



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:31 pm GMT

PDB ID : 1WC6  
Title : Soluble adenylyl cyclase CyaC from *S. platensis* in complex with Rp- ATPal-phaS in presence of bicarbonate  
Authors : Steegborn, C.; Litvin, T.N.; Levin, L.R.; Buck, J.; Wu, H.  
Deposited on : 2004-11-08  
Resolution : 2.51 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

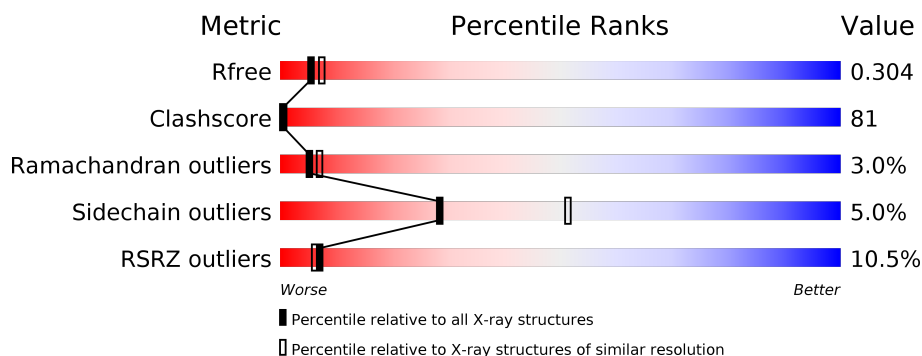
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	226	<div> <div>5%</div> <div>19%</div> <div>62%</div> <div>5%</div> <div>14%</div> </div>
1	B	226	<div> <div>6%</div> <div>23%</div> <div>57%</div> <div>6%</div> <div>15%</div> </div>
1	C	226	<div> <div>16%</div> <div>20%</div> <div>61%</div> <div>5%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

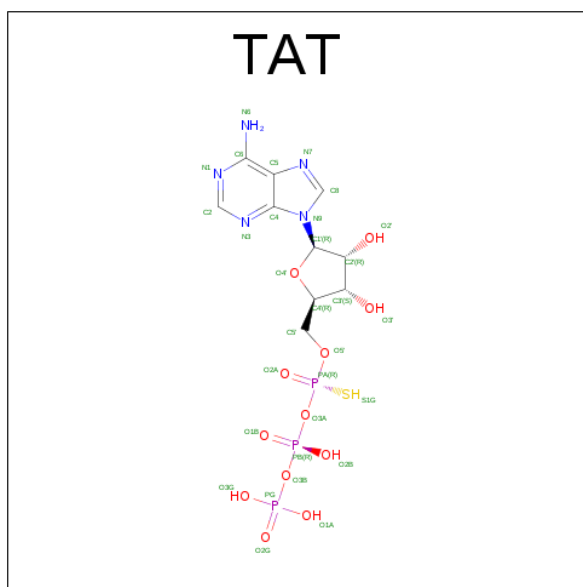
There are 4 unique types of molecules in this entry. The entry contains 4631 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	3	0	1
			1485	935	259	279	12			
1	B	193	Total	C	N	O	S	0	0	1
			1477	930	258	278	11			
1	C	194	Total	C	N	O	S	15	0	1
			1485	935	259	279	12			

- Molecule 2 is ADENOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: TAT) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	35	Total	O	0	0
			35	35		
4	C	27	Total	O	0	0
			27	27		



Q1168	E1173	E1174	I1175	I1176	K1177	R1178	E1179	F1180	L1181	E1182	L1183	K1184	G1185	I1186	D1187	E1188	P1189	M1190	M1191	T1192	C1193	V1194	I1195	M1196	P1197	N1198	M1199	L1200	ASN	GLN																					
Y1040	L1041	G1042	E1043	M1044	T1045	R1046	A1047	V1048	F1049	E1050	N1051	Q1052	G1053	T1054	V1055	D1056	K1057	F1058	V1059	G1060	D1061	A1062	I1063	M1064	A1065	L1066	Y1067	G1068	A1069																						
G1104	L1105	V1106	G1107	ARG	ASN	GLU	V1111	P1112	P1113	V1114	R1115	F1116	R1117	C1118	G1119	I1120	H1121	Q1122	G1123	M1124	A1125	V1126	V1127	F1130	G1131	S1132	S1136	D1137	F1138	T1139	A1140	T1141	G1142	P1143	S1144	V1145	M1146	T1147													
E1023	M1024	S1025	N1026	A1027	L1028	Q1029	S1030	Q1031	G1032	V1033	A1034	L1037	M1038	E1039	E1072	M1073	S1074	P1075	S1076	E1077	Q1078	V1079	R1080	R1081	A1082	I1083	A1084	T1085	A1086	R1087	Q1088	M1089	L1090	V1091	A1092	L1093	E1094	K1095	L1096	W1100	R1103										
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	GLY	ASP	L1004	R1005	P1006	L1010	I1011	T1012	I1013	L1014	F1015	S1016	D1017	I1018	V1019	G1020	F1021	T1022	R1023	S1024	N1025	A1026	L1027	Q1028	S1029	Q1030	G1031	G1032	V1033	A1034	L1037	M1038	E1039

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.15Å 73.97Å 266.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.51 38.03 – 2.51	Depositor EDS
% Data completeness (in resolution range)	66.0 (14.99-2.51) 73.6 (38.03-2.51)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.291 0.257 , 0.304	Depositor DCC
$R_{free}$ test set	928 reflections (7.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: TAT, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/1508	0.68	0/2040
1	B	0.50	0/1500	0.67	0/2030
1	C	0.49	0/1508	0.67	0/2040
All	All	0.50	0/4516	0.67	0/6110

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	1485	0	1496	279	0
1	B	1477	0	1487	250	0
1	C	1485	0	1496	254	1
2	A	31	0	14	2	0
2	B	31	0	14	1	0
2	C	31	0	14	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	35	0	0	5	0
4	C	27	0	0	8	0
All	All	4631	0	4521	730	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 81.

All (730) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:ALA:HA	1:B:1168:GLN:HE22	1.01	1.10
1:A:1164:ALA:CA	1:B:1168:GLN:HE22	1.69	1.05
1:A:1168:GLN:CD	1:B:1165:MET:HG2	1.77	1.05
1:A:1164:ALA:HB1	1:B:1168:GLN:OE1	1.60	1.01
1:C:1155:THR:HB	1:C:1161:MET:HB2	1.44	0.98
1:A:1164:ALA:HA	1:B:1168:GLN:NE2	1.81	0.96
1:B:1155:THR:HB	1:B:1161:MET:HB2	1.42	0.96
1:A:1155:THR:HB	1:A:1161:MET:HB2	1.46	0.95
1:A:1168:GLN:NE2	1:B:1165:MET:HG2	1.81	0.94
1:A:1180:PHE:HE2	1:B:1076:SER:HB3	1.31	0.92
1:A:1057:LYS:HE2	1:C:1058:PHE:O	1.74	0.88
1:A:1141:ILE:HG12	1:C:1037:LEU:CD2	2.05	0.86
1:A:1120:ILE:HB	1:A:1162:VAL:HG12	1.57	0.86
1:C:1079:VAL:HG13	1:C:1166:VAL:HG13	1.56	0.85
1:A:1058:PHE:O	1:C:1057:LYS:HE2	1.76	0.85
1:A:1079:VAL:HG13	1:A:1166:VAL:HG13	1.56	0.85
1:B:1156:ALA:O	1:B:1159:SER:HB3	1.77	0.84
1:B:1079:VAL:HG13	1:B:1166:VAL:HG13	1.59	0.83
1:C:1120:ILE:HB	1:C:1162:VAL:HG12	1.59	0.83
1:A:1028:LEU:H	1:A:1028:LEU:HD23	1.45	0.82
1:C:1156:ALA:O	1:C:1159:SER:HB3	1.80	0.82
1:A:1156:ALA:O	1:A:1159:SER:HB3	1.79	0.82
1:A:1042:GLY:HA2	1:C:1132:SER:HB3	1.62	0.81
1:C:1028:LEU:HD23	1:C:1028:LEU:H	1.46	0.81
1:A:1130:PHE:CD2	1:C:1037:LEU:HD23	2.16	0.81
1:A:1130:PHE:HA	1:C:1038:ASN:OD1	1.81	0.80
1:B:1028:LEU:H	1:B:1028:LEU:HD23	1.46	0.79
1:A:1080:ARG:NH2	1:A:1081:ARG:HE	1.80	0.79
1:A:1164:ALA:HB1	1:B:1168:GLN:CD	2.02	0.79
1:A:1132:SER:HB3	1:C:1042:GLY:HA2	1.63	0.78
1:A:1143:PRO:O	1:A:1147:ILE:HG12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:ARG:HG2	1:B:1080:ARG:HH11	1.48	0.78
1:A:1090:LEU:HD21	1:A:1158:ASN:HA	1.66	0.78
1:B:1120:ILE:HB	1:B:1162:VAL:HG12	1.64	0.78
1:C:1056:ASP:HB2	1:C:1066:LEU:HG	1.64	0.78
1:B:1077:GLU:OE2	1:B:1080:ARG:NE	2.16	0.77
1:C:1086:ALA:HB2	1:C:1120:ILE:HD11	1.65	0.77
1:B:1080:ARG:NH2	1:B:1081:ARG:HE	1.82	0.76
1:C:1080:ARG:HG2	1:C:1080:ARG:HH11	1.49	0.76
1:C:1143:PRO:O	1:C:1147:ILE:HG12	1.85	0.76
1:A:1180:PHE:CE2	1:B:1076:SER:HB3	2.18	0.76
1:C:1080:ARG:NH2	1:C:1081:ARG:HE	1.84	0.76
1:A:1005:ARG:HG2	1:A:1006:PRO:HD2	1.67	0.76
1:B:1075:PRO:HB3	1:B:1122:GLN:NE2	2.00	0.76
1:B:1069:ALA:HB1	1:B:1138:PHE:HZ	1.50	0.76
1:B:1090:LEU:HD21	1:B:1158:ASN:HA	1.65	0.76
1:C:1090:LEU:HD21	1:C:1158:ASN:HA	1.68	0.76
1:B:1075:PRO:HB3	1:B:1122:GLN:HE22	1.51	0.75
1:C:1117:ARG:HB3	1:C:1152:GLN:O	1.86	0.75
1:A:1164:ALA:CB	1:B:1168:GLN:HE22	1.98	0.75
1:A:1056:ASP:HB2	1:A:1066:LEU:HG	1.66	0.75
1:B:1056:ASP:HB2	1:B:1066:LEU:HG	1.68	0.75
1:A:1077:GLU:OE2	1:A:1080:ARG:NE	2.16	0.75
1:B:1024:MET:HB3	1:B:1028:LEU:HD21	1.68	0.75
1:C:1077:GLU:OE2	1:C:1080:ARG:NE	2.18	0.74
1:C:1075:PRO:HB3	1:C:1122:GLN:NE2	2.02	0.74
1:A:1024:MET:HB3	1:A:1028:LEU:HD21	1.69	0.74
1:B:1143:PRO:O	1:B:1147:ILE:HG12	1.87	0.74
1:A:1124:MET:HG2	1:B:1124:MET:CE	2.18	0.74
1:A:1124:MET:HG2	1:B:1124:MET:HE2	1.70	0.74
1:B:1130:PHE:CE1	1:B:1141:ILE:HD13	2.22	0.74
1:A:1075:PRO:HB3	1:A:1122:GLN:NE2	2.03	0.73
1:C:1024:MET:HB3	1:C:1028:LEU:HD21	1.69	0.73
1:A:1040:TYR:CE2	1:A:1063:ILE:HD11	2.22	0.73
1:A:1086:ALA:HB2	1:A:1120:ILE:HD11	1.70	0.73
1:B:1155:THR:HB	1:B:1161:MET:CB	2.18	0.73
1:A:1124:MET:CG	1:B:1124:MET:HE2	2.18	0.73
1:B:1086:ALA:HB2	1:B:1120:ILE:HD11	1.70	0.73
1:B:1117:ARG:HB3	1:B:1152:GLN:O	1.89	0.73
1:A:1117:ARG:HB3	1:A:1152:GLN:O	1.89	0.73
1:A:1080:ARG:HG2	1:A:1080:ARG:HH11	1.54	0.73
1:C:1122:GLN:HG2	1:C:1165:MET:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:LEU:CD2	1:C:1141:ILE:HG12	2.19	0.72
1:A:1150:ARG:NH1	1:A:1184:LYS:HD2	2.03	0.72
1:B:1040:TYR:CE2	1:B:1063:ILE:HD11	2.25	0.72
1:C:1040:TYR:CE2	1:C:1063:ILE:HD11	2.25	0.72
1:C:1155:THR:HB	1:C:1161:MET:CB	2.20	0.71
1:C:1130:PHE:CE1	1:C:1141:ILE:HD13	2.25	0.71
1:C:1150:ARG:NH1	1:C:1184:LYS:HD2	2.04	0.71
1:A:1130:PHE:CE1	1:A:1141:ILE:HD13	2.25	0.71
1:B:1147:ILE:O	1:B:1151:LEU:HG	1.91	0.71
1:A:1069:ALA:HB1	1:A:1138:PHE:HZ	1.56	0.70
1:C:1069:ALA:HB1	1:C:1138:PHE:HZ	1.54	0.70
1:A:1037:LEU:HD23	1:C:1130:PHE:CD2	2.26	0.70
1:A:1155:THR:HB	1:A:1161:MET:CB	2.20	0.70
1:A:1142:GLY:HA2	1:C:1025:SER:HB3	1.74	0.70
1:A:1038:ASN:OD1	1:C:1130:PHE:HA	1.92	0.70
1:C:1052:GLN:HG3	1:C:1081:ARG:CZ	2.21	0.70
1:A:1116:PHE:HE1	1:A:1118:CYS:HB2	1.57	0.69
1:B:1005:ARG:HG3	1:B:1005:ARG:HH11	1.56	0.69
1:A:1147:ILE:O	1:A:1151:LEU:HG	1.92	0.69
1:A:1176:ILE:HB	1:A:1194:VAL:HG22	1.74	0.69
1:C:1075:PRO:HB3	1:C:1122:GLN:HE22	1.57	0.69
1:A:1075:PRO:HB3	1:A:1122:GLN:HE22	1.57	0.69
1:A:1122:GLN:HG2	1:A:1165:MET:HE3	1.74	0.69
1:C:1147:ILE:O	1:C:1151:LEU:HG	1.93	0.69
1:A:1164:ALA:CA	1:B:1168:GLN:NE2	2.49	0.69
1:A:1019:VAL:HG21	1:A:1157:PRO:HG3	1.75	0.69
1:A:1141:ILE:HG12	1:C:1037:LEU:HD22	1.76	0.68
1:B:1052:GLN:HG3	1:B:1081:ARG:CZ	2.24	0.68
1:A:1167:ALA:HA	1:A:1170:VAL:HG12	1.77	0.67
1:C:1176:ILE:HB	1:C:1194:VAL:HG22	1.76	0.67
1:A:1164:ALA:CB	1:B:1168:GLN:NE2	2.57	0.67
1:C:1093:LEU:HD22	1:C:1116:PHE:HD2	1.59	0.67
1:A:1052:GLN:HG3	1:A:1081:ARG:CZ	2.24	0.67
1:B:1093:LEU:HD22	1:B:1116:PHE:HD2	1.57	0.67
1:B:1122:GLN:HG2	1:B:1165:MET:HE3	1.76	0.67
1:A:1164:ALA:HB2	1:A:1191:MET:HB3	1.77	0.67
1:C:1116:PHE:HE1	1:C:1118:CYS:HB2	1.58	0.67
1:C:1140:ALA:C	1:C:1141:ILE:HD12	2.15	0.67
1:A:1186:ILE:HG21	1:A:1190:VAL:CG2	2.25	0.67
1:A:1126:VAL:HG11	1:C:1034:ALA:HB2	1.77	0.67
1:C:1167:ALA:HA	1:C:1170:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:VAL:HG11	1:B:1169:TYR:HB2	1.75	0.66
1:C:1019:VAL:HG21	1:C:1157:PRO:HG3	1.77	0.66
1:C:1174:GLU:O	1:C:1196:ASN:N	2.27	0.66
1:B:1176:ILE:HB	1:B:1194:VAL:HG22	1.76	0.66
1:B:1116:PHE:HE1	1:B:1118:CYS:HB2	1.60	0.66
1:C:1186:ILE:HG21	1:C:1190:VAL:CG2	2.25	0.66
1:A:1120:ILE:O	1:A:1162:VAL:HA	1.95	0.66
1:B:1085:THR:O	1:B:1089:MET:HG3	1.95	0.66
1:C:1079:VAL:HG11	1:C:1169:TYR:HB2	1.76	0.66
1:C:1116:PHE:H	1:C:1158:ASN:ND2	1.94	0.66
1:B:1120:ILE:O	1:B:1162:VAL:HA	1.96	0.66
1:B:1171:PRO:HB2	1:B:1173:GLU:HG2	1.78	0.66
1:A:1093:LEU:HD22	1:A:1116:PHE:HD2	1.61	0.66
1:C:1080:ARG:HG2	1:C:1080:ARG:NH1	2.12	0.65
1:B:1019:VAL:HG21	1:B:1157:PRO:HG3	1.78	0.65
1:C:1120:ILE:O	1:C:1162:VAL:HA	1.96	0.65
1:C:1074:SER:OG	1:C:1077:GLU:HB2	1.96	0.65
1:B:1074:SER:OG	1:B:1077:GLU:HB2	1.95	0.65
1:B:1080:ARG:NH1	1:B:1080:ARG:HG2	2.11	0.65
1:B:1186:ILE:HG21	1:B:1190:VAL:CG2	2.26	0.65
1:A:1116:PHE:H	1:A:1158:ASN:ND2	1.95	0.65
1:A:1162:VAL:HB	1:A:1166:VAL:HB	1.78	0.65
1:C:1085:THR:O	1:C:1089:MET:HG3	1.96	0.65
1:A:1079:VAL:HG11	1:A:1169:TYR:HB2	1.79	0.65
1:B:1167:ALA:HA	1:B:1170:VAL:HG12	1.78	0.65
1:C:1052:GLN:HG3	1:C:1081:ARG:NH1	2.11	0.64
1:B:1116:PHE:H	1:B:1158:ASN:ND2	1.95	0.64
1:B:1052:GLN:HG3	1:B:1081:ARG:NH1	2.12	0.64
1:B:1164:ALA:HB2	1:B:1191:MET:HB3	1.78	0.64
1:A:1074:SER:OG	1:A:1077:GLU:HB2	1.96	0.64
1:A:1140:ALA:C	1:A:1141:ILE:HD12	2.18	0.64
1:C:1164:ALA:HB2	1:C:1191:MET:HB3	1.79	0.64
1:B:1093:LEU:HD22	1:B:1116:PHE:CD2	2.33	0.64
1:C:1073:MET:HG2	1:C:1077:GLU:HB3	1.80	0.64
1:C:1024:MET:HG2	1:C:1111:VAL:HG13	1.79	0.64
1:B:1013:ILE:N	1:B:1013:ILE:HD12	2.12	0.64
1:B:1011:ILE:HG21	1:B:1127:VAL:HG11	1.80	0.64
1:B:1140:ALA:C	1:B:1141:ILE:HD12	2.18	0.64
1:A:1132:SER:OG	1:C:1045:THR:HG21	1.97	0.64
1:C:1162:VAL:HB	1:C:1166:VAL:HB	1.78	0.63
1:C:1020:GLY:HA2	4:C:2027:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1162:VAL:HB	1:B:1166:VAL:HB	1.81	0.63
1:C:1064:MET:HE2	1:C:1066:LEU:HD21	1.80	0.63
1:A:1168:GLN:HB3	1:B:1165:MET:HA	1.81	0.62
1:A:1174:GLU:O	1:A:1196:ASN:N	2.27	0.62
1:B:1140:ALA:O	1:B:1145:VAL:HG21	1.99	0.62
1:C:1093:LEU:HD22	1:C:1116:PHE:CD2	2.34	0.62
1:C:1018:ILE:HD11	1:C:1040:TYR:CD2	2.34	0.62
1:B:1122:GLN:HE21	1:B:1165:MET:HE3	1.64	0.62
1:B:1063:ILE:N	1:B:1063:ILE:HD12	2.15	0.62
1:C:1171:PRO:HB2	1:C:1173:GLU:HG2	1.79	0.62
1:A:1093:LEU:HD22	1:A:1116:PHE:CD2	2.35	0.62
1:A:1011:ILE:HG21	1:A:1127:VAL:HG11	1.82	0.61
1:A:1040:TYR:HE2	1:A:1063:ILE:HD11	1.62	0.61
1:B:1087:ARG:O	1:B:1091:VAL:HG23	1.99	0.61
1:C:1178:ARG:HG3	1:C:1178:ARG:HH11	1.66	0.61
1:A:1122:GLN:HE21	1:A:1165:MET:CE	2.13	0.61
1:B:1024:MET:HG2	1:B:1111:VAL:HG13	1.82	0.61
1:B:1174:GLU:O	1:B:1196:ASN:N	2.27	0.61
1:C:1013:ILE:HD12	1:C:1013:ILE:N	2.16	0.61
1:A:1063:ILE:N	1:A:1063:ILE:HD12	2.15	0.61
1:C:1046:ARG:HA	4:C:2008:HOH:O	2.00	0.61
1:A:1081:ARG:HG3	1:A:1081:ARG:HH11	1.64	0.61
1:A:1052:GLN:HG3	1:A:1081:ARG:NH1	2.15	0.61
1:A:1174:GLU:HG2	1:A:1200:LEU:N	2.16	0.61
1:A:1085:THR:O	1:A:1089:MET:HG3	2.01	0.60
1:A:1024:MET:HG2	1:A:1111:VAL:HG13	1.83	0.60
1:A:1171:PRO:HB2	1:A:1173:GLU:HG2	1.82	0.60
1:A:1045:THR:HG23	1:A:1049:PHE:CE2	2.36	0.60
1:A:1019:VAL:HG21	1:A:1157:PRO:CB	2.31	0.60
1:A:1080:ARG:HG2	1:A:1080:ARG:NH1	2.17	0.60
1:B:1073:MET:HG2	1:B:1077:GLU:HB3	1.82	0.60
1:A:1073:MET:HG2	1:A:1077:GLU:HB3	1.84	0.60
1:C:1011:ILE:HG21	1:C:1127:VAL:HG11	1.83	0.60
1:B:1045:THR:HG23	1:B:1049:PHE:CE2	2.37	0.60
1:B:1117:ARG:NH2	2:B:2199:TAT:O3G	2.35	0.60
1:C:1115:ARG:HA	1:C:1158:ASN:HD21	1.66	0.60
1:A:1116:PHE:CE1	1:A:1118:CYS:HB2	2.35	0.59
1:A:1140:ALA:O	1:A:1145:VAL:HG21	2.01	0.59
1:B:1040:TYR:HA	1:B:1096:LEU:HD13	1.85	0.59
1:A:1087:ARG:O	1:A:1091:VAL:HG23	2.02	0.59
1:B:1122:GLN:HE21	1:B:1165:MET:CE	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1063:ILE:HD12	1:C:1063:ILE:N	2.18	0.59
1:B:1040:TYR:HE2	1:B:1063:ILE:HD11	1.67	0.59
1:B:1115:ARG:HA	1:B:1158:ASN:HD21	1.68	0.59
1:C:1021:PHE:HD1	1:C:1024:MET:HE3	1.67	0.59
1:C:1019:VAL:HG21	1:C:1157:PRO:CB	2.33	0.59
1:B:1178:ARG:HG3	1:B:1178:ARG:HH11	1.67	0.59
1:C:1064:MET:HE3	1:C:1145:VAL:HG13	1.85	0.59
1:A:1024:MET:C	1:A:1026:ASN:H	2.05	0.58
1:B:1013:ILE:H	1:B:1013:ILE:HD12	1.68	0.58
1:B:1016:SER:OG	1:B:1063:ILE:HD13	2.03	0.58
1:B:1024:MET:C	1:B:1026:ASN:H	2.07	0.58
1:B:1043:GLU:HB2	1:B:1096:LEU:HD11	1.84	0.58
1:B:1069:ALA:HB1	1:B:1138:PHE:CZ	2.34	0.58
1:A:1164:ALA:HB1	1:B:1168:GLN:NE2	2.17	0.58
1:B:1116:PHE:CE1	1:B:1118:CYS:HB2	2.39	0.58
1:C:1116:PHE:CE1	1:C:1118:CYS:HB2	2.37	0.58
1:A:1019:VAL:HG21	1:A:1157:PRO:CG	2.34	0.58
1:A:1013:ILE:N	1:A:1013:ILE:HD12	2.18	0.58
1:A:1018:ILE:HD11	1:A:1040:TYR:CD2	2.38	0.58
1:A:1041:LEU:HD22	1:A:1058:PHE:CD2	2.39	0.58
1:A:1018:ILE:HG23	1:A:1114:VAL:HG13	1.86	0.58
1:C:1122:GLN:HE21	1:C:1165:MET:CE	2.17	0.58
1:A:1115:ARG:HA	1:A:1158:ASN:HD21	1.68	0.58
1:B:1018:ILE:HD11	1:B:1040:TYR:CD2	2.38	0.58
1:B:1117:ARG:CZ	1:B:1152:GLN:OE1	2.52	0.58
1:C:1069:ALA:HB1	1:C:1138:PHE:CZ	2.38	0.58
1:A:1014:LEU:C	1:A:1014:LEU:HD23	2.25	0.57
1:C:1041:LEU:HD22	1:C:1058:PHE:CD2	2.38	0.57
1:B:1041:LEU:HD22	1:B:1058:PHE:CD2	2.40	0.57
1:B:1079:VAL:HG21	1:B:1169:TYR:CD1	2.38	0.57
1:C:1087:ARG:O	1:C:1091:VAL:HG23	2.04	0.57
1:A:1041:LEU:O	1:A:1045:THR:HB	2.04	0.57
1:A:1043:GLU:HB2	1:A:1096:LEU:HD11	1.85	0.57
1:A:1173:GLU:H	1:A:1173:GLU:CD	2.06	0.57
1:B:1019:VAL:HG21	1:B:1157:PRO:CB	2.34	0.57
1:B:1041:LEU:O	1:B:1045:THR:HB	2.03	0.57
1:C:1139:THR:HG23	1:C:1141:ILE:HD11	1.86	0.57
1:B:1151:LEU:CD2	1:B:1192:THR:HG22	2.35	0.57
1:C:1049:PHE:HB2	4:C:2008:HOH:O	2.04	0.57
1:B:1005:ARG:NH1	1:B:1005:ARG:HG3	2.16	0.57
1:C:1117:ARG:CZ	1:C:1152:GLN:OE1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:SER:HB3	1:C:1142:GLY:HA2	1.87	0.57
1:B:1081:ARG:HH11	1:B:1081:ARG:HG3	1.69	0.57
1:A:1016:SER:OG	1:A:1063:ILE:HD13	2.05	0.57
1:A:1024:MET:CB	1:A:1028:LEU:HD21	2.35	0.56
1:A:1040:TYR:CZ	1:A:1044:MET:HG3	2.40	0.56
1:B:1161:MET:HA	1:B:1194:VAL:HA	1.87	0.56
1:B:1170:VAL:HG22	1:B:1174:GLU:HB2	1.87	0.56
1:C:1043:GLU:HB2	1:C:1096:LEU:HD11	1.86	0.56
1:C:1161:MET:HA	1:C:1194:VAL:HA	1.87	0.56
1:A:1086:ALA:HB1	1:A:1160:ILE:HG12	1.87	0.56
1:B:1024:MET:CB	1:B:1028:LEU:HD21	2.34	0.56
1:B:1018:ILE:HG23	1:B:1114:VAL:HG13	1.86	0.56
1:C:1018:ILE:HG23	1:C:1114:VAL:HG13	1.87	0.56
1:C:1139:THR:HG23	1:C:1141:ILE:CD1	2.35	0.56
1:B:1121:HIS:HD2	1:B:1144:SER:O	1.88	0.56
1:B:1173:GLU:CD	1:B:1173:GLU:H	2.08	0.56
1:A:1040:TYR:HA	1:A:1096:LEU:HD13	1.87	0.56
1:B:1022:THR:C	1:B:1024:MET:H	2.07	0.56
1:C:1041:LEU:O	1:C:1045:THR:HB	2.06	0.56
1:A:1022:THR:C	1:A:1024:MET:H	2.07	0.56
1:A:1079:VAL:HG21	1:A:1169:TYR:CD1	2.41	0.56
1:C:1024:MET:C	1:C:1026:ASN:H	2.07	0.56
1:C:1151:LEU:CD2	1:C:1192:THR:HG22	2.36	0.56
1:A:1047:ALA:HA	1:A:1088:GLN:NE2	2.21	0.56
1:B:1064:MET:HE2	1:B:1066:LEU:HD21	1.88	0.56
1:C:1012:THR:HB	1:C:1067:TYR:HB2	1.88	0.56
1:C:1024:MET:CB	1:C:1028:LEU:HD21	2.34	0.56
1:B:1014:LEU:HD23	1:B:1014:LEU:C	2.26	0.56
1:C:1079:VAL:HG21	1:C:1169:TYR:CD1	2.41	0.56
1:A:1019:VAL:CG2	1:A:1117:ARG:HG3	2.36	0.56
1:C:1045:THR:HG23	1:C:1049:PHE:CE2	2.41	0.55
1:A:1047:ALA:O	1:A:1051:ASN:ND2	2.32	0.55
1:C:1090:LEU:HG	1:C:1116:PHE:CZ	2.41	0.55
1:A:1186:ILE:C	1:A:1188:GLU:H	2.09	0.55
1:B:1021:PHE:HD1	1:B:1024:MET:HE3	1.71	0.55
1:B:1093:LEU:HD11	1:B:1114:VAL:HG12	1.87	0.55
1:C:1019:VAL:CG2	1:C:1117:ARG:HG3	2.36	0.55
1:C:1019:VAL:HG21	1:C:1157:PRO:CG	2.36	0.55
1:C:1087:ARG:HD2	4:C:2014:HOH:O	2.06	0.55
1:C:1173:GLU:H	1:C:1173:GLU:CD	2.08	0.55
1:B:1040:TYR:CZ	1:B:1044:MET:HG3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:VAL:HG22	1:A:1174:GLU:HB2	1.88	0.55
1:A:1180:PHE:CE2	1:B:1076:SER:CB	2.89	0.55
1:B:1005:ARG:HG2	1:B:1006:PRO:HD2	1.89	0.55
1:A:1139:THR:HG23	1:A:1141:ILE:HD11	1.88	0.55
1:C:1014:LEU:HD23	1:C:1014:LEU:C	2.27	0.55
1:A:1161:MET:HA	1:A:1194:VAL:HA	1.88	0.55
1:C:1093:LEU:HD11	1:C:1114:VAL:HG12	1.89	0.55
1:A:1178:ARG:HG3	1:A:1178:ARG:HH11	1.71	0.55
1:B:1139:THR:HG23	1:B:1141:ILE:HD11	1.89	0.55
1:A:1165:MET:SD	1:B:1165:MET:HE2	2.47	0.55
1:C:1081:ARG:HG3	1:C:1081:ARG:HH11	1.71	0.55
1:C:1140:ALA:O	1:C:1145:VAL:HG21	2.06	0.55
1:A:1139:THR:HG23	1:A:1141:ILE:CD1	2.37	0.55
1:C:1005:ARG:HG2	1:C:1006:PRO:HD2	1.90	0.55
1:B:1162:VAL:HG22	1:B:1193:CYS:O	2.07	0.54
1:C:1022:THR:C	1:C:1024:MET:H	2.08	0.54
1:C:1169:TYR:HB3	4:C:2013:HOH:O	2.07	0.54
1:A:1012:THR:HB	1:A:1067:TYR:HB2	1.90	0.54
1:B:1167:ALA:O	1:B:1170:VAL:HG12	2.07	0.54
1:C:1013:ILE:H	1:C:1013:ILE:HD12	1.71	0.54
1:C:1037:LEU:HD11	1:C:1061:ASP:HA	1.88	0.54
1:C:1186:ILE:C	1:C:1188:GLU:H	2.11	0.54
1:C:1081:ARG:HD3	4:C:2009:HOH:O	2.08	0.54
1:C:1177:LYS:HE3	1:C:1179:GLU:OE1	2.07	0.54
1:A:1013:ILE:HD12	1:A:1013:ILE:H	1.73	0.54
1:A:1011:ILE:HD13	1:A:1127:VAL:HG11	1.90	0.54
1:A:1175:ILE:HD12	1:A:1178:ARG:NH2	2.23	0.54
1:B:1019:VAL:HG22	1:B:1117:ARG:HG3	1.90	0.54
1:C:1167:ALA:O	1:C:1170:VAL:HG12	2.07	0.54
1:B:1043:GLU:HB3	1:B:1092:ALA:HB1	1.90	0.54
1:C:1040:TYR:CZ	1:C:1044:MET:HG3	2.42	0.54
1:B:1037:LEU:HD11	1:B:1061:ASP:HA	1.90	0.54
1:C:1019:VAL:HG22	1:C:1117:ARG:HG3	1.89	0.54
1:A:1057:LYS:HD2	2:C:2200:TAT:H1	1.90	0.54
1:C:1090:LEU:HD13	1:C:1197:PRO:HB2	1.90	0.54
1:A:1045:THR:HG23	1:A:1049:PHE:CD2	2.43	0.54
1:C:1040:TYR:HA	1:C:1096:LEU:HD13	1.90	0.54
1:C:1080:ARG:HH22	1:C:1081:ARG:HE	1.56	0.53
1:A:1117:ARG:CZ	1:A:1152:GLN:OE1	2.55	0.53
1:B:1019:VAL:CG2	1:B:1117:ARG:HG3	2.38	0.53
1:A:1019:VAL:HG22	1:A:1117:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:LYS:HE3	1:B:1179:GLU:OE1	2.07	0.53
1:A:1037:LEU:HD11	1:A:1061:ASP:HA	1.90	0.53
1:A:1090:LEU:HG	1:A:1116:PHE:CZ	2.44	0.53
1:B:1019:VAL:HG21	1:B:1157:PRO:CG	2.38	0.53
1:C:1056:ASP:N	1:C:1064:MET:O	2.41	0.53
1:A:1167:ALA:O	1:A:1170:VAL:HG12	2.09	0.53
1:A:1151:LEU:CD2	1:A:1192:THR:HG22	2.38	0.53
1:B:1047:ALA:HA	1:B:1088:GLN:NE2	2.24	0.53
1:B:1139:THR:HG23	1:B:1141:ILE:CD1	2.38	0.53
1:B:1183:LEU:HD12	1:B:1190:VAL:HG21	1.91	0.53
1:C:1121:HIS:HD2	1:C:1144:SER:O	1.92	0.53
1:A:1122:GLN:HE21	1:A:1165:MET:HE3	1.73	0.53
1:C:1183:LEU:HD12	1:C:1190:VAL:HG21	1.90	0.53
1:A:1064:MET:HE2	1:A:1066:LEU:HD21	1.90	0.53
1:B:1080:ARG:HH22	1:B:1081:ARG:HE	1.56	0.53
1:C:1016:SER:OG	1:C:1063:ILE:HD13	2.09	0.53
1:C:1086:ALA:HB1	1:C:1160:ILE:HG12	1.91	0.53
1:A:1124:MET:CG	1:B:1124:MET:CE	2.83	0.53
1:C:1162:VAL:HG22	1:C:1193:CYS:O	2.09	0.52
1:B:1011:ILE:HD13	1:B:1127:VAL:HG11	1.91	0.52
1:C:1040:TYR:HE2	1:C:1063:ILE:HD11	1.70	0.52
1:B:1090:LEU:HG	1:B:1116:PHE:CZ	2.44	0.52
1:A:1080:ARG:HH22	1:A:1081:ARG:HE	1.55	0.52
1:B:1186:ILE:C	1:B:1188:GLU:H	2.12	0.52
1:C:1047:ALA:HA	1:C:1088:GLN:NE2	2.25	0.52
1:B:1052:GLN:HB2	1:B:1073:MET:HE1	1.92	0.52
1:B:1086:ALA:HB1	1:B:1160:ILE:HG12	1.90	0.52
1:A:1093:LEU:HD11	1:A:1114:VAL:HG12	1.91	0.52
1:A:1121:HIS:HD2	1:A:1144:SER:O	1.93	0.52
1:A:1168:GLN:OE1	1:B:1165:MET:HG2	2.09	0.52
1:A:1010:LEU:HD13	1:B:1124:MET:HG3	1.91	0.52
1:B:1121:HIS:CD2	1:B:1147:ILE:HB	2.45	0.52
1:C:1165:MET:O	1:C:1168:GLN:HG2	2.09	0.52
1:C:1121:HIS:CD2	1:C:1147:ILE:HB	2.44	0.52
1:A:1162:VAL:HG22	1:A:1193:CYS:O	2.09	0.52
1:B:1005:ARG:O	1:B:1007:GLU:HG2	2.10	0.52
1:A:1021:PHE:HD1	1:A:1024:MET:HE3	1.75	0.52
1:A:1017:ASP:HA	1:A:1062:ALA:HA	1.92	0.51
1:A:1037:LEU:HD22	1:C:1141:ILE:HG12	1.92	0.51
1:A:1059:VAL:HG12	2:A:2200:TAT:H8	1.92	0.51
1:B:1083:ILE:HG23	1:B:1195:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:ARG:NE	1:B:1196:ASN:O	2.38	0.51
1:C:1043:GLU:HB3	1:C:1092:ALA:HB1	1.91	0.51
1:C:1083:ILE:HG23	1:C:1195:ILE:HD13	1.92	0.51
1:A:1043:GLU:HB3	1:A:1092:ALA:HB1	1.91	0.51
1:C:1122:GLN:HE21	1:C:1165:MET:HE3	1.74	0.51
1:B:1045:THR:HG23	1:B:1049:PHE:CD2	2.45	0.51
1:B:1119:GLY:HA2	1:B:1161:MET:O	2.11	0.51
1:A:1069:ALA:HB1	1:A:1138:PHE:CZ	2.40	0.51
1:A:1177:LYS:HE3	1:A:1179:GLU:OE1	2.11	0.51
1:B:1170:VAL:HG13	1:B:1175:ILE:HD11	1.93	0.51
1:A:1083:ILE:HG23	1:A:1195:ILE:HD13	1.92	0.51
1:A:1011:ILE:HD12	1:A:1066:LEU:HD22	1.93	0.51
1:C:1021:PHE:HA	1:C:1024:MET:CE	2.41	0.51
1:C:1170:VAL:HG22	1:C:1174:GLU:HB2	1.92	0.51
1:A:1079:VAL:CG1	1:A:1166:VAL:HG13	2.34	0.51
1:B:1015:PHE:O	1:B:1118:CYS:HA	2.11	0.51
1:A:1183:LEU:HD12	1:A:1190:VAL:HG21	1.92	0.50
1:B:1116:PHE:H	1:B:1158:ASN:HD22	1.59	0.50
1:C:1079:VAL:CG1	1:C:1166:VAL:HG13	2.34	0.50
1:A:1188:GLU:OE1	1:B:1074:SER:HA	2.10	0.50
1:B:1155:THR:CB	1:B:1161:MET:HB2	2.30	0.50
1:A:1142:GLY:HA2	1:C:1025:SER:CB	2.40	0.50
1:C:1120:ILE:HG22	1:C:1166:VAL:HG21	1.92	0.50
1:A:1080:ARG:NH2	1:A:1081:ARG:NE	2.56	0.50
1:B:1079:VAL:CG1	1:B:1166:VAL:HG13	2.38	0.50
1:C:1045:THR:HG23	1:C:1049:PHE:CD2	2.47	0.50
1:B:1175:ILE:HG23	1:B:1193:CYS:HB3	1.93	0.50
1:A:1056:ASP:N	1:A:1064:MET:O	2.40	0.50
1:A:1130:PHE:CZ	1:A:1141:ILE:HD13	2.47	0.50
1:B:1040:TYR:HB2	1:B:1100:TRP:HH2	1.76	0.50
1:C:1017:ASP:HA	1:C:1062:ALA:HA	1.93	0.50
1:A:1175:ILE:HG23	1:A:1193:CYS:HB3	1.94	0.49
1:B:1047:ALA:O	1:B:1051:ASN:ND2	2.33	0.49
1:B:1090:LEU:HD13	1:B:1197:PRO:HB2	1.93	0.49
1:B:1175:ILE:HD12	1:B:1178:ARG:NH2	2.27	0.49
1:C:1116:PHE:H	1:C:1158:ASN:HD22	1.58	0.49
1:C:1175:ILE:HG23	1:C:1193:CYS:HB3	1.94	0.49
1:A:1187:ASP:O	1:A:1188:GLU:HG3	2.12	0.49
1:B:1048:VAL:CG2	1:B:1049:PHE:N	2.74	0.49
1:B:1011:ILE:HD12	1:B:1066:LEU:HD22	1.94	0.49
1:C:1113:PRO:O	1:C:1114:VAL:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1040:TYR:HB2	1:B:1100:TRP:CH2	2.47	0.49
1:A:1083:ILE:HG23	1:A:1195:ILE:CD1	2.43	0.49
1:B:1080:ARG:NH2	1:B:1081:ARG:NE	2.58	0.49
2:A:2200:TAT:H1	1:C:1057:LYS:HD2	1.95	0.49
1:A:1024:MET:C	1:A:1026:ASN:N	2.66	0.49
1:A:1044:MET:SD	1:A:1089:MET:HB3	2.52	0.49
1:B:1012:THR:HB	1:B:1067:TYR:HB2	1.94	0.49
1:C:1040:TYR:HB2	1:C:1100:TRP:CH2	2.48	0.49
1:C:1047:ALA:O	1:C:1051:ASN:ND2	2.34	0.49
1:C:1079:VAL:HG13	1:C:1166:VAL:CG1	2.37	0.49
1:A:1034:ALA:HB2	1:C:1126:VAL:HG11	1.93	0.49
1:A:1076:SER:HA	1:A:1169:TYR:CD2	2.47	0.49
1:A:1121:HIS:ND1	1:A:1163:SER:CB	2.76	0.49
1:C:1150:ARG:HA	1:C:1153:GLU:HG2	1.95	0.49
1:B:1017:ASP:HA	1:B:1062:ALA:HA	1.93	0.49
1:A:1119:GLY:HA2	1:A:1161:MET:O	2.13	0.49
1:C:1016:SER:O	1:C:1062:ALA:HA	2.12	0.49
1:C:1017:ASP:CG	1:C:1117:ARG:HH21	2.16	0.49
1:A:1016:SER:O	1:A:1062:ALA:HA	2.13	0.49
1:A:1121:HIS:CD2	1:A:1147:ILE:HB	2.47	0.49
1:B:1083:ILE:HG23	1:B:1195:ILE:CD1	2.43	0.49
1:C:1048:VAL:CG2	1:C:1049:PHE:N	2.76	0.49
1:C:1178:ARG:HG3	1:C:1178:ARG:NH1	2.28	0.49
1:C:1175:ILE:HD12	1:C:1178:ARG:NH2	2.28	0.49
1:B:1076:SER:HA	1:B:1169:TYR:CD2	2.47	0.48
1:C:1087:ARG:NE	1:C:1196:ASN:O	2.41	0.48
1:C:1011:ILE:HD13	1:C:1127:VAL:HG11	1.95	0.48
1:C:1187:ASP:O	1:C:1188:GLU:HG3	2.13	0.48
1:A:1040:TYR:HB2	1:A:1100:TRP:CH2	2.48	0.48
1:A:1150:ARG:HA	1:A:1153:GLU:HG2	1.95	0.48
1:B:1130:PHE:CZ	1:B:1141:ILE:HD13	2.49	0.48
1:B:1150:ARG:HA	1:B:1153:GLU:HG2	1.95	0.48
1:C:1040:TYR:HB2	1:C:1100:TRP:HH2	1.78	0.48
1:A:1019:VAL:HG21	1:A:1157:PRO:HB3	1.94	0.48
1:A:1025:SER:HA	1:A:1033:VAL:HG21	1.96	0.48
1:A:1141:ILE:CG2	1:C:1021:PHE:HE2	2.26	0.48
1:A:1040:TYR:HB2	1:A:1100:TRP:HH2	1.78	0.48
1:A:1011:ILE:HD13	1:A:1127:VAL:CG1	2.44	0.48
1:A:1005:ARG:O	1:A:1007:GLU:HG2	2.13	0.48
1:B:1016:SER:O	1:B:1062:ALA:HA	2.13	0.48
1:C:1083:ILE:HG23	1:C:1195:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:GLN:HB2	4:B:2012:HOH:O	2.14	0.48
1:A:1164:ALA:CB	1:B:1168:GLN:OE1	2.49	0.48
1:C:1021:PHE:HA	1:C:1024:MET:HE3	1.96	0.48
1:B:1056:ASP:N	1:B:1064:MET:O	2.40	0.48
1:B:1044:MET:SD	1:B:1089:MET:HB3	2.53	0.48
1:B:1103:ARG:NH2	1:B:1105:LEU:HD11	2.29	0.47
1:C:1015:PHE:O	1:C:1118:CYS:HA	2.14	0.47
1:C:1076:SER:HA	1:C:1169:TYR:CD2	2.48	0.47
1:C:1121:HIS:ND1	1:C:1163:SER:CB	2.77	0.47
1:A:1113:PRO:O	1:A:1114:VAL:C	2.52	0.47
1:A:1171:PRO:HB2	1:A:1173:GLU:OE2	2.14	0.47
1:C:1024:MET:C	1:C:1026:ASN:N	2.68	0.47
1:A:1015:PHE:O	1:A:1118:CYS:HA	2.14	0.47
1:A:1052:GLN:HB2	1:A:1073:MET:HE1	1.95	0.47
1:A:1017:ASP:CG	1:A:1117:ARG:HH21	2.17	0.47
1:A:1064:MET:HE3	1:A:1145:VAL:HG13	1.95	0.47
1:A:1122:GLN:HE21	1:A:1165:MET:HE1	1.79	0.47
1:A:1117:ARG:NH1	1:A:1153:GLU:HA	2.29	0.47
1:A:1120:ILE:HG22	1:A:1166:VAL:HG21	1.95	0.47
1:B:1117:ARG:NH1	1:B:1153:GLU:HA	2.29	0.47
1:C:1018:ILE:CG2	1:C:1114:VAL:HG13	2.44	0.47
1:C:1067:TYR:OH	1:C:1085:THR:HG21	2.15	0.47
1:A:1056:ASP:HB3	1:A:1064:MET:O	2.15	0.47
1:A:1096:LEU:HB3	1:A:1100:TRP:CH2	2.50	0.47
1:B:1064:MET:HE3	1:B:1145:VAL:HG13	1.95	0.47
1:B:1017:ASP:CG	1:B:1117:ARG:HH21	2.18	0.47
1:B:1160:ILE:HD12	1:B:1197:PRO:HA	1.96	0.47
1:A:1031:GLN:NE2	4:A:2002:HOH:O	2.47	0.47
1:A:1051:ASN:C	1:A:1053:GLY:H	2.18	0.47
1:A:1079:VAL:HG13	1:A:1166:VAL:CG1	2.37	0.47
1:A:1116:PHE:H	1:A:1158:ASN:HD22	1.61	0.47
1:B:1024:MET:C	1:B:1026:ASN:N	2.67	0.47
1:A:1170:VAL:HG13	1:A:1175:ILE:HD11	1.96	0.47
1:B:1021:PHE:HA	1:B:1024:MET:CE	2.44	0.47
1:C:1130:PHE:CZ	1:C:1141:ILE:HD13	2.49	0.47
1:A:1018:ILE:HB	1:A:1061:ASP:HB2	1.97	0.47
1:A:1164:ALA:CB	1:B:1169:TYR:OH	2.63	0.47
1:B:1071:GLU:HA	4:B:2010:HOH:O	2.15	0.47
1:B:1165:MET:O	1:B:1168:GLN:HG2	2.15	0.47
1:A:1093:LEU:HD21	1:A:1114:VAL:O	2.15	0.47
1:A:1165:MET:O	1:A:1168:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:PRO:O	1:B:1115:ARG:HG3	2.15	0.47
1:C:1021:PHE:CD1	1:C:1024:MET:HE3	2.49	0.47
1:C:1103:ARG:NH2	1:C:1105:LEU:HD11	2.30	0.47
1:C:1019:VAL:HG21	1:C:1157:PRO:HB3	1.97	0.47
1:B:1048:VAL:HG22	1:B:1049:PHE:N	2.30	0.46
1:B:1011:ILE:HD13	1:B:1127:VAL:CG1	2.45	0.46
1:C:1170:VAL:HG13	1:C:1175:ILE:HD11	1.96	0.46
1:A:1180:PHE:HE2	1:B:1076:SER:CB	2.14	0.46
1:C:1073:MET:CG	1:C:1077:GLU:HB3	2.45	0.46
1:C:1117:ARG:NH1	1:C:1153:GLU:HA	2.30	0.46
1:A:1048:VAL:HG12	1:A:1089:MET:HE3	1.98	0.46
1:A:1067:TYR:OH	1:A:1085:THR:HG21	2.16	0.46
1:A:1103:ARG:NH2	1:A:1105:LEU:HD11	2.30	0.46
1:B:1025:SER:HA	1:B:1033:VAL:HG21	1.97	0.46
1:C:1119:GLY:HA2	1:C:1161:MET:O	2.15	0.46
1:A:1139:THR:OG1	1:A:1140:ALA:N	2.49	0.46
1:A:1162:VAL:HB	1:A:1166:VAL:CB	2.45	0.46
1:A:1087:ARG:NE	1:A:1196:ASN:O	2.41	0.46
1:B:1004:LEU:HB3	4:B:2001:HOH:O	2.15	0.46
1:A:1026:ASN:OD1	1:A:1027:ALA:N	2.48	0.46
1:A:1048:VAL:CG2	1:A:1049:PHE:N	2.79	0.46
1:B:1051:ASN:C	1:B:1053:GLY:H	2.18	0.46
1:B:1161:MET:CG	1:B:1192:THR:HB	2.46	0.46
1:B:1021:PHE:HA	1:B:1024:MET:HE3	1.97	0.46
1:B:1113:PRO:O	1:B:1114:VAL:C	2.54	0.46
1:B:1018:ILE:CG2	1:B:1114:VAL:HG13	2.45	0.46
1:C:1026:ASN:OD1	1:C:1027:ALA:N	2.49	0.46
1:C:1124:MET:O	1:C:1144:SER:OG	2.30	0.46
1:C:1141:ILE:N	1:C:1141:ILE:HD12	2.31	0.46
1:C:1121:HIS:CD2	1:C:1144:SER:HA	2.50	0.46
1:A:1018:ILE:CG2	1:A:1114:VAL:HG13	2.45	0.46
1:B:1130:PHE:CD1	1:B:1141:ILE:HD13	2.51	0.46
1:B:1178:ARG:NH1	1:B:1178:ARG:HG3	2.29	0.46
1:C:1080:ARG:NH2	1:C:1081:ARG:NE	2.60	0.46
1:C:1044:MET:SD	1:C:1089:MET:HB3	2.56	0.46
1:C:1051:ASN:C	1:C:1053:GLY:H	2.19	0.46
1:A:1155:THR:CB	1:A:1161:MET:HB2	2.32	0.46
1:B:1019:VAL:HG21	1:B:1157:PRO:HB3	1.97	0.46
1:C:1161:MET:CG	1:C:1192:THR:HB	2.46	0.46
1:A:1191:MET:HB3	4:A:2021:HOH:O	2.16	0.45
1:A:1087:ARG:HG2	1:A:1197:PRO:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:THR:C	1:B:1024:MET:N	2.69	0.45
1:B:1067:TYR:OH	1:B:1085:THR:HG21	2.16	0.45
1:B:1121:HIS:ND1	1:B:1163:SER:CB	2.79	0.45
1:B:1171:PRO:HB2	1:B:1173:GLU:CG	2.45	0.45
1:C:1010:LEU:HD23	1:C:1075:PRO:HG3	1.98	0.45
1:A:1081:ARG:HG3	1:A:1081:ARG:NH1	2.31	0.45
1:B:1056:ASP:HB3	1:B:1064:MET:O	2.15	0.45
1:B:1120:ILE:HG22	1:B:1166:VAL:HG21	1.97	0.45
1:B:1141:ILE:HD12	1:B:1141:ILE:N	2.30	0.45
1:C:1025:SER:HA	1:C:1033:VAL:HG21	1.98	0.45
1:A:1006:PRO:HG3	1:C:1038:ASN:HD21	1.81	0.45
1:C:1093:LEU:HD21	1:C:1114:VAL:O	2.17	0.45
1:A:1021:PHE:HA	1:A:1024:MET:CE	2.47	0.45
1:A:1168:GLN:NE2	1:B:1165:MET:CG	2.67	0.45
1:B:1079:VAL:HG23	1:B:1122:GLN:OE1	2.16	0.45
1:B:1093:LEU:HD11	1:B:1114:VAL:CG1	2.46	0.45
1:C:1018:ILE:HB	1:C:1061:ASP:HB2	1.98	0.45
1:C:1113:PRO:O	1:C:1115:ARG:HG3	2.16	0.45
1:A:1021:PHE:HA	1:A:1024:MET:HE2	1.97	0.45
1:A:1150:ARG:HH12	1:A:1184:LYS:HD2	1.77	0.45
1:B:1044:MET:O	1:B:1047:ALA:HB3	2.17	0.45
1:B:1171:PRO:HB2	1:B:1173:GLU:OE2	2.16	0.45
1:C:1079:VAL:HG23	1:C:1122:GLN:OE1	2.17	0.45
1:C:1130:PHE:O	1:C:1136:SER:HA	2.17	0.45
1:A:1022:THR:C	1:A:1024:MET:N	2.70	0.45
1:B:1121:HIS:CD2	1:B:1144:SER:HA	2.51	0.45
1:B:1122:GLN:O	1:B:1165:MET:HG3	2.16	0.45
1:A:1131:GLY:HA2	1:C:1041:LEU:CB	2.47	0.45
1:A:1178:ARG:HG3	1:A:1178:ARG:NH1	2.31	0.45
1:B:1018:ILE:CG1	1:B:1061:ASP:HB2	2.47	0.45
1:B:1170:VAL:CG2	1:B:1174:GLU:HB2	2.46	0.45
1:A:1186:ILE:O	1:A:1188:GLU:N	2.50	0.45
1:B:1142:GLY:HA3	4:B:2016:HOH:O	2.16	0.45
1:B:1040:TYR:HA	1:B:1096:LEU:CD1	2.47	0.45
1:B:1054:THR:O	1:B:1065:ALA:HA	2.17	0.45
1:C:1150:ARG:NH1	1:C:1153:GLU:OE2	2.47	0.45
1:C:1155:THR:CB	1:C:1161:MET:HB2	2.32	0.45
1:A:1038:ASN:OD1	1:C:1131:GLY:N	2.50	0.45
1:C:1146:ASN:HB2	4:C:2017:HOH:O	2.17	0.45
1:C:1150:ARG:HH12	1:C:1184:LYS:HD2	1.78	0.45
1:B:1051:ASN:O	1:B:1081:ARG:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1093:LEU:HA	1:C:1096:LEU:HB2	1.99	0.44
1:C:1116:PHE:C	1:C:1116:PHE:CD1	2.91	0.44
1:A:1051:ASN:C	1:A:1053:GLY:N	2.70	0.44
1:C:1056:ASP:HB3	1:C:1064:MET:O	2.17	0.44
1:C:1051:ASN:O	1:C:1081:ARG:HB3	2.17	0.44
1:C:1096:LEU:HB3	1:C:1100:TRP:CH2	2.51	0.44
1:A:1113:PRO:O	1:A:1115:ARG:HG3	2.17	0.44
1:A:1171:PRO:HB2	1:A:1173:GLU:CG	2.48	0.44
1:B:1194:VAL:HG22	1:B:1194:VAL:O	2.17	0.44
1:C:1052:GLN:HB2	1:C:1073:MET:HE1	1.98	0.44
1:C:1087:ARG:HD3	1:C:1198:ASN:O	2.18	0.44
1:A:1100:TRP:HZ3	1:A:1114:VAL:HB	1.83	0.44
1:A:1012:THR:HA	1:A:1122:GLN:HA	2.00	0.44
1:A:1178:ARG:O	1:A:1179:GLU:HB2	2.18	0.44
1:B:1056:ASP:OD2	1:B:1064:MET:HE2	2.17	0.44
1:B:1196:ASN:OD1	1:B:1198:ASN:HB2	2.18	0.44
1:C:1048:VAL:HG22	1:C:1049:PHE:N	2.32	0.44
1:A:1116:PHE:CD1	1:A:1116:PHE:C	2.90	0.44
1:A:1198:ASN:O	1:A:1199:MET:HB2	2.17	0.44
1:B:1018:ILE:HB	1:B:1061:ASP:HB2	1.99	0.44
1:C:1044:MET:O	1:C:1047:ALA:HB3	2.17	0.44
1:C:1171:PRO:HB2	1:C:1173:GLU:OE2	2.17	0.44
1:A:1141:ILE:N	1:A:1141:ILE:HD12	2.32	0.44
1:B:1051:ASN:C	1:B:1053:GLY:N	2.70	0.44
1:B:1093:LEU:HD21	1:B:1114:VAL:O	2.17	0.44
1:C:1017:ASP:HB3	1:C:1117:ARG:HH21	1.83	0.44
1:C:1018:ILE:HD11	1:C:1040:TYR:CG	2.53	0.44
1:C:1119:GLY:HA3	1:C:1152:GLN:N	2.33	0.44
1:C:1171:PRO:HB2	1:C:1173:GLU:CG	2.46	0.44
1:C:1178:ARG:O	1:C:1179:GLU:CB	2.66	0.44
1:C:1178:ARG:O	1:C:1179:GLU:HB2	2.17	0.44
1:A:1056:ASP:OD1	1:A:1057:LYS:HG2	2.17	0.44
1:B:1096:LEU:HB3	1:B:1100:TRP:CH2	2.53	0.44
1:B:1160:ILE:O	1:B:1194:VAL:HA	2.18	0.44
1:C:1117:ARG:CB	1:C:1152:GLN:O	2.63	0.44
1:C:1198:ASN:O	1:C:1199:MET:HB2	2.18	0.44
1:B:1056:ASP:OD1	1:B:1057:LYS:HG2	2.18	0.43
1:C:1024:MET:SD	1:C:1114:VAL:HG22	2.58	0.43
1:A:1068:GLY:HA2	1:A:1073:MET:HB3	1.99	0.43
1:A:1051:ASN:O	1:A:1081:ARG:HB3	2.19	0.43
1:A:1019:VAL:CG2	1:A:1157:PRO:HG3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:MET:CG	1:A:1192:THR:HB	2.48	0.43
1:B:1130:PHE:O	1:B:1136:SER:HA	2.18	0.43
1:C:1011:ILE:HD13	1:C:1127:VAL:CG1	2.48	0.43
1:C:1051:ASN:C	1:C:1053:GLY:N	2.71	0.43
1:C:1041:LEU:HD23	1:C:1063:ILE:HD11	2.00	0.43
1:C:1093:LEU:HD11	1:C:1114:VAL:CG1	2.48	0.43
1:C:1122:GLN:O	1:C:1165:MET:HG3	2.17	0.43
1:B:1026:ASN:OD1	1:B:1027:ALA:N	2.51	0.43
1:C:1011:ILE:HD12	1:C:1066:LEU:HD22	2.00	0.43
1:A:1130:PHE:O	1:A:1136:SER:HA	2.17	0.43
1:A:1170:VAL:CG2	1:A:1174:GLU:HB2	2.48	0.43
1:B:1071:GLU:HG3	4:B:2010:HOH:O	2.17	0.43
1:B:1119:GLY:HA3	1:B:1152:GLN:N	2.33	0.43
1:C:1056:ASP:OD1	1:C:1057:LYS:HG2	2.19	0.43
1:C:1100:TRP:HZ3	1:C:1114:VAL:HB	1.84	0.43
1:C:1150:ARG:HA	1:C:1150:ARG:HD3	1.81	0.43
1:A:1195:ILE:HD12	1:A:1196:ASN:O	2.19	0.43
1:B:1100:TRP:HZ3	1:B:1114:VAL:HB	1.84	0.43
1:B:1195:ILE:HD12	1:B:1196:ASN:O	2.18	0.43
1:C:1168:GLN:HB2	1:C:1168:GLN:HE21	1.62	0.43
1:B:1013:ILE:HG12	1:B:1145:VAL:HG22	2.00	0.43
1:B:1021:PHE:O	1:B:1024:MET:HB2	2.19	0.43
1:B:1093:LEU:HD21	1:B:1115:ARG:HA	2.01	0.43
1:B:1187:ASP:O	1:B:1188:GLU:HG3	2.18	0.43
1:C:1077:GLU:O	1:C:1081:ARG:HG2	2.17	0.43
1:C:1195:ILE:HD12	1:C:1196:ASN:O	2.19	0.43
1:A:1121:HIS:CD2	1:A:1144:SER:HA	2.52	0.43
1:A:1178:ARG:O	1:A:1179:GLU:CB	2.67	0.43
1:C:1022:THR:C	1:C:1024:MET:N	2.71	0.43
1:A:1044:MET:O	1:A:1047:ALA:HB3	2.18	0.43
1:A:1093:LEU:HD21	1:A:1115:ARG:HA	2.01	0.43
1:B:1162:VAL:HB	1:B:1166:VAL:CB	2.47	0.43
1:C:1018:ILE:HB	1:C:1061:ASP:OD2	2.19	0.43
1:C:1139:THR:OG1	1:C:1140:ALA:N	2.52	0.43
1:A:1040:TYR:HA	1:A:1096:LEU:CD1	2.49	0.43
1:A:1128:GLY:HA2	1:A:1138:PHE:CE1	2.53	0.43
1:B:1178:ARG:O	1:B:1179:GLU:CB	2.66	0.43
1:A:1006:PRO:HG3	1:C:1038:ASN:ND2	2.34	0.43
1:A:1056:ASP:C	1:A:1056:ASP:OD1	2.57	0.42
1:A:1079:VAL:HG23	1:A:1122:GLN:OE1	2.19	0.42
1:B:1077:GLU:O	1:B:1081:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:ARG:O	1:B:1179:GLU:HB2	2.19	0.42
1:C:1170:VAL:CG2	1:C:1174:GLU:HB2	2.48	0.42
1:B:1093:LEU:HA	1:B:1096:LEU:HB2	2.01	0.42
1:C:1162:VAL:HB	1:C:1166:VAL:CB	2.45	0.42
1:A:1017:ASP:HB3	1:A:1117:ARG:HH21	1.84	0.42
1:A:1051:ASN:O	1:A:1053:GLY:N	2.52	0.42
1:B:1116:PHE:CD1	1:B:1116:PHE:C	2.93	0.42
1:C:1021:PHE:O	1:C:1024:MET:HB2	2.19	0.42
1:A:1018:ILE:CG1	1:A:1061:ASP:HB2	2.50	0.42
1:A:1194:VAL:HG22	1:A:1194:VAL:O	2.19	0.42
1:B:1059:VAL:N	1:B:1062:ALA:O	2.48	0.42
1:C:1054:THR:O	1:C:1065:ALA:HA	2.18	0.42
1:A:1139:THR:OG1	2:C:2200:TAT:N6	2.51	0.42
1:B:1012:THR:HA	1:B:1122:GLN:HA	2.01	0.42
1:B:1112:PRO:HA	1:B:1113:PRO:HD3	1.96	0.42
1:B:1024:MET:SD	1:B:1114:VAL:HG22	2.59	0.42
1:B:1017:ASP:HB3	1:B:1117:ARG:HH21	1.84	0.42
1:B:1010:LEU:HD23	1:B:1075:PRO:HG3	2.01	0.42
1:C:1160:ILE:HD12	1:C:1197:PRO:HA	2.00	0.42
1:A:1054:THR:O	1:A:1065:ALA:HA	2.19	0.42
1:A:1130:PHE:CD1	1:A:1141:ILE:HD13	2.54	0.42
1:A:1150:ARG:HD3	1:A:1150:ARG:HA	1.80	0.42
1:A:1188:GLU:OE1	1:B:1074:SER:HB3	2.20	0.42
1:C:1122:GLN:HE21	1:C:1165:MET:HE1	1.85	0.42
1:A:1093:LEU:HA	1:A:1096:LEU:HB2	2.01	0.42
1:A:1073:MET:SD	1:A:1078:GLN:HA	2.60	0.42
1:B:1021:PHE:CD1	1:B:1024:MET:HE3	2.52	0.42
1:A:1048:VAL:HG22	1:A:1049:PHE:N	2.34	0.42
1:A:1087:ARG:NH2	1:A:1174:GLU:OE1	2.48	0.42
1:B:1056:ASP:OD1	1:B:1056:ASP:C	2.58	0.42
1:C:1165:MET:O	1:C:1168:GLN:CG	2.68	0.41
1:C:1194:VAL:HG22	1:C:1194:VAL:O	2.20	0.41
1:A:1160:ILE:HD12	1:A:1197:PRO:HA	2.02	0.41
1:B:1180:PHE:HA	1:B:1190:VAL:O	2.20	0.41
1:A:1063:ILE:N	1:A:1063:ILE:CD1	2.84	0.41
1:B:1081:ARG:NH1	1:B:1081:ARG:HG3	2.35	0.41
1:B:1162:VAL:HG22	1:B:1195:ILE:HG23	2.03	0.41
1:C:1068:GLY:HA3	1:C:1078:GLN:NE2	2.35	0.41
1:A:1150:ARG:NH1	1:A:1153:GLU:OE2	2.50	0.41
1:C:1130:PHE:CD1	1:C:1141:ILE:HD13	2.55	0.41
1:A:1021:PHE:O	1:A:1024:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:THR:HG21	1:C:1132:SER:OG	2.19	0.41
1:A:1010:LEU:HD23	1:A:1075:PRO:HG3	2.03	0.41
1:A:1176:ILE:HD11	1:A:1196:ASN:HA	2.02	0.41
1:B:1139:THR:OG1	1:B:1140:ALA:N	2.54	0.41
1:C:1105:LEU:HD23	4:C:2003:HOH:O	2.21	0.41
1:C:1093:LEU:HD21	1:C:1115:ARG:HA	2.03	0.41
1:C:1161:MET:SD	1:C:1192:THR:HB	2.61	0.41
1:A:1112:PRO:HA	1:A:1113:PRO:HD3	1.94	0.41
1:B:1019:VAL:CG2	1:B:1157:PRO:HG3	2.48	0.41
1:A:1064:MET:SD	2:C:2200:TAT:C2	3.09	0.41
1:A:1152:GLN:CD	1:A:1152:GLN:C	2.80	0.41
1:A:1162:VAL:HB	1:A:1166:VAL:CG1	2.50	0.41
1:B:1031:GLN:OE1	1:B:1031:GLN:HA	2.21	0.41
1:B:1036:LEU:HD23	1:B:1036:LEU:C	2.41	0.41
1:B:1162:VAL:HB	1:B:1166:VAL:CG1	2.50	0.41
1:C:1170:VAL:HG11	1:C:1195:ILE:HG21	2.01	0.41
1:B:1079:VAL:HG13	1:B:1166:VAL:CG1	2.40	0.41
1:C:1044:MET:O	1:C:1048:VAL:HG13	2.21	0.41
1:A:1036:LEU:HD23	1:A:1036:LEU:C	2.41	0.41
1:A:1093:LEU:HD11	1:A:1114:VAL:CG1	2.49	0.41
1:A:1117:ARG:NH1	4:A:2012:HOH:O	2.54	0.41
1:C:1013:ILE:HG12	1:C:1145:VAL:HG22	2.02	0.41
1:C:1059:VAL:HG12	2:C:2200:TAT:H8	2.02	0.41
1:C:1019:VAL:CG2	1:C:1157:PRO:HG3	2.46	0.41
1:C:1162:VAL:HB	1:C:1166:VAL:CG1	2.51	0.41
1:A:1013:ILE:HG12	1:A:1145:VAL:HG22	2.03	0.40
1:B:1165:MET:O	1:B:1168:GLN:CG	2.69	0.40
1:C:1031:GLN:OE1	1:C:1031:GLN:HA	2.21	0.40
1:B:1051:ASN:C	1:B:1052:GLN:HG2	2.41	0.40
1:A:1096:LEU:HD23	1:A:1096:LEU:HA	1.96	0.40
1:A:1096:LEU:HD22	1:A:1100:TRP:CZ2	2.56	0.40
1:B:1010:LEU:HD11	1:B:1122:GLN:HG2	2.04	0.40
1:B:1017:ASP:OD1	1:B:1117:ARG:NH2	2.55	0.40
1:C:1028:LEU:HD22	1:C:1111:VAL:HG21	2.04	0.40
1:A:1130:PHE:CA	1:C:1038:ASN:OD1	2.61	0.40
1:C:1186:ILE:O	1:C:1188:GLU:N	2.51	0.40
1:A:1056:ASP:OD2	1:A:1064:MET:HE2	2.22	0.40
1:A:1102:GLU:O	1:A:1102:GLU:HG3	2.22	0.40
1:A:1177:LYS:HG3	1:A:1194:VAL:HG13	2.03	0.40
1:B:1129:LEU:HD23	1:B:1138:PHE:CA	2.52	0.40
1:C:1018:ILE:O	1:C:1061:ASP:OD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1087:ARG:NH1	1:C:1174:GLU:OE1	2.54	0.40
1:C:1180:PHE:HA	1:C:1190:VAL:O	2.21	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:C:1072:GLU:OE1	1:C:1072:GLU:OE1[3_555]	1.90	0.30

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/226 (84%)	170 (90%)	14 (7%)	6 (3%)	5	6
1	B	189/226 (84%)	170 (90%)	14 (7%)	5 (3%)	6	9
1	C	190/226 (84%)	169 (89%)	15 (8%)	6 (3%)	5	6
All	All	569/678 (84%)	509 (90%)	43 (8%)	17 (3%)	5	7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1199	MET
1	C	1199	MET
1	A	1114	VAL
1	A	1179	GLU
1	A	1187	ASP
1	B	1114	VAL
1	B	1179	GLU
1	B	1187	ASP
1	C	1114	VAL
1	C	1179	GLU

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Mol	Chain	Res	Type
1	C	1187	ASP
1	A	1027	ALA
1	B	1027	ALA
1	C	1027	ALA
1	C	1113	PRO
1	A	1113	PRO
1	B	1113	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	160/189 (85%)	153 (96%)	7 (4%)	33	57
1	B	159/189 (84%)	149 (94%)	10 (6%)	21	38
1	C	160/189 (85%)	153 (96%)	7 (4%)	33	57
All	All	479/567 (84%)	455 (95%)	24 (5%)	28	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	LEU
1	A	1029	GLN
1	A	1048	VAL
1	A	1077	GLU
1	A	1152	GLN
1	A	1168	GLN
1	A	1177	LYS
1	B	1005	ARG
1	B	1028	LEU
1	B	1029	GLN
1	B	1048	VAL
1	B	1077	GLU
1	B	1152	GLN
1	B	1165	MET
1	B	1168	GLN

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Mol	Chain	Res	Type
1	B	1177	LYS
1	B	1184	LYS
1	C	1028	LEU
1	C	1029	GLN
1	C	1048	VAL
1	C	1077	GLU
1	C	1152	GLN
1	C	1168	GLN
1	C	1177	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1029	GLN
1	A	1122	GLN
1	A	1133	GLN
1	A	1158	ASN
1	A	1168	GLN
1	B	1029	GLN
1	B	1098	GLN
1	B	1122	GLN
1	B	1133	GLN
1	B	1158	ASN
1	B	1168	GLN
1	C	1029	GLN
1	C	1122	GLN
1	C	1133	GLN
1	C	1158	ASN
1	C	1168	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	TAT	A	2200	3	25,33,33	1.31	2 (8%)	25,52,52	1.17	4 (16%)
2	TAT	B	2199	3	25,33,33	1.54	2 (8%)	25,52,52	1.13	3 (12%)
2	TAT	C	2200	3	25,33,33	1.34	2 (8%)	25,52,52	1.25	4 (16%)

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	TAT	A	2200	3	-	0/14/38/38	0/3/3/3
2	TAT	B	2199	3	-	0/14/38/38	0/3/3/3
2	TAT	C	2200	3	-	0/14/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2200	TAT	C2-N1	3.59	1.40	1.33
2	A	2200	TAT	C2-N1	3.61	1.40	1.33
2	C	2200	TAT	O4'-C1'	3.72	1.46	1.41
2	A	2200	TAT	O4'-C1'	3.73	1.46	1.41
2	B	2199	TAT	C2-N1	4.31	1.42	1.33
2	B	2199	TAT	O4'-C1'	4.52	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2200	TAT	PB-O3A-PA	-3.45	120.92	132.29
2	B	2199	TAT	PB-O3A-PA	-3.20	121.73	132.29
2	A	2200	TAT	C4'-O4'-C1'	-2.92	106.66	109.77
2	A	2200	TAT	PB-O3A-PA	-2.22	124.97	132.29
2	C	2200	TAT	C4'-O4'-C1'	-2.17	107.46	109.77
2	A	2200	TAT	N3-C2-N1	-2.06	127.06	128.86
2	B	2199	TAT	C4-C5-N7	2.10	111.44	109.41
2	C	2200	TAT	O3A-PA-O5'	2.21	109.44	101.34
2	B	2199	TAT	O3A-PA-O5'	2.41	110.18	101.34
2	A	2200	TAT	C4-C5-N7	2.45	111.77	109.41
2	C	2200	TAT	C4-C5-N7	2.66	111.98	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2200	TAT	2	0
2	B	2199	TAT	1	0
2	C	2200	TAT	4	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	194/226 (85%)	0.64	11 (5%) 24 25	11, 25, 50, 57	1 (0%)
1	B	193/226 (85%)	0.63	14 (7%) 16 16	5, 24, 48, 64	0
1	C	194/226 (85%)	1.21	36 (18%) 1 1	11, 28, 58, 63	4 (2%)
All	All	581/678 (85%)	0.83	61 (10%) 7 6	5, 25, 53, 64	5 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1106	VAL	12.6
1	C	1105	LEU	9.7
1	C	1104	GLY	8.1
1	C	1107	GLY	7.0
1	C	1112	PRO	6.9
1	C	1025	SER	6.7
1	C	1111	VAL	5.8
1	C	1026	ASN	4.7
1	A	1200	LEU	4.6
1	C	1175	ILE	4.5
1	C	1031	GLN	4.4
1	C	1181	LEU	4.1
1	B	1112	PRO	4.1
1	C	1028	LEU	3.8
1	C	1187	ASP	3.8
1	C	1190	VAL	3.7
1	C	1116	PHE	3.6
1	B	1187	ASP	3.6
1	C	1191	MET	3.4
1	A	1187	ASP	3.4
1	B	1028	LEU	3.2
1	C	1114	VAL	3.2
1	C	1024	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1184	LYS	3.2
1	A	1105	LEU	3.2
1	A	1029	GLN	3.0
1	B	1029	GLN	3.0
1	A	1004	LEU	3.0
1	B	1101	GLN	2.9
1	C	1182	GLU	2.9
1	C	1030	SER	2.8
1	A	1199	MET	2.8
1	C	1186	ILE	2.8
1	C	1172	ASP	2.8
1	C	1183	LEU	2.8
1	C	1170	VAL	2.6
1	B	1092	ALA	2.6
1	B	1052	GLN	2.5
1	C	1164	ALA	2.5
1	C	1021	PHE	2.4
1	A	1025	SER	2.4
1	C	1195	ILE	2.4
1	A	1134	GLU	2.4
1	B	1071	GLU	2.4
1	C	1094	GLU	2.3
1	B	1105	LEU	2.3
1	C	1113	PRO	2.3
1	B	1102	GLU	2.3
1	B	1176	ILE	2.2
1	C	1180	PHE	2.2
1	B	1096	LEU	2.2
1	C	1199	MET	2.2
1	C	1184	LYS	2.1
1	A	1081	ARG	2.1
1	C	1032	GLY	2.1
1	C	1151	LEU	2.1
1	A	1189	PRO	2.1
1	C	1166	VAL	2.0
1	B	1035	GLU	2.0
1	C	1193	CYS	2.0
1	B	1023	ARG	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
3	MG	C	2202	1/1	0.95	0.20	-0.50	21,21,21,21	0
2	TAT	B	2199	31/31	0.94	0.17	-0.53	22,31,46,46	0
2	TAT	A	2200	31/31	0.94	0.15	-0.83	22,30,41,42	0
2	TAT	C	2200	31/31	0.88	0.16	-0.85	17,29,57,58	0
3	MG	A	2202	1/1	0.95	0.08	-2.62	7,7,7,7	0
3	MG	B	2201	1/1	0.95	0.08	-2.80	8,8,8,8	0
3	MG	A	2201	1/1	0.92	0.16	-	17,17,17,17	0
3	MG	B	2200	1/1	0.54	0.31	-	43,43,43,43	0
3	MG	C	2201	1/1	0.80	0.17	-	36,36,36,36	0

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

There are no such residues in this entry.