL:HB	2.37	0.44
1:D:46:PRO:O	1:D:49:GLY:N	2.50	0.44
1:D:52:LEU:O	1:D:53:TRP:C	2.56	0.44
1:C:288:HIS:ND1	1:C:367:VAL:HG23	2.33	0.44
1:B:158:ASP:OD1	1:B:376:LEU:HD23	2.18	0.44
1:D:151:ILE:HG23	1:D:202:VAL:HG22	1.99	0.44
1:A:129:ASN:HB3	1:A:145:TYR:CG	2.52	0.44
1:B:122:TYR:O	1:B:126:LEU:HD22	2.18	0.44
1:A:212:PRO:HD2	1:A:288:HIS:NE2	2.33	0.44
1:B:66:PRO:HA	1:B:67:PRO:HD2	1.87	0.44
1:D:71:LEU:HD23	1:D:71:LEU:N	2.32	0.44
1:D:65:VAL:O	1:D:109:ARG:NH2	2.50	0.44
1:D:55:VAL:HG11	1:D:126:LEU:CD1	2.44	0.44
1:D:245:PHE:HD1	1:D:250:GLN:HB2	1.83	0.44
1:C:179:ASN:OD1	1:C:179:ASN:N	2.49	0.44
1:A:281:TYR:HD1	1:A:372:LEU:CD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:HIS:HA	1:D:173:ILE:CG1	2.48	0.44
1:A:261:ILE:O	1:A:264:GLU:N	2.50	0.44
1:A:239:THR:O	1:A:239:THR:HG22	2.18	0.44
1:B:219:LEU:HD22	1:B:415:PHE:HE2	1.83	0.43
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.87	0.43
1:A:108:PHE:O	1:A:112:ARG:NH1	2.51	0.43
1:D:159:ILE:O	1:D:162:MET:CB	2.66	0.43
1:D:93:ASN:C	1:D:93:ASN:OD1	2.56	0.43
1:B:145:TYR:CZ	1:B:146:ASP:OD1	2.71	0.43
1:B:273:LEU:C	1:B:278:ILE:HB	2.37	0.43
1:C:247:ASN:OD1	1:C:248:LYS:N	2.51	0.43
1:C:287:ILE:CG2	1:C:366:GLU:OE2	2.66	0.43
1:D:109:ARG:O	1:D:112:ARG:HB2	2.19	0.43
1:C:101:LYS:HB2	1:C:190:ARG:HH21	1.83	0.43
1:C:83:LYS:HG3	1:C:99:LYS:HE3	2.01	0.43
1:D:49:GLY:O	1:D:94:LEU:HD21	2.19	0.43
1:D:404:HIS:N	1:D:404:HIS:HD1	2.16	0.43
1:C:83:LYS:CB	1:C:99:LYS:HE3	2.48	0.43
1:C:45:ASP:HA	1:C:46:PRO:HD3	1.60	0.43
1:B:170:HIS:O	1:B:174:VAL:HG23	2.17	0.43
1:C:414:ASP:HA	1:C:417:THR:HG22	2.00	0.43
1:D:284:LEU:O	1:D:370:MET:HA	2.19	0.43
1:A:373:ILE:O	1:A:375:ILE:N	2.47	0.43
1:D:180:THR:HG22	1:D:268:ARG:HH12	1.83	0.43
1:B:243:MET:O	1:B:247:ASN:OD1	2.37	0.43
1:A:220:LYS:HD2	1:A:280:ASP:CG	2.38	0.43
1:A:412:PHE:CE2	1:A:416:ILE:HD12	2.54	0.43
1:A:51:PHE:CZ	1:A:151:ILE:HG21	2.54	0.43
1:A:51:PHE:O	1:A:55:VAL:HG23	2.19	0.43
1:C:158:ASP:OD1	1:C:376:LEU:HD13	2.19	0.43
1:C:129:ASN:HB2	1:C:145:TYR:CD1	2.53	0.43
1:C:281:TYR:HA	1:C:374:ASP:HB3	2.01	0.43
1:B:283:LEU:CD2	1:B:370:MET:CE	2.89	0.43
1:C:215:ARG:NH1	1:C:248:LYS:NZ	2.67	0.43
1:A:285:LEU:HD22	1:A:286:GLY:N	2.33	0.43
1:B:207:PHE:CD2	1:B:213:VAL:HG21	2.54	0.43
1:C:140:ARG:HH12	1:C:142:LEU:HD21	1.84	0.43
1:B:140:ARG:O	1:B:152:LYS:HG3	2.19	0.43
1:D:261:ILE:H	1:D:261:ILE:CD1	2.27	0.43
1:D:176:CYS:HB2	1:D:268:ARG:NH1	2.34	0.43
1:C:45:ASP:HB3	1:C:48:VAL:CG1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.79	0.43
1:D:123:LEU:O	1:D:126:LEU:N	2.50	0.43
1:B:54:GLY:HA3	1:B:100:PHE:CD2	2.54	0.43
1:B:54:GLY:O	1:B:57:HIS:N	2.52	0.43
1:B:195:ASN:O	1:B:195:ASN:OD1	2.37	0.43
1:D:128:ARG:HE	1:D:128:ARG:HB3	1.69	0.43
1:C:270:VAL:CG2	1:C:412:PHE:CD2	3.02	0.42
1:A:185:PHE:HZ	1:A:375:ILE:HD11	1.84	0.42
1:A:47:LEU:CD1	1:A:198:SER:HB2	2.47	0.42
1:C:126:LEU:HD22	1:C:126:LEU:HA	1.84	0.42
1:D:159:ILE:HG13	1:D:199:TYR:CD2	2.54	0.42
1:D:162:MET:O	1:D:166:LEU:N	2.50	0.42
1:C:259:LYS:HZ3	1:C:263:LEU:HD21	1.84	0.42
1:B:70:MET:CE	1:B:72:LEU:HG	2.49	0.42
1:C:183:PRO:HB2	1:C:185:PHE:CZ	2.55	0.42
1:C:278:ILE:HD13	1:C:375:ILE:HG23	2.00	0.42
1:B:179:ASN:O	1:B:265:LYS:HG2	2.20	0.42
1:A:270:VAL:HG22	1:A:281:TYR:CE1	2.54	0.42
1:A:184:GLN:O	1:A:186:LEU:HG	2.20	0.42
1:A:55:VAL:HG12	1:A:59:ILE:HD12	2.00	0.42
1:B:163:HIS:NE2	1:B:188:MET:CE	2.82	0.42
1:A:162:MET:HB3	1:A:188:MET:HE1	2.02	0.42
1:A:141:PHE:N	1:A:151:ILE:O	2.53	0.42
1:A:112:ARG:NH1	1:A:186:LEU:O	2.50	0.42
1:B:273:LEU:HB2	1:B:278:ILE:HB	2.01	0.42
1:A:214:HIS:N	1:A:287:ILE:O	2.43	0.42
1:C:124:VAL:O	1:C:124:VAL:HG22	2.19	0.42
1:B:86:ASN:HD22	1:B:89:PHE:HB3	1.83	0.42
1:A:56:ALA:C	1:A:60:ASN:HD22	2.22	0.42
1:D:213:VAL:HG22	1:D:287:ILE:H	1.85	0.42
1:A:405:PRO:O	1:A:409:ALA:HB2	2.19	0.42
1:A:117:ILE:HD13	1:A:186:LEU:CD1	2.49	0.42
1:A:65:VAL:HG23	1:D:90:HIS:ND1	2.34	0.42
1:A:60:ASN:O	1:A:64:GLN:NE2	2.50	0.42
1:B:405:PRO:O	1:B:409:ALA:HB2	2.19	0.42
1:C:273:LEU:HD12	1:C:278:ILE:CB	2.49	0.42
1:D:111:LEU:CD2	1:D:173:ILE:HG21	2.50	0.42
1:C:83:LYS:HB2	1:C:99:LYS:HE3	2.02	0.42
1:A:48:VAL:HG12	1:A:49:GLY:N	2.34	0.42
1:B:277:LYS:CD	1:B:277:LYS:O	2.68	0.42
1:C:283:LEU:HD12	1:C:372:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLU:HB2	1:B:200:MET:HE1	2.02	0.42
1:C:201:LEU:HD23	1:C:202:VAL:H	1.83	0.42
1:D:154:VAL:CG2	1:D:159:ILE:HD11	2.50	0.42
1:B:279:MET:O	1:B:408:TYR:CE2	2.73	0.42
1:C:270:VAL:CA	1:C:273:LEU:HD23	2.50	0.42
1:C:211:LEU:HD22	1:C:288:HIS:CE1	2.55	0.42
1:B:103:TYR:CD1	1:B:188:MET:CG	3.02	0.42
1:C:174:VAL:HG13	1:C:175:LYS:N	2.35	0.42
1:A:52:LEU:HD23	1:A:126:LEU:O	2.20	0.42
1:A:133:GLU:CB	1:A:142:LEU:HD23	2.49	0.42
1:D:79:SER:CB	1:D:101:LYS:HE2	2.49	0.42
1:B:207:PHE:CD1	1:B:369:PHE:HB2	2.54	0.42
1:D:115:PHE:CZ	1:D:184:GLN:HA	2.55	0.42
1:D:147:ARG:HB3	1:D:147:ARG:HE	1.56	0.42
1:C:143:ILE:HG22	1:C:147:ARG:HA	2.01	0.42
1:B:366:GLU:O	1:B:368:TYR:CE1	2.73	0.41
1:B:412:PHE:CE1	1:B:416:ILE:HG21	2.55	0.41
1:D:83:LYS:HG3	1:D:99:LYS:HG3	2.01	0.41
1:A:81:LYS:HB2	1:D:85:ASN:ND2	2.32	0.41
1:A:71:LEU:HD22	1:A:75:ASP:OD2	2.20	0.41
1:D:49:GLY:HA2	1:D:52:LEU:HD12	2.01	0.41
1:B:162:MET:O	1:B:166:LEU:HB2	2.20	0.41
1:C:82:ILE:O	1:C:99:LYS:HA	2.21	0.41
1:D:99:LYS:HB2	1:D:192:SER:OG	2.21	0.41
1:A:287:ILE:HG12	1:A:368:TYR:CE2	2.54	0.41
1:B:169:TYR:CZ	1:B:173:ILE:HD11	2.55	0.41
1:B:102:GLU:OE1	1:B:105:PRO:HB3	2.21	0.41
1:C:258:GLU:H	1:C:258:GLU:HG2	1.51	0.41
1:D:414:ASP:O	1:D:417:THR:HB	2.20	0.41
1:A:94:LEU:HA	1:A:95:PRO:HD3	1.80	0.41
1:C:284:LEU:CB	1:C:373:ILE:HG21	2.42	0.41
1:D:285:LEU:HA	1:D:369:PHE:O	2.21	0.41
1:B:151:ILE:CG1	1:B:202:VAL:HG13	2.47	0.41
1:C:45:ASP:CG	1:C:46:PRO:CD	2.88	0.41
1:C:165:ASN:HB2	1:C:276:LEU:CD2	2.47	0.41
1:C:269:ASP:HB3	1:C:372:LEU:HD11	2.03	0.41
1:C:265:LYS:O	1:C:269:ASP:OD1	2.38	0.41
1:B:283:LEU:HB2	1:B:412:PHE:CE1	2.55	0.41
1:D:125:SER:HA	1:D:145:TYR:CE1	2.55	0.41
1:B:101:LYS:HD3	1:B:190:ARG:HD3	2.01	0.41
1:B:159:ILE:HG23	1:B:163:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:VAL:C	1:C:273:LEU:HD23	2.41	0.41
1:C:268:ARG:NH1	1:C:268:ARG:HG2	2.36	0.41
1:D:287:ILE:HG12	1:D:368:TYR:HD2	1.85	0.41
1:B:50:VAL:HG21	1:B:98:PHE:CB	2.48	0.41
1:C:270:VAL:O	1:C:273:LEU:HD23	2.20	0.41
1:D:285:LEU:CD2	1:D:370:MET:HB3	2.40	0.41
1:B:48:VAL:HG12	1:B:49:GLY:N	2.35	0.41
1:D:255:GLY:O	1:D:259:LYS:CB	2.64	0.41
1:B:73:PRO:O	1:B:76:PHE:N	2.52	0.41
1:D:404:HIS:N	1:D:404:HIS:ND1	2.68	0.41
1:C:283:LEU:HD23	1:C:283:LEU:O	2.20	0.41
1:A:215:ARG:HB3	1:A:287:ILE:HD12	2.00	0.41
1:C:270:VAL:HG22	1:C:412:PHE:CD2	2.56	0.41
1:A:190:ARG:HD2	1:A:197:ASP:HB3	2.01	0.41
1:D:169:TYR:CE2	1:D:185:PHE:HD2	2.39	0.41
1:B:217:TYR:CD1	1:B:285:LEU:HD12	2.55	0.41
1:C:126:LEU:CD2	1:C:144:SER:CB	2.93	0.41
1:B:65:VAL:HA	1:B:66:PRO:HD2	1.86	0.41
1:A:59:ILE:HD11	1:A:122:TYR:CE2	2.55	0.40
1:D:65:VAL:O	1:D:65:VAL:HG12	2.20	0.40
1:B:51:PHE:CZ	1:B:151:ILE:HG21	2.56	0.40
1:D:412:PHE:O	1:D:415:PHE:N	2.54	0.40
1:D:221:GLY:HA2	1:D:415:PHE:CD1	2.56	0.40
1:A:81:LYS:C	1:A:82:ILE:HD13	2.42	0.40
1:C:216:LYS:HG2	1:C:239:THR:N	2.36	0.40
1:A:71:LEU:HD13	1:A:107:VAL:HG22	2.02	0.40
1:B:261:ILE:HG22	1:B:265:LYS:HE2	2.04	0.40
1:B:265:LYS:HA	1:B:268:ARG:HE	1.86	0.40
1:D:282:SER:OG	1:D:374:ASP:HB2	2.20	0.40
1:B:404:HIS:HA	1:B:405:PRO:HD3	1.79	0.40
1:C:103:TYR:OH	1:C:199:TYR:HE2	2.05	0.40
1:A:259:LYS:HG2	1:A:263:LEU:HD11	2.02	0.40
1:B:163:HIS:NE2	1:B:188:MET:HE3	2.36	0.40
1:C:115:PHE:CZ	1:C:184:GLN:HB3	2.56	0.40
1:B:261:ILE:O	1:B:264:GLU:N	2.54	0.40
1:A:372:LEU:HD22	1:A:372:LEU:HA	1.79	0.40
1:B:141:PHE:O	1:B:142:LEU:HG	2.22	0.40
1:D:267:LYS:O	1:D:271:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/392 (58%)	189 (82%)	39 (17%)	1 (0%)	39	74
1	B	240/392 (61%)	203 (85%)	37 (15%)	0	100	100
1	C	233/392 (59%)	197 (84%)	35 (15%)	1 (0%)	39	74
1	D	240/392 (61%)	194 (81%)	45 (19%)	1 (0%)	39	74
All	All	942/1568 (60%)	783 (83%)	156 (17%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	375	ILE
1	C	241	ARG
1	A	95	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/348 (66%)	175 (76%)	56 (24%)	1	2
1	B	237/348 (68%)	182 (77%)	55 (23%)	1	3
1	C	233/348 (67%)	181 (78%)	52 (22%)	1	3
1	D	237/348 (68%)	177 (75%)	60 (25%)	1	2
All	All	938/1392 (67%)	715 (76%)	223 (24%)	1	2

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	47	LEU
1	A	48	VAL
1	A	52	LEU
1	A	62	LEU
1	A	65	VAL
1	A	70	MET
1	A	77	LYS
1	A	80	SER
1	A	81	LYS
1	A	96	SER
1	A	97	HIS
1	A	120	GLN
1	A	128	ARG
1	A	141	PHE
1	A	151	ILE
1	A	156	SER
1	A	162	MET
1	A	164	SER
1	A	174	VAL
1	A	176	CYS
1	A	191	VAL
1	A	192	SER
1	A	193	VAL
1	A	195	ASN
1	A	196	GLU
1	A	197	ASP
1	A	201	LEU
1	A	204	ARG
1	A	210	ARG
1	A	216	LYS
1	A	220	LYS
1	A	240	LEU
1	A	242	ASP
1	A	243	MET
1	A	248	LYS
1	A	253	TYR
1	A	268	ARG
1	A	272	PHE
1	A	279	MET
1	A	283	LEU
1	A	285	LEU
1	A	289	ASP

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Mol	Chain	Res	Type
1	A	366	GLU
1	A	367	VAL
1	A	370	MET
1	A	372	LEU
1	A	373	ILE
1	A	374	ASP
1	A	404	HIS
1	A	407	GLN
1	A	408	TYR
1	A	410	LYS
1	A	413	LEU
1	A	416	ILE
1	A	417	THR
1	B	48	VAL
1	B	65	VAL
1	B	70	MET
1	B	71	LEU
1	B	77	LYS
1	B	79	SER
1	B	91	ARG
1	B	92	GLU
1	B	93	ASN
1	B	94	LEU
1	B	109	ARG
1	B	114	ARG
1	B	124	VAL
1	B	126	LEU
1	B	128	ARG
1	B	132	SER
1	B	140	ARG
1	B	141	PHE
1	B	146	ASP
1	B	157	GLU
1	B	164	SER
1	B	165	ASN
1	B	168	ASN
1	B	179	ASN
1	B	180	THR
1	B	189	TYR
1	B	191	VAL
1	B	192	SER
1	B	196	GLU

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Mol	Chain	Res	Type
1	B	201	LEU
1	B	210	ARG
1	B	215	ARG
1	B	216	LYS
1	B	245	PHE
1	B	246	LEU
1	B	247	ASN
1	B	252	VAL
1	B	256	GLU
1	B	260	LYS
1	B	266	LEU
1	B	267	LYS
1	B	274	VAL
1	B	278	ILE
1	B	285	LEU
1	B	289	ASP
1	B	366	GLU
1	B	368	TYR
1	B	370	MET
1	B	373	ILE
1	B	375	ILE
1	B	407	GLN
1	B	408	TYR
1	B	410	LYS
1	B	413	LEU
1	B	416	ILE
1	C	47	LEU
1	C	48	VAL
1	C	62	LEU
1	C	63	SER
1	C	69	VAL
1	C	70	MET
1	C	77	LYS
1	C	79	SER
1	C	80	SER
1	C	85	ASN
1	C	92	GLU
1	C	99	LYS
1	C	109	ARG
1	C	126	LEU
1	C	128	ARG
1	C	132	SER

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Mol	Chain	Res	Type
1	C	146	ASP
1	C	147	ARG
1	C	149	LEU
1	C	150	VAL
1	C	152	LYS
1	C	156	SER
1	C	163	HIS
1	C	164	SER
1	C	165	ASN
1	C	167	SER
1	C	180	THR
1	C	192	SER
1	C	196	GLU
1	C	203	MET
1	C	210	ARG
1	C	240	LEU
1	C	242	ASP
1	C	243	MET
1	C	251	LYS
1	C	253	TYR
1	C	258	GLU
1	C	268	ARG
1	C	273	LEU
1	C	274	VAL
1	C	276	LEU
1	C	282	SER
1	C	285	LEU
1	C	289	ASP
1	C	369	PHE
1	C	370	MET
1	C	373	ILE
1	C	377	THR
1	C	406	GLU
1	C	408	TYR
1	C	410	LYS
1	C	413	LEU
1	D	45	ASP
1	D	47	LEU
1	D	61	GLU
1	D	62	LEU
1	D	64	GLN
1	D	65	VAL

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Mol	Chain	Res	Type
1	D	70	MET
1	D	77	LYS
1	D	79	SER
1	D	82	ILE
1	D	83	LYS
1	D	85	ASN
1	D	90	HIS
1	D	94	LEU
1	D	109	ARG
1	D	114	ARG
1	D	119	ASP
1	D	120	GLN
1	D	121	ASP
1	D	126	LEU
1	D	128	ARG
1	D	132	SER
1	D	135	GLU
1	D	144	SER
1	D	147	ARG
1	D	153	GLU
1	D	163	HIS
1	D	165	ASN
1	D	166	LEU
1	D	167	SER
1	D	180	THR
1	D	186	LEU
1	D	192	SER
1	D	200	MET
1	D	203	MET
1	D	210	ARG
1	D	213	VAL
1	D	216	LYS
1	D	217	TYR
1	D	220	LYS
1	D	245	PHE
1	D	246	LEU
1	D	250	GLN
1	D	252	VAL
1	D	258	GLU
1	D	266	LEU
1	D	273	LEU
1	D	279	MET

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Mol	Chain	Res	Type
1	D	282	SER
1	D	283	LEU
1	D	284	LEU
1	D	289	ASP
1	D	370	MET
1	D	372	LEU
1	D	373	ILE
1	D	404	HIS
1	D	407	GLN
1	D	408	TYR
1	D	410	LYS
1	D	416	ILE

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

Mol	Chain	Res	Type
1	A	57	HIS
1	A	60	ASN
1	A	184	GLN
1	A	195	ASN
1	A	209	HIS
1	A	404	HIS
1	B	57	HIS
1	B	60	ASN
1	B	64	GLN
1	B	86	ASN
1	B	195	ASN
1	B	247	ASN
1	C	87	HIS
1	C	129	ASN
1	C	163	HIS
1	C	195	ASN
1	D	85	ASN
1	D	87	HIS
1	D	195	ASN
1	D	209	HIS
1	D	214	HIS
1	D	288	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	243/392 (61%)	-0.09	3 (1%) 81 73	24, 58, 114, 158	0
1	B	250/392 (63%)	0.03	12 (4%) 34 23	24, 58, 138, 152	0
1	C	245/392 (62%)	-0.06	10 (4%) 41 29	25, 59, 128, 158	0
1	D	250/392 (63%)	-0.05	9 (3%) 46 34	24, 60, 144, 158	0
All	All	988/1568 (63%)	-0.04	34 (3%) 49 36	24, 59, 136, 158	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ASN	5.3
1	B	416	ILE	4.8
1	A	405	PRO	4.2
1	A	253	TYR	4.2
1	B	253	TYR	3.7
1	B	219	LEU	3.7
1	B	255	GLY	3.6
1	D	212	PRO	3.5
1	D	416	ILE	3.5
1	B	143	ILE	3.4
1	B	412	PHE	3.4
1	C	368	TYR	3.3
1	C	405	PRO	3.2
1	B	406	GLU	3.1
1	C	151	ILE	3.0
1	C	216	LYS	2.9
1	C	279	MET	2.7
1	B	165	ASN	2.7
1	D	142	LEU	2.7
1	D	413	LEU	2.5
1	C	217	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	251	LYS	2.5
1	D	412	PHE	2.5
1	D	134	SER	2.4
1	C	126	LEU	2.4
1	C	241	ARG	2.4
1	B	258	GLU	2.3
1	B	69	VAL	2.3
1	C	369	PHE	2.3
1	B	413	LEU	2.3
1	D	65	VAL	2.2
1	D	213	VAL	2.2
1	A	240	LEU	2.2
1	B	254	ILE	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.