



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2016 – 04:55 AM EDT

PDB ID : 5L0C  
Title : Human metavinculin (residues 959-1134) in complex with PIP2  
Authors : Chinthalapudi, K.; Izard, T.  
Deposited on : 2016-07-27  
Resolution : 3.10 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

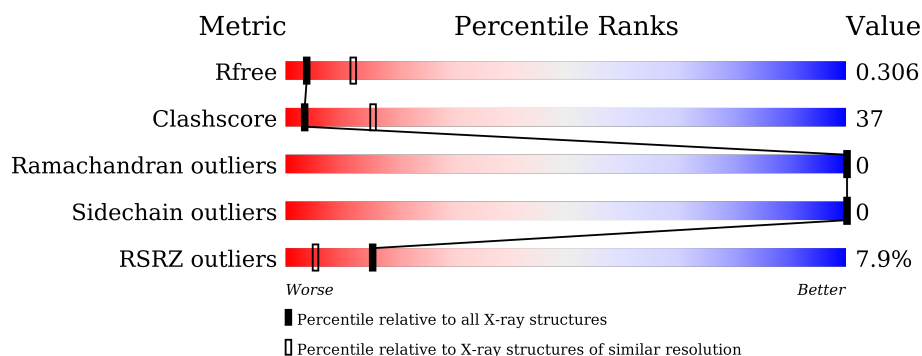
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	176	
1	B	176	
1	C	176	
1	D	176	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PIO	B	1202	-	-	-	X
2	PIO	C	1201	-	-	-	X

## 2 Entry composition i

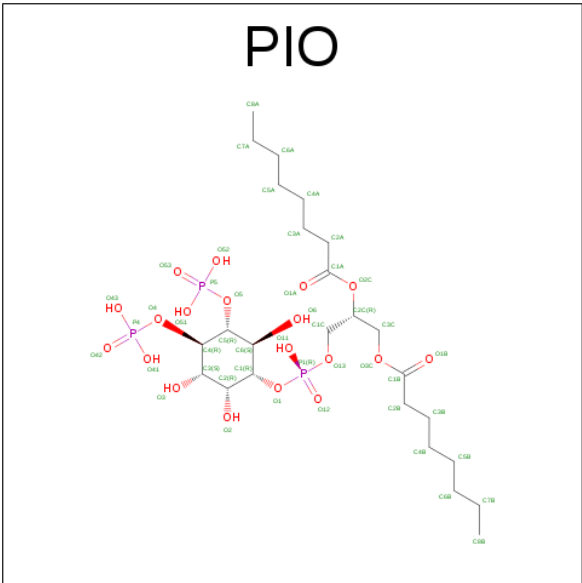
There are 4 unique types of molecules in this entry. The entry contains 5588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1368	843	257	259	9			
1	B	175	Total	C	N	O	S	0	1	0
			1362	842	255	256	9			
1	C	175	Total	C	N	O	S	0	0	0
			1358	838	255	256	9			
1	D	166	Total	C	N	O	S	0	1	0
			1299	799	246	245	9			

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>).



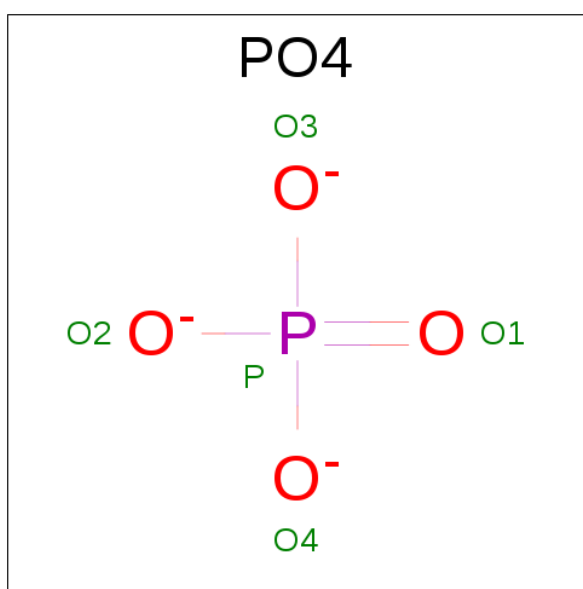
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			29	9	17	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			24	6	15	3		
2	B	1	Total	C	O	P	0	0
			24	6	15	3		
2	C	1	Total	C	O	P	0	0
			24	6	15	3		
2	D	1	Total	C	O	P	0	0
			24	6	15	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	19	Total	O	0	0
			19	19		

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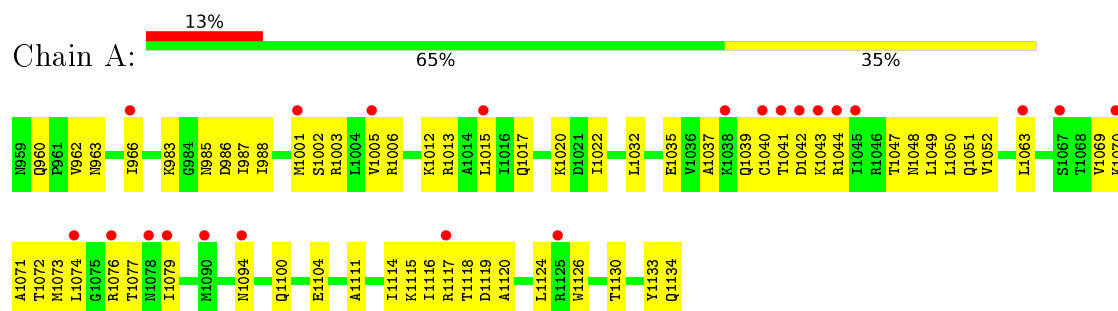
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	18	Total	O	0	0
			18	18		
4	D	13	Total	O	0	0
			13	13		

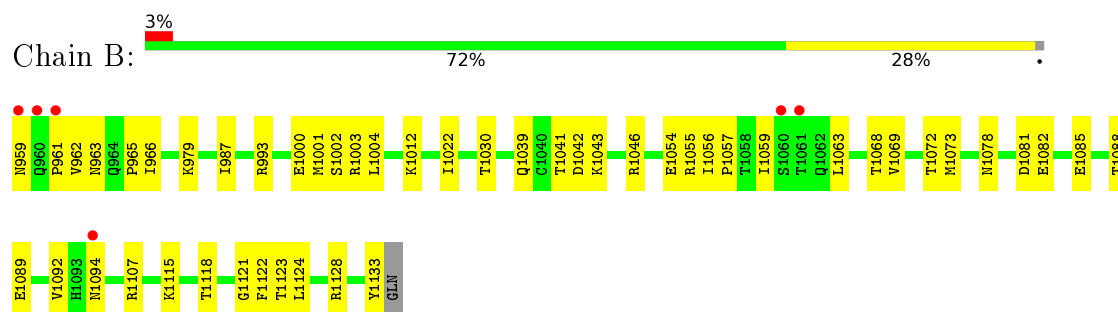
### 3 Residue-property plots [i](#)

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

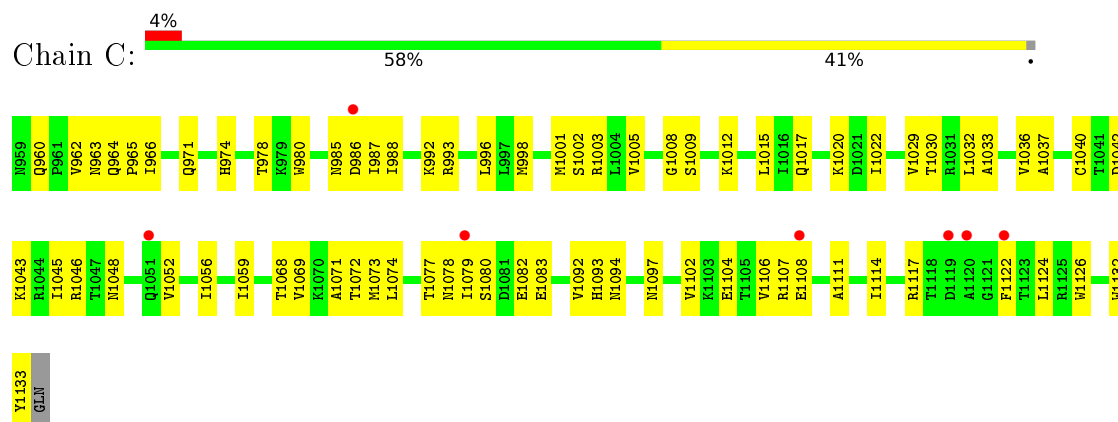
#### • Molecule 1: Vinculin



#### • Molecule 1: Vinculin

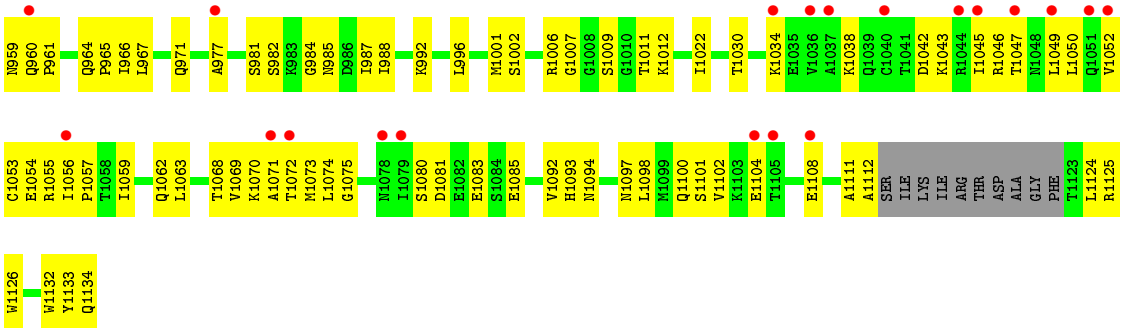


#### • Molecule 1: Vinculin



#### • Molecule 1: Vinculin







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.52Å 100.68Å 105.61Å 90.00° 122.49° 90.00°	Depositor
Resolution (Å)	30.45 – 3.10 48.30 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.45-3.10) 97.8 (48.30-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.235 , 0.261 0.299 , 0.306	Depositor DCC
$R_{free}$ test set	923 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 92.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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, PIO

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	0.45	0/1381	0.68	0/1858
1	B	0.47	0/1378	0.66	0/1856
1	C	0.45	0/1371	0.64	0/1846
1	D	0.46	0/1313	0.64	0/1765
All	All	0.46	0/5443	0.66	0/7325

There are no bond length outliers.

There are no bond angle outliers.

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	1368	0	1428	108	1
1	B	1362	0	1429	73	1
1	C	1358	0	1420	117	0
1	D	1299	0	1359	126	0
2	A	29	0	14	0	0
2	B	48	0	18	13	0
2	C	24	0	9	6	0
2	D	24	0	9	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
4	A	11	0	0	0	0
4	B	19	0	0	1	0
4	C	18	0	0	1	0
4	D	13	0	0	2	0
All	All	5588	0	5686	413	1

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 37.

All (413) 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:1009:SER:CB	1:D:1074:LEU:HD22	1.68	1.22
1:A:1017:GLN:HE22	1:A:1020:LYS:NZ	1.45	1.14
1:C:985:ASN:ND2	1:C:988:ILE:HG12	1.61	1.13
1:C:1040:CYS:SG	1:C:1045:ILE:HD11	1.90	1.12
1:A:1073:MET:HB2	1:A:1079:ILE:CD1	1.81	1.10
1:B:987:ILE:HD12	1:B:1124:LEU:CD1	1.82	1.09
1:D:1104:GLU:O	1:D:1108:GLU:HG2	1.51	1.07
1:D:966:ILE:CG2	1:D:1002:SER:HB3	1.86	1.06
1:D:1054:GLU:O	1:D:1057:PRO:HD2	1.55	1.06
1:A:1069:VAL:O	1:A:1073:MET:HG2	1.60	1.01
1:D:1009:SER:OG	1:D:1074:LEU:HD22	1.59	1.01
1:D:987:ILE:HD12	1:D:1124:LEU:HD11	1.38	1.01
1:B:959:ASN:HD21	1:C:993:ARG:NH2	1.57	1.00
1:B:1078:ASN:HB3	1:C:960:GLN:NE2	1.76	1.00
1:B:1078:ASN:HB3	1:C:960:GLN:HE22	1.25	0.99
1:D:1030:THR:HG21	1:D:1057:PRO:HG3	1.41	0.98
1:D:1042:ASP:OD2	1:D:1045:ILE:HD12	1.63	0.98
1:C:1124:LEU:CD2	1:C:1126:TRP:NE1	2.27	0.98
1:D:985:ASN:O	1:D:988:ILE:HG22	1.61	0.97
1:D:966:ILE:HG22	1:D:1002:SER:HB3	1.42	0.97
1:B:987:ILE:HD12	1:B:1124:LEU:HD11	1.44	0.95
1:C:1124:LEU:HD22	1:C:1126:TRP:HE1	1.28	0.94
1:B:1063:LEU:N	1:B:1094:ASN:HD21	1.66	0.94
1:D:1050:LEU:HA	1:D:1053:CYS:SG	2.08	0.94
1:D:987:ILE:HD12	1:D:1124:LEU:CD1	1.97	0.93
1:A:960:GLN:OE1	1:A:1003:ARG:HD3	1.69	0.93
1:A:1012:LYS:HG3	1:A:1071:ALA:C	1.89	0.93
1:C:1124:LEU:HD22	1:C:1126:TRP:NE1	1.85	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASN:CG	1:A:988:ILE:HG12	1.89	0.91
1:B:1133:TYR:O	1:B:1133:TYR:CD1	2.23	0.91
1:C:987:ILE:HG12	1:C:1032:LEU:HD11	1.51	0.90
1:A:1040:CYS:SG	1:A:1042:ASP:HB2	2.11	0.90
1:B:966:ILE:HG22	1:B:1002:SER:HB3	1.54	0.89
1:C:985:ASN:ND2	1:C:988:ILE:CG1	2.35	0.89
1:C:1117:ARG:HG2	1:C:1117:ARG:HH11	1.33	0.89
1:A:1073:MET:HB2	1:A:1079:ILE:HD12	1.53	0.89
1:C:992:LYS:O	1:C:996:LEU:HD13	1.72	0.89
1:A:1042:ASP:OD1	1:A:1115:LYS:HD2	1.72	0.89
1:D:1043:LYS:O	1:D:1046:ARG:HG2	1.72	0.87
1:D:965:PRO:HB2	1:D:1092:VAL:HG13	1.55	0.87
1:A:985:ASN:OD1	1:A:988:ILE:HG12	1.73	0.87
1:D:1009:SER:OG	1:D:1074:LEU:CD2	2.22	0.86
1:D:1056:ILE:HG23	1:D:1098:LEU:CD1	2.04	0.86
1:C:985:ASN:CG	1:C:988:ILE:HG12	1.95	0.86
1:D:982:SER:HA	1:D:988:ILE:CG2	2.07	0.85
1:B:1078:ASN:CB	1:C:960:GLN:HE22	1.89	0.85
1:A:1017:GLN:HE22	1:A:1020:LYS:CE	1.90	0.84
1:C:1073:MET:HB3	1:C:1079:ILE:CD1	2.07	0.84
1:C:962:VAL:HG22	1:C:1003:ARG:HG2	1.57	0.84
1:D:1074:LEU:HD12	1:D:1075:GLY:N	1.93	0.84
1:A:1012:LYS:HG3	1:A:1071:ALA:O	1.78	0.84
1:A:963:ASN:N	1:A:1006:ARG:HG3	1.92	0.84
1:A:1070:LYS:HE3	1:A:1074:LEU:HD11	1.60	0.84
1:D:964:GLN:HB3	4:D:1302:HOH:O	1.77	0.83
1:D:1009:SER:HB2	1:D:1074:LEU:HD22	1.58	0.83
1:C:1017:GLN:HE22	1:C:1020:LYS:HD3	1.44	0.82
1:B:966:ILE:CG2	1:B:1002:SER:HB3	2.08	0.82
1:B:987:ILE:CD1	1:B:1124:LEU:HD11	2.09	0.81
1:A:1124:LEU:O	1:A:1124:LEU:HD12	1.80	0.81
1:D:977:ALA:O	1:D:988:ILE:HD11	1.80	0.81
1:A:1073:MET:CB	1:A:1079:ILE:CD1	2.59	0.81
1:A:1017:GLN:NE2	1:A:1020:LYS:NZ	2.28	0.81
1:D:987:ILE:CD1	1:D:1124:LEU:HD11	2.10	0.81
1:C:1036:VAL:HG22	1:C:1122:PHE:CE2	2.17	0.80
1:D:1030:THR:HG21	1:D:1057:PRO:CG	2.12	0.79
1:C:987:ILE:CG1	1:C:1032:LEU:HD11	2.12	0.79
1:C:987:ILE:CG2	1:C:1106:VAL:HG22	2.13	0.79
1:D:1063:LEU:N	1:D:1094:ASN:HD21	1.78	0.79
1:C:962:VAL:HG13	1:C:1002:SER:HB3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:992:LYS:O	1:D:996:LEU:HD13	1.82	0.79
1:D:1009:SER:CB	1:D:1074:LEU:CD2	2.57	0.78
1:A:1017:GLN:NE2	1:A:1020:LYS:CE	2.47	0.78
1:D:984:GLY:HA3	1:D:1125:ARG:HD2	1.66	0.78
1:A:1017:GLN:HE22	1:A:1020:LYS:HZ1	1.29	0.77
1:C:987:ILE:HG13	1:C:1032:LEU:HD13	1.66	0.77
1:A:1073:MET:HB2	1:A:1079:ILE:HD13	1.66	0.77
1:B:963:ASN:ND2	1:B:965:PRO:HD2	2.00	0.77
1:D:1042:ASP:O	1:D:1046:ARG:HD2	1.84	0.76
1:B:1063:LEU:HA	1:B:1094:ASN:ND2	2.00	0.76
1:D:1069:VAL:HB	1:D:1073:MET:HE3	1.66	0.76
1:C:987:ILE:CG1	1:C:1032:LEU:CD1	2.62	0.76
1:A:1017:GLN:CD	1:A:1020:LYS:HE3	2.05	0.76
1:A:1005:VAL:HB	1:A:1070:LYS:HE2	1.67	0.76
1:B:1107:ARG:NH1	2:B:1202:PIO:O11	2.18	0.76
1:D:965:PRO:HB2	1:D:1092:VAL:CG1	2.17	0.75
1:C:1009:SER:O	1:C:1012:LYS:HG2	1.86	0.75
1:C:980:TRP:CZ2	2:C:1201:PIO:O43	2.40	0.75
1:D:1054:GLU:C	1:D:1057:PRO:HD2	2.07	0.74
1:B:1063:LEU:CA	1:B:1094:ASN:HD21	2.01	0.74
1:A:1012:LYS:CG	1:A:1071:ALA:HB1	2.18	0.73
1:A:1017:GLN:NE2	1:A:1020:LYS:HE3	2.03	0.73
1:B:1000:GLU:O	1:B:1004:LEU:HG	1.87	0.73
1:A:1017:GLN:OE1	1:A:1020:LYS:HE3	1.88	0.73
1:B:1063:LEU:CA	1:B:1094:ASN:ND2	2.52	0.72
1:C:1073:MET:HB3	1:C:1079:ILE:HD13	1.70	0.72
1:C:1032:LEU:HD12	1:C:1033:ALA:N	2.05	0.71
1:D:965:PRO:CB	1:D:1092:VAL:CG1	2.68	0.71
1:A:1069:VAL:O	1:A:1073:MET:CG	2.38	0.71
1:A:1012:LYS:HD3	1:A:1072:THR:HA	1.71	0.71
1:A:1043:LYS:NZ	1:D:960:GLN:NE2	2.39	0.71
1:A:1117:ARG:HG2	1:A:1118:THR:HG23	1.72	0.71
1:D:1104:GLU:O	1:D:1108:GLU:CG	2.36	0.71
1:A:1017:GLN:OE1	1:A:1020:LYS:CE	2.38	0.70
1:C:998:MET:HE2	1:C:1022:ILE:HD13	1.72	0.70
1:D:1055:ARG:O	1:D:1059:ILE:HG13	1.90	0.70
1:C:963:ASN:HD22	1:C:966:ILE:HG13	1.55	0.70
1:D:1009:SER:CA	1:D:1074:LEU:HD22	2.21	0.70
1:C:971:GLN:HG2	1:D:1132:TRP:HZ2	1.57	0.70
1:B:1081:ASP:OD1	1:B:1082:GLU:N	2.24	0.69
1:C:1043:LYS:HG2	1:C:1046:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:ASN:ND2	1:D:988:ILE:HB	2.08	0.69
1:B:959:ASN:ND2	1:C:993:ARG:NH2	2.39	0.69
1:A:1048:ASN:O	1:A:1052:VAL:HG23	1.92	0.69
1:C:1043:LYS:HG2	1:C:1046:ARG:NH2	2.07	0.69
1:D:1100:GLN:O	1:D:1104:GLU:HG3	1.93	0.69
1:B:962:VAL:HG22	1:B:963:ASN:N	2.08	0.69
1:B:1068:THR:O	1:B:1072:THR:HG23	1.93	0.69
1:C:1069:VAL:O	1:C:1073:MET:HG3	1.92	0.68
1:D:966:ILE:HG21	1:D:1002:SER:N	2.08	0.68
1:A:1070:LYS:O	1:A:1074:LEU:HG	1.94	0.68
1:B:1078:ASN:CB	1:C:960:GLN:NE2	2.52	0.68
1:B:1081:ASP:O	1:B:1085:GLU:HG3	1.93	0.68
1:D:1124:LEU:O	1:D:1126:TRP:CD1	2.47	0.68
1:D:1050:LEU:CA	1:D:1053:CYS:SG	2.83	0.67
1:C:987:ILE:HG13	1:C:1032:LEU:CD1	2.24	0.67
1:D:966:ILE:CB	1:D:1002:SER:HB3	2.25	0.67
1:A:1042:ASP:OD1	1:A:1115:LYS:CD	2.43	0.67
1:D:1056:ILE:HG23	1:D:1098:LEU:HD11	1.74	0.67
1:A:1043:LYS:NZ	1:D:960:GLN:HE22	1.93	0.67
1:A:1043:LYS:O	1:A:1044:ARG:HB2	1.95	0.67
1:B:1043:LYS:NZ	4:B:1301:HOH:O	2.29	0.66
1:C:1073:MET:CE	1:C:1079:ILE:HD13	2.25	0.66
1:A:1043:LYS:HZ2	1:D:960:GLN:HE22	1.44	0.66
1:A:1012:LYS:HG3	1:A:1071:ALA:HB1	1.78	0.65
1:B:1001:MET:HE3	1:B:1022:ILE:HD12	1.79	0.65
1:C:1008:GLY:C	1:C:1074:LEU:HD21	2.18	0.65
1:C:1030:THR:CG2	1:C:1056:ILE:HB	2.27	0.64
1:C:1037:ALA:O	1:C:1046:ARG:HD3	1.96	0.64
1:C:965:PRO:HB2	1:C:1092:VAL:HG13	1.79	0.64
1:B:959:ASN:HD21	1:C:993:ARG:CZ	2.10	0.64
1:C:971:GLN:HG2	1:D:1132:TRP:CZ2	2.32	0.64
1:A:1017:GLN:HE22	1:A:1020:LYS:HZ2	1.42	0.64
1:C:1073:MET:CE	1:C:1079:ILE:HG21	2.28	0.64
1:C:1036:VAL:HG22	1:C:1122:PHE:HE2	1.61	0.64
1:C:987:ILE:HG21	1:C:1106:VAL:HG22	1.78	0.63
1:B:1063:LEU:N	1:B:1094:ASN:ND2	2.42	0.63
1:D:1043:LYS:O	1:D:1047:THR:HG23	1.99	0.63
1:D:1050:LEU:O	1:D:1053:CYS:SG	2.55	0.62
1:D:1069:VAL:O	1:D:1073:MET:HG2	1.99	0.62
1:D:961:PRO:HB2	1:D:1006:ARG:NE	2.13	0.62
1:C:1124:LEU:CD2	1:C:1126:TRP:CE2	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:980:TRP:HZ2	2:C:1201:PIO:O43	1.82	0.62
1:A:960:GLN:OE1	1:A:1003:ARG:CD	2.46	0.62
1:A:988:ILE:HD11	1:A:1126:TRP:CZ3	2.34	0.62
1:C:1073:MET:CB	1:C:1079:ILE:CD1	2.77	0.62
1:A:1070:LYS:CE	1:A:1074:LEU:HD11	2.29	0.62
1:C:998:MET:CE	1:C:1022:ILE:HD13	2.30	0.62
1:D:965:PRO:CB	1:D:1092:VAL:HG11	2.30	0.62
1:D:982:SER:HA	1:D:988:ILE:HG23	1.80	0.62
1:A:1069:VAL:HG12	1:A:1073:MET:SD	2.40	0.62
1:A:986:ASP:OD2	1:B:993:ARG:NH2	2.33	0.61
2:B:1202:PIO:O43	2:B:1202:PIO:H3	2.00	0.61
1:C:988:ILE:HG22	1:C:992:LYS:HD2	1.82	0.61
1:B:1069:VAL:O	1:B:1072:THR:OG1	2.18	0.61
1:B:962:VAL:HG22	1:B:963:ASN:H	1.65	0.61
2:B:1202:PIO:O12	2:B:1202:PIO:O2	2.16	0.61
1:C:965:PRO:HB2	1:C:1092:VAL:CG1	2.30	0.61
1:D:1009:SER:HB2	1:D:1074:LEU:CD2	2.25	0.61
1:A:962:VAL:CG2	1:A:1002:SER:OG	2.49	0.61
1:B:1042:ASP:HB2	1:B:1115:LYS:HD2	1.81	0.61
1:A:1100:GLN:HE21	1:A:1104:GLU:HG3	1.65	0.61
1:A:1040:CYS:SG	1:A:1042:ASP:CB	2.86	0.61
1:C:998:MET:O	1:C:1001:MET:HB3	2.01	0.60
1:D:985:ASN:OD1	1:D:1124:LEU:HD22	2.01	0.60
1:A:1130:THR:OG1	1:A:1134:GLN:HA	2.01	0.60
1:A:1070:LYS:HG2	1:A:1074:LEU:HD11	1.84	0.60
1:C:1012:LYS:HB2	1:C:1071:ALA:HB1	1.84	0.60
1:D:1043:LYS:O	1:D:1046:ARG:CG	2.46	0.60
1:B:1012:LYS:NZ	2:B:1201:PIO:O2	2.24	0.60
1:D:1009:SER:HB2	1:D:1074:LEU:HD13	1.84	0.60
1:A:1063:LEU:HB2	1:A:1094:ASN:HD21	1.67	0.60
1:C:1030:THR:HG21	1:C:1056:ILE:HB	1.82	0.60
1:D:1034:LYS:O	1:D:1038:LYS:HG2	2.02	0.59
1:D:965:PRO:CB	1:D:1092:VAL:HG13	2.26	0.59
1:C:966:ILE:CD1	1:C:1005:VAL:HG21	2.32	0.59
1:C:1073:MET:HE3	1:C:1079:ILE:HD13	1.84	0.59
1:A:1124:LEU:HD13	1:A:1126:TRP:CD1	2.38	0.59
1:A:985:ASN:ND2	1:A:988:ILE:HG12	2.18	0.59
1:C:966:ILE:HG22	1:C:1002:SER:OG	2.02	0.59
1:C:987:ILE:CG1	1:C:1032:LEU:HD13	2.30	0.59
1:D:982:SER:HA	1:D:988:ILE:HG21	1.81	0.59
1:D:961:PRO:O	1:D:1006:ARG:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:980:TRP:CH2	2:C:1201:PIO:O43	2.55	0.58
1:D:1053:CYS:O	1:D:1057:PRO:HD3	2.03	0.58
1:C:962:VAL:CG2	1:C:1003:ARG:HG2	2.33	0.58
1:D:1030:THR:O	1:D:1034:LYS:HG3	2.03	0.58
1:A:1017:GLN:CD	1:A:1020:LYS:CE	2.73	0.57
1:A:962:VAL:C	1:A:1006:ARG:HG3	2.25	0.57
1:B:962:VAL:HG23	1:B:1002:SER:O	2.05	0.57
2:B:1202:PIO:O4	2:B:1202:PIO:O53	2.23	0.57
1:C:1017:GLN:NE2	1:C:1020:LYS:HD3	2.19	0.57
1:C:964:GLN:HB2	1:C:965:PRO:HD3	1.87	0.57
1:D:1043:LYS:C	1:D:1046:ARG:HG2	2.25	0.57
1:C:1104:GLU:O	1:C:1107:ARG:HG2	2.04	0.57
1:A:1041:THR:O	1:A:1041:THR:HG22	2.04	0.57
1:A:1073:MET:HA	1:A:1076:ARG:CD	2.35	0.57
1:A:1076:ARG:O	1:A:1077:THR:HB	2.04	0.57
1:C:1079:ILE:HG22	1:C:1080:SER:O	2.05	0.56
1:D:1056:ILE:HD13	1:D:1102:VAL:HG22	1.87	0.56
1:D:966:ILE:CG2	1:D:1002:SER:CB	2.72	0.56
1:A:1073:MET:HA	1:A:1076:ARG:HD3	1.87	0.56
1:B:1133:TYR:O	1:B:1133:TYR:CG	2.54	0.56
1:C:1042:ASP:OD1	1:C:1045:ILE:CG1	2.54	0.56
1:D:987:ILE:HD12	1:D:1124:LEU:HD13	1.86	0.56
1:C:1117:ARG:HG2	1:C:1117:ARG:NH1	2.09	0.56
1:C:963:ASN:CG	1:C:965:PRO:HD2	2.26	0.56
1:D:1069:VAL:HB	1:D:1073:MET:CE	2.34	0.56
1:D:1056:ILE:HG23	1:D:1098:LEU:HD12	1.86	0.56
1:C:1124:LEU:HD23	1:C:1126:TRP:NE1	2.19	0.56
1:D:1056:ILE:HD11	1:D:1101:SER:C	2.26	0.56
1:D:1063:LEU:N	1:D:1094:ASN:ND2	2.51	0.56
1:A:1005:VAL:CB	1:A:1070:LYS:HE2	2.36	0.55
1:C:962:VAL:CG1	1:C:1002:SER:HB3	2.33	0.55
1:A:1077:THR:O	1:A:1077:THR:HG22	2.07	0.55
2:C:1201:PIO:O3	2:C:1201:PIO:O43	2.23	0.55
1:D:967:LEU:O	1:D:971:GLN:HG3	2.06	0.55
1:C:1036:VAL:CG2	1:C:1122:PHE:CE2	2.89	0.55
1:D:1111:ALA:O	1:D:1112:ALA:HB3	2.07	0.54
1:B:959:ASN:ND2	1:C:993:ARG:CZ	2.71	0.54
1:D:966:ILE:HB	1:D:1002:SER:CB	2.38	0.54
1:D:1056:ILE:HG13	1:D:1101:SER:HB3	1.88	0.54
1:A:1119:ASP:O	1:A:1120:ALA:HB3	2.07	0.54
1:D:1081:ASP:O	1:D:1085:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:LYS:NZ	2:B:1202:PIO:O5	2.39	0.54
1:D:966:ILE:HB	1:D:1002:SER:HB3	1.88	0.54
1:D:1049:LEU:O	1:D:1053:CYS:SG	2.66	0.54
1:D:966:ILE:HG21	1:D:1002:SER:CA	2.37	0.54
1:A:1111:ALA:O	1:A:1114:ILE:HG12	2.08	0.54
1:C:1068:THR:O	1:C:1072:THR:HG23	2.08	0.54
1:D:1133:TYR:O	1:D:1134:GLN:HB2	2.06	0.54
1:A:1114:ILE:HG13	1:A:1115:LYS:HG3	1.89	0.54
1:B:966:ILE:CG2	1:B:1002:SER:CB	2.84	0.54
2:C:1201:PIO:HO3	2:C:1201:PIO:P4	2.31	0.54
1:D:1080:SER:OG	1:D:1083:GLU:HG3	2.08	0.54
1:A:1012:LYS:HG2	1:A:1071:ALA:HB1	1.88	0.54
1:A:987:ILE:HG12	1:A:1032:LEU:HB2	1.88	0.54
1:D:1043:LYS:HA	1:D:1046:ARG:CD	2.38	0.54
1:A:1070:LYS:HG2	1:A:1074:LEU:CD1	2.38	0.54
1:B:1118:THR:O	1:B:1118:THR:HG23	2.07	0.54
1:C:986:ASP:HB3	1:C:1032:LEU:HD22	1.91	0.53
1:B:1107:ARG:NH1	2:B:1202:PIO:O6	2.41	0.53
1:A:1070:LYS:CG	1:A:1074:LEU:HD11	2.38	0.53
1:C:1043:LYS:HA	1:C:1046:ARG:NH2	2.24	0.53
1:A:963:ASN:HB2	1:A:1006:ARG:HG2	1.91	0.53
1:A:1017:GLN:OE1	1:A:1020:LYS:HE2	2.08	0.53
1:C:1017:GLN:HE22	1:C:1020:LYS:CD	2.19	0.53
1:A:1015:LEU:HD23	1:A:1071:ALA:HB2	1.91	0.52
1:C:1048:ASN:O	1:C:1052:VAL:HG12	2.10	0.52
1:D:1068:THR:O	1:D:1072:THR:HG23	2.09	0.52
1:A:1073:MET:CB	1:A:1079:ILE:HD12	2.34	0.52
1:B:1054:GLU:O	1:B:1057:PRO:HD2	2.10	0.52
1:C:1133:TYR:CD1	1:C:1133:TYR:O	2.63	0.52
1:D:1001:MET:CE	1:D:1022:ILE:HD12	2.39	0.52
1:D:1056:ILE:CG1	1:D:1101:SER:HB3	2.39	0.52
1:B:1089:GLU:HA	1:B:1092:VAL:HG22	1.92	0.52
1:D:1009:SER:HA	1:D:1074:LEU:HD22	1.92	0.52
1:C:992:LYS:O	1:C:996:LEU:CD1	2.52	0.51
1:D:1073:MET:O	1:D:1073:MET:HG3	2.09	0.51
1:A:1012:LYS:HE2	1:A:1071:ALA:O	2.10	0.51
1:D:1043:LYS:HA	1:D:1046:ARG:HG2	1.93	0.51
1:B:1122:PHE:CD2	1:B:1123:THR:N	2.79	0.51
1:C:963:ASN:OD1	1:C:965:PRO:HD2	2.11	0.51
1:C:966:ILE:CG2	1:C:1002:SER:OG	2.58	0.51
1:A:1012:LYS:CD	1:A:1072:THR:HA	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:ILE:HG13	1:A:1032:LEU:HD13	1.94	0.50
1:C:986:ASP:CB	1:C:1032:LEU:HD22	2.41	0.50
1:C:1117:ARG:HH11	1:C:1117:ARG:CG	2.11	0.50
1:D:1056:ILE:HG12	1:D:1101:SER:HB2	1.92	0.50
1:D:1012:LYS:HG3	1:D:1071:ALA:HB1	1.93	0.50
1:C:1009:SER:O	1:C:1012:LYS:CG	2.59	0.50
1:C:965:PRO:CB	1:C:1092:VAL:CG1	2.89	0.50
1:C:966:ILE:HD12	1:C:1005:VAL:HG21	1.92	0.50
1:B:1128:ARG:NH2	2:B:1202:PIO:O43	2.45	0.50
1:D:1042:ASP:OD1	1:D:1043:LYS:N	2.43	0.50
1:B:1122:PHE:CG	1:B:1123:THR:N	2.80	0.50
1:D:977:ALA:CA	1:D:988:ILE:HD11	2.42	0.50
1:C:1124:LEU:HD21	1:C:1126:TRP:CE2	2.46	0.50
1:C:1042:ASP:OD1	1:C:1045:ILE:HG13	2.12	0.50
1:A:1117:ARG:C	1:A:1118:THR:HG23	2.32	0.49
1:D:1042:ASP:OD2	1:D:1045:ILE:CD1	2.50	0.49
1:A:1012:LYS:HG3	1:A:1071:ALA:CB	2.40	0.49
1:A:1073:MET:HE3	1:A:1079:ILE:HD13	1.93	0.49
1:A:1043:LYS:O	1:A:1044:ARG:CB	2.59	0.49
1:C:1117:ARG:CG	1:C:1117:ARG:NH1	2.72	0.49
1:B:987:ILE:HD12	1:B:1124:LEU:HD13	1.86	0.49
1:C:1093:HIS:CD2	1:C:1097:ASN:HD21	2.31	0.49
1:A:1070:LYS:HE3	1:A:1074:LEU:CD1	2.36	0.48
1:B:979:LYS:NZ	2:B:1202:PIO:C5	2.76	0.48
1:A:1037:ALA:HA	1:A:1049:LEU:HD23	1.95	0.48
1:B:966:ILE:HD12	1:B:1002:SER:HA	1.95	0.48
1:A:1013:ARG:NE	1:B:1121:GLY:HA2	2.28	0.48
1:A:1124:LEU:C	1:A:1124:LEU:HD12	2.34	0.48
1:C:1079:ILE:HG23	1:C:1083:GLU:HB2	1.95	0.48
1:D:1059:ILE:HG22	1:D:1094:ASN:OD1	2.13	0.48
1:D:1009:SER:HB2	1:D:1074:LEU:CD1	2.44	0.48
1:D:1030:THR:HG21	1:D:1057:PRO:CD	2.44	0.48
1:A:1043:LYS:HZ2	1:D:960:GLN:NE2	2.05	0.48
1:A:966:ILE:HD12	1:A:1005:VAL:HG21	1.95	0.48
1:C:1102:VAL:O	1:C:1106:VAL:HG23	2.14	0.48
1:D:961:PRO:HB3	1:D:1006:ARG:NH2	2.28	0.48
1:C:1030:THR:HG22	1:C:1056:ILE:HD12	1.96	0.48
1:A:1017:GLN:NE2	1:A:1020:LYS:HZ2	2.05	0.47
1:A:1047:THR:O	1:A:1051:GLN:HG3	2.15	0.47
1:B:966:ILE:HG21	1:B:1002:SER:CA	2.43	0.47
1:A:1001:MET:HE1	1:A:1022:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ILE:HG13	1:A:1116:ILE:O	2.13	0.47
1:A:1005:VAL:CA	1:A:1070:LYS:HE2	2.45	0.47
1:D:977:ALA:HA	1:D:988:ILE:HD11	1.97	0.47
1:D:1001:MET:HE3	1:D:1022:ILE:HD12	1.96	0.47
1:A:985:ASN:CG	1:A:988:ILE:CG1	2.72	0.47
1:B:962:VAL:HG23	1:B:1002:SER:C	2.36	0.47
1:B:962:VAL:HB	1:B:1003:ARG:HG2	1.97	0.46
1:B:1069:VAL:O	1:B:1073:MET:HG2	2.16	0.46
1:B:961:PRO:HA	4:C:1306:HOH:O	2.15	0.46
1:C:1132:TRP:HZ3	1:D:996:LEU:HA	1.79	0.46
1:B:966:ILE:HB	1:B:1002:SER:CB	2.46	0.46
1:A:1117:ARG:O	1:A:1118:THR:CG2	2.63	0.46
1:D:1050:LEU:C	1:D:1053:CYS:SG	2.94	0.46
1:D:985:ASN:HD22	1:D:988:ILE:HB	1.80	0.46
1:B:962:VAL:CG2	1:B:963:ASN:H	2.29	0.46
1:A:963:ASN:HB2	1:A:1006:ARG:CG	2.45	0.46
1:A:987:ILE:CG1	1:A:1032:LEU:HB2	2.47	0.45
1:A:1133:TYR:O	1:A:1133:TYR:CD1	2.69	0.45
1:B:962:VAL:CG2	1:B:963:ASN:N	2.75	0.45
1:C:965:PRO:CB	1:C:1092:VAL:HG11	2.46	0.45
1:C:1093:HIS:CD2	1:C:1097:ASN:ND2	2.84	0.45
1:C:974:HIS:O	1:C:978:THR:HG22	2.17	0.45
1:C:1015:LEU:HD12	1:C:1015:LEU:O	2.17	0.45
1:C:1029:VAL:O	1:C:1032:LEU:HG	2.17	0.45
1:B:979:LYS:NZ	2:B:1202:PIO:H5	2.31	0.45
1:D:1052:VAL:HG11	1:D:1108:GLU:HG3	1.99	0.45
1:A:1001:MET:CE	1:A:1022:ILE:HD12	2.47	0.45
1:A:1073:MET:CE	1:A:1079:ILE:HD13	2.46	0.45
1:C:1111:ALA:HA	1:C:1114:ILE:HD12	1.97	0.45
1:C:1003:ARG:NH1	1:D:1134:GLN:HB2	2.31	0.44
1:A:962:VAL:HG23	1:A:1002:SER:OG	2.15	0.44
1:B:1088:THR:O	1:B:1092:VAL:HG13	2.16	0.44
1:C:1030:THR:CG2	1:C:1056:ILE:HD12	2.48	0.44
1:A:986:ASP:O	1:A:987:ILE:C	2.55	0.44
1:B:1107:ARG:CZ	2:B:1202:PIO:O6	2.65	0.44
1:D:1063:LEU:CA	1:D:1094:ASN:ND2	2.81	0.44
1:C:1077:THR:O	1:C:1078:ASN:HB3	2.17	0.44
1:D:1043:LYS:HA	1:D:1046:ARG:HD3	1.99	0.44
1:C:1037:ALA:HB1	1:C:1046:ARG:HG3	2.00	0.44
1:B:962:VAL:CG2	1:B:1003:ARG:HG2	2.48	0.43
1:C:1073:MET:HA	1:C:1079:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:966:ILE:HB	1:C:1002:SER:OG	2.18	0.43
1:D:1043:LYS:CA	1:D:1046:ARG:HG2	2.47	0.43
1:B:1089:GLU:HA	1:B:1092:VAL:CG2	2.48	0.43
1:C:1080:SER:C	1:C:1082:GLU:N	2.70	0.43
1:A:1005:VAL:O	1:A:1070:LYS:CE	2.66	0.43
1:B:1088:THR:O	1:B:1092:VAL:HG22	2.17	0.43
1:D:1074:LEU:HD12	1:D:1074:LEU:C	2.36	0.43
1:B:1041:THR:HB	1:B:1115:LYS:HB3	2.01	0.43
1:B:1122:PHE:O	1:B:1123:THR:HB	2.17	0.43
1:C:980:TRP:HB2	1:C:988:ILE:CD1	2.49	0.43
1:D:965:PRO:CG	1:D:1092:VAL:HG11	2.49	0.43
1:A:1042:ASP:CG	1:A:1115:LYS:HD2	2.35	0.43
1:D:1062:GLN:C	1:D:1094:ASN:HD21	2.20	0.43
1:D:961:PRO:O	1:D:1006:ARG:CB	2.67	0.43
1:C:1073:MET:HE2	1:C:1079:ILE:HD13	1.98	0.43
1:D:1063:LEU:HA	1:D:1094:ASN:ND2	2.34	0.43
1:D:965:PRO:HG2	1:D:1092:VAL:HG11	2.00	0.43
1:D:1006:ARG:HD3	4:D:1303:HOH:O	2.19	0.43
1:A:1012:LYS:CG	1:A:1071:ALA:O	2.60	0.43
1:B:1030:THR:CG2	1:B:1056:ILE:HB	2.49	0.42
1:A:1076:ARG:O	1:A:1077:THR:CB	2.68	0.42
1:A:987:ILE:HD11	1:A:1032:LEU:HB3	2.00	0.42
1:D:1056:ILE:CG1	1:D:1101:SER:CB	2.97	0.42
1:D:1056:ILE:HG12	1:D:1101:SER:CB	2.50	0.42
1:D:1069:VAL:O	1:D:1073:MET:HE2	2.20	0.42
1:B:1039:GLN:OE1	1:B:1118:THR:HG22	2.20	0.42
2:B:1202:PIO:O51	2:B:1202:PIO:H4	2.19	0.42
1:C:1107:ARG:HG3	1:C:1108:GLU:N	2.35	0.42
1:C:966:ILE:HG21	1:C:1002:SER:N	2.34	0.42
1:B:1089:GLU:CA	1:B:1092:VAL:HG22	2.50	0.42
1:B:979:LYS:HZ3	2:B:1202:PIO:C5	2.33	0.42
1:C:1122:PHE:CE2	1:C:1124:LEU:HB2	2.54	0.42
1:D:965:PRO:HB3	1:D:1092:VAL:CG1	2.48	0.42
1:A:1117:ARG:C	1:A:1118:THR:CG2	2.88	0.42
1:C:1124:LEU:HD23	1:C:1126:TRP:CD1	2.55	0.42
1:D:1093:HIS:CD2	1:D:1097:ASN:HD21	2.38	0.42
1:B:1055:ARG:O	1:B:1059:ILE:HG13	2.20	0.41
1:D:1007:GLY:HA3	1:D:1011:THR:HG21	2.01	0.41
1:D:959:ASN:O	1:D:959:ASN:OD1	2.38	0.41
1:A:1069:VAL:O	1:A:1073:MET:SD	2.78	0.41
1:B:966:ILE:CD1	1:B:1002:SER:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1030:THR:HG21	1:D:1057:PRO:HD3	2.03	0.41
1:B:1001:MET:CE	1:B:1022:ILE:HD12	2.46	0.41
1:B:1043:LYS:HG2	1:B:1046:ARG:HH22	1.85	0.41
1:A:1012:LYS:CE	1:A:1072:THR:HA	2.50	0.41
1:D:1070:LYS:HA	1:D:1073:MET:HG2	2.03	0.41
1:D:981:SER:O	1:D:988:ILE:HG21	2.21	0.41
1:A:1037:ALA:HB1	1:A:1050:LEU:HG	2.03	0.41
1:A:1035:GLU:O	1:A:1039:GLN:HG2	2.21	0.41
1:C:966:ILE:HD11	1:C:1005:VAL:HG21	2.02	0.41
1:A:1012:LYS:HG3	1:A:1071:ALA:CA	2.49	0.41
1:C:1042:ASP:CG	1:C:1045:ILE:HG12	2.41	0.41
1:D:1056:ILE:HD11	1:D:1102:VAL:N	2.36	0.40
1:C:1059:ILE:HG23	1:C:1094:ASN:OD1	2.22	0.40
2:C:1201:PIO:P4	2:C:1201:PIO:O3	2.79	0.40
1:B:1118:THR:CG2	1:B:1118:THR:O	2.68	0.40
1:C:988:ILE:CG2	1:C:992:LYS:NZ	2.85	0.40

All (1) 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)
1:A:983:LYS:NZ	1:B:1133:TYR:C[2_655]	2.19	0.01

## 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	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
1	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
1	C	173/176 (98%)	168 (97%)	5 (3%)	0	100	100
1	D	163/176 (93%)	160 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	684/704 (97%)	668 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	148/148 (100%)	148 (100%)	0	100	100
1	B	148/148 (100%)	148 (100%)	0	100	100
1	C	147/148 (99%)	147 (100%)	0	100	100
1	D	141/148 (95%)	141 (100%)	0	100	100
All	All	584/592 (99%)	584 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1017	GLN
1	A	1086	GLN
1	A	1094	ASN
1	A	1100	GLN
1	B	959	ASN
1	B	1094	ASN
1	C	960	GLN
1	C	963	ASN
1	C	1017	GLN
1	D	960	GLN
1	D	963	ASN
1	D	1094	ASN
1	D	1100	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 ⓘ

8 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	PIO	A	1201	-	27,29,47	0.64	0	41,45,65	1.62	8 (19%)
3	PO4	A	1202	-	4,4,4	0.69	0	6,6,6	0.23	0
2	PIO	B	1201	-	21,24,47	0.72	0	39,39,65	1.78	11 (28%)
2	PIO	B	1202	-	21,24,47	0.70	0	39,39,65	1.71	10 (25%)
3	PO4	B	1203	-	4,4,4	0.69	0	6,6,6	0.23	0
3	PO4	B	1204	-	4,4,4	0.68	0	6,6,6	0.23	0
2	PIO	C	1201	-	21,24,47	0.72	0	39,39,65	1.78	11 (28%)
2	PIO	D	1201	-	21,24,47	0.94	1 (4%)	39,39,65	1.78	11 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIO	A	1201	-	-	0/23/47/68	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1202	-	-	0/0/0/0	0/0/0/0
2	PIO	B	1201	-	-	0/15/39/68	0/1/1/1
2	PIO	B	1202	-	-	1/15/39/68	0/1/1/1
3	PO4	B	1203	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1204	-	-	0/0/0/0	0/0/0/0
2	PIO	C	1201	-	-	0/15/39/68	0/1/1/1
2	PIO	D	1201	-	-	1/15/39/68	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	PIO	P1-O12	3.28	1.61	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	PIO	O5-P5-O53	-4.23	97.38	107.48
2	A	1201	PIO	O5-P5-O53	-4.21	97.42	107.48
2	C	1201	PIO	O1-P1-O12	-3.80	98.41	107.48
2	B	1201	PIO	O1-P1-O12	-3.79	98.43	107.48
2	B	1201	PIO	O4-P4-O42	-3.29	99.62	107.48
2	C	1201	PIO	O4-P4-O42	-3.29	99.63	107.48
2	A	1201	PIO	O4-P4-O42	-3.28	99.64	107.48
2	D	1201	PIO	O11-P1-O12	-3.20	100.18	110.63
2	C	1201	PIO	O13-P1-O12	-3.19	100.21	110.63
2	B	1201	PIO	O13-P1-O12	-3.19	100.23	110.63
2	B	1201	PIO	O52-P5-O5	-3.09	97.37	106.62
2	C	1201	PIO	O52-P5-O5	-3.09	97.39	106.62
2	D	1201	PIO	O52-P5-O5	-3.08	97.42	106.62
2	B	1202	PIO	O11-P1-O1	-2.76	98.36	106.62
2	D	1201	PIO	O11-P1-O1	-2.75	98.39	106.62
2	A	1201	PIO	O1-P1-O12	-2.67	98.39	109.34
2	B	1202	PIO	O43-P4-O4	-2.34	99.63	106.62
2	D	1201	PIO	O43-P4-O4	-2.33	99.66	106.62
2	A	1201	PIO	O13-P1-O12	-2.20	100.19	109.21
2	B	1202	PIO	O4-P4-O42	-2.07	102.54	107.48
2	B	1201	PIO	O13-P1-O11	2.02	114.86	107.44
2	C	1201	PIO	O13-P1-O11	2.04	114.92	107.44
2	D	1201	PIO	C3-C2-C1	2.09	114.25	109.63
2	B	1201	PIO	O11-P1-O12	2.23	117.90	110.63
2	B	1202	PIO	O11-P1-O12	2.23	117.90	110.63
2	C	1201	PIO	O11-P1-O12	2.23	117.92	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	PIO	O11-P1-O1	2.49	114.05	106.62
2	B	1201	PIO	O11-P1-O1	2.49	114.08	106.62
2	D	1201	PIO	O13-P1-O1	2.50	114.09	106.62
2	B	1202	PIO	O1-P1-O12	2.78	114.12	107.48
2	D	1201	PIO	O13-P1-O11	2.84	117.88	107.44
2	B	1201	PIO	P5-O5-C5	2.97	129.16	121.56
2	C	1201	PIO	P5-O5-C5	2.98	129.20	121.56
2	B	1202	PIO	P5-O5-C5	2.99	129.21	121.56
2	D	1201	PIO	P5-O5-C5	2.99	129.22	121.56
2	A	1201	PIO	P5-O5-C5	3.00	129.24	121.56
2	A	1201	PIO	O52-P5-O5	3.32	116.55	106.62
2	D	1201	PIO	O51-P5-O5	3.34	116.61	106.62
2	B	1202	PIO	O52-P5-O5	3.35	116.63	106.62
2	B	1201	PIO	P4-O4-C4	3.59	130.77	121.56
2	A	1201	PIO	P4-O4-C4	3.60	130.79	121.56
2	B	1202	PIO	P4-O4-C4	3.61	130.80	121.56
2	D	1201	PIO	P4-O4-C4	3.61	130.81	121.56
2	C	1201	PIO	P4-O4-C4	3.69	131.01	121.56
2	A	1201	PIO	O43-P4-O4	3.74	117.82	106.62
2	B	1202	PIO	O41-P4-O4	3.74	117.82	106.62
2	C	1201	PIO	O43-P4-O4	3.75	117.83	106.62
2	B	1201	PIO	O43-P4-O4	3.76	117.85	106.62
2	B	1201	PIO	O5-P5-O53	3.82	116.58	107.48
2	C	1201	PIO	O5-P5-O53	3.84	116.63	107.48
2	D	1201	PIO	O4-P4-O42	4.33	117.82	107.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1202	PIO	P5-O5-C5-C4
2	D	1201	PIO	P5-O5-C5-C4

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	PIO	1	0
2	B	1202	PIO	12	0
2	C	1201	PIO	6	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	176/176 (100%)	0.83	22 (12%) 5 2	82, 117, 173, 198	0
1	B	175/176 (99%)	0.47	6 (3%) 49 24	30, 99, 146, 164	0
1	C	175/176 (99%)	0.41	7 (4%) 42 20	67, 105, 149, 171	0
1	D	166/176 (94%)	0.73	20 (12%) 6 2	30, 111, 156, 171	0
All	All	692/704 (98%)	0.61	55 (7%) 15 5	30, 108, 158, 198	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	CYS	6.3
1	A	1041	THR	6.0
1	A	1042	ASP	5.8
1	D	960	GLN	4.2
1	D	1056	ILE	4.2
1	A	1043	LYS	3.9
1	A	1117	ARG	3.8
1	D	1049	LEU	3.8
1	C	1108	GLU	3.6
1	A	1001	MET	3.6
1	C	1120	ALA	3.4
1	D	1036	VAL	3.4
1	D	1045	ILE	3.3
1	C	986	ASP	3.0
1	D	1040	CYS	3.0
1	D	1052	VAL	2.9
1	D	1051	GLN	2.8
1	A	1090	MET	2.7
1	A	1076	ARG	2.7
1	B	961	PRO	2.7
1	C	1051	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1074	LEU	2.6
1	C	1119	ASP	2.6
1	B	1094	ASN	2.5
1	A	1005	VAL	2.5
1	D	1079	ILE	2.5
1	D	1108	GLU	2.5
1	A	1070	LYS	2.5
1	D	1072	THR	2.4
1	A	1038	LYS	2.4
1	C	1122	PHE	2.4
1	D	1044	ARG	2.4
1	D	1105	THR	2.4
1	B	959	ASN	2.4
1	A	1015	LEU	2.4
1	D	977	ALA	2.3
1	A	1079	ILE	2.3
1	B	1060	SER	2.3
1	A	966	ILE	2.3
1	A	1063	LEU	2.3
1	D	1078	ASN	2.3
1	D	1071	ALA	2.3
1	B	960	GLN	2.3
1	D	1104	GLU	2.2
1	A	1078	ASN	2.2
1	A	1044	ARG	2.2
1	A	1045	ILE	2.2
1	A	1094	ASN	2.2
1	D	1034	LYS	2.1
1	D	1037	ALA	2.1
1	D	1047	THR	2.1
1	C	1079	ILE	2.0
1	A	1067	SER	2.0
1	A	1125	ARG	2.0
1	B	1061	THR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PIO	C	1201	24/47	0.46	0.54	5.21	133,134,137,137	24
2	PIO	B	1202	24/47	0.52	0.52	2.77	115,120,128,128	24
2	PIO	B	1201	24/47	0.42	0.39	0.92	146,150,155,156	24
3	PO4	A	1202	5/5	0.90	0.28	0.46	167,168,168,169	0
3	PO4	B	1203	5/5	0.68	0.30	0.12	146,148,148,149	0
2	PIO	D	1201	24/47	0.74	0.33	0.03	145,148,155,155	24
2	PIO	A	1201	29/47	0.60	0.26	-0.26	158,180,184,185	29
3	PO4	B	1204	5/5	0.94	0.43	-	30,30,30,30	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.