Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 03:36 PM EDT

PDB ID	:	1YNT
Title	:	Structure of the monomeric form of T. gondii SAG1 surface antigen bound to a human Fab
Authors	:	Graille, M.; Stura, E.A.; Bossus, M.; Muller, B.H.; Letourneur, O.; Battail-Poirot, N.; Sibai, G.; Rolland, D.; Le Du, M.H.; Ducancel, F.
Deposited on	:	2005-01-25
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

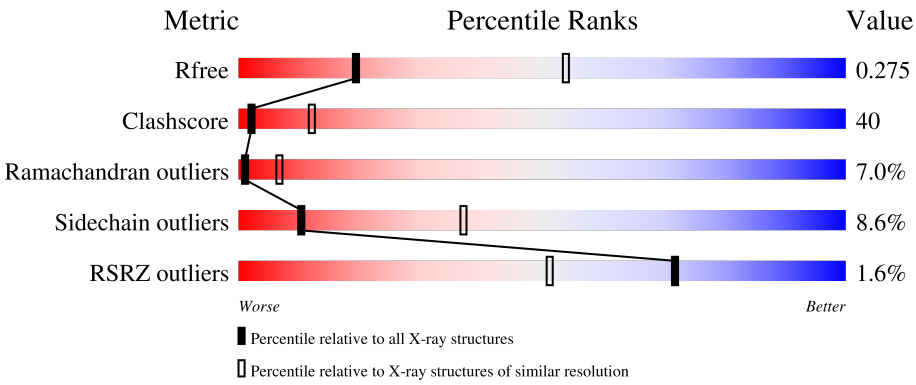
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	213	% 34% 59% 8%
1	C	213	32% 61% 8%
2	B	218	45% 44% 10% •
2	D	218	47% 42% 10% •
3	E	61	31% 64% 5%

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Mol	Chain	Length	Quality of chain
4	F	254	3% 33% 56% 9%
4	G	254	5% 32% 57% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10802 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 4F11E12 Fab variable light chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	1658	1027	280	346	5	0	0	0
1	C	213	1658	1027	280	346	5	0	0	0

- Molecule 2 is a protein called 4F11E12 Fab variable heavy chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1657	1048	269	332	8	0	0	0
2	D	218	1657	1048	269	332	8	0	0	0

- Molecule 3 is a protein called protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	61	476	302	76	97	1	0	0	0

- Molecule 4 is a protein called Major surface antigen p30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	252	1847	1151	308	374	14	0	0	0
4	G	252	1847	1151	308	374	14	0	0	0

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
5	B	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
5	D	1	1	1	0	0

3 Residue-property plots (i)

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

• Molecule 1: 4F11E12 Fab variable light chain region

Chain A: % 34% 59% 8%

D1 I2 Q3 V4 T5 Q6 T7 T8 S9 S10 L11 S12 A13 S14 L15 G16 D17 R18 V19 C23 R24 A25 S26 Q27 D28 I29 S30 N31 Y32 L33 N34 W35 Y36 Q37 Q38 K39 P40 D41 G42 T43 V44 K45 L46 L47 T48 Y49 Y50 T51 S52 R53 L54 H55 V58 F62 S63 G64 S65

G66 S67 G68 T69 D70 Y71 S72 L73 T74 I75 S76 N77 L78 E79 Q80 E81 D82 I83 A84 T85 Y86 F87 C88 Q89 Q90 G91 D92 N93 T94 L95 Y96 T97 F98 G99 G100 G101 T102 K103 L104 E105 I106 K107 R108 A109 D110 A111 A112 P113 T114 V115 S116 I117 F118 P119 P120 S121 S122 E123 Q124 L125

V133 C134 F135 L136 N137 N138 F139 Y140 P141 I144 N145 V146 K147 W148 K149 I150 D151 E154 R155 N161 S162 D165 D170 S171 S174 M175 S176 S177 T178 L179 R188 H189 N190 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 S201 P204 I205 V206 K207 S208 F209 N210

R211 N212 E213

• Molecule 1: 4F11E12 Fab variable light chain region

Chain C: 32% 61% 8%

D1001 I1002 Q1003 V1004 T1005 Q1006 T1007 L1011 S1012 A1013 S1014 L1015 G1016 D1017 R1018 V1019 C1023 R1024 A1025 S1026 Q1027 D1028 I1029 S1030 N1031 Y1032 L1033 N1034 W1035 Y1036 Q1037 Q1038 K1039 P1040 D1041 G1042 T1043 V1044 K1045 L1046 L1047 I1048 Y1049 Y1050 T1051 S1052 R1053 L1054 H1055 V1058 R1061 F1062 S1063 G1064 S1065 G1066

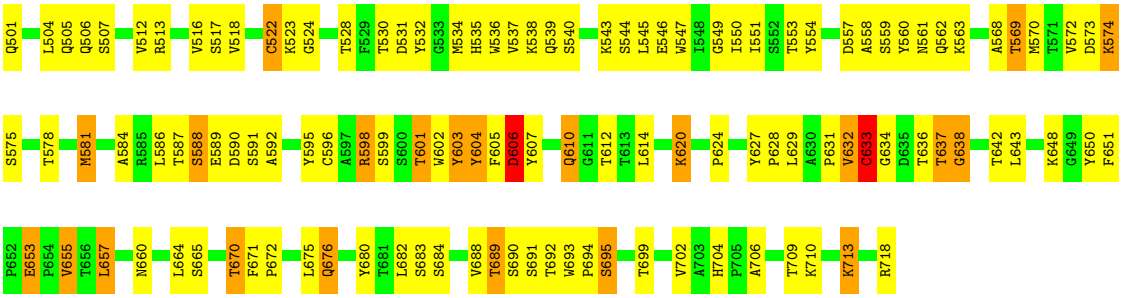
S1067 G1068 T1069 D1070 Y1071 S1072 L1073 T1074 I1075 S1076 N1077 L1078 E1081 D1082 I1083 A1084 T1085 Y1086 F1087 C1088 Q1089 Q1090 G1091 N1092 T1093 L1094 P1095 Y1096 T1097 F1098 G1099 G1100 G1101 T1102 K1103 L1104 E1105 I1106 K1107 R1108 A1109 D1110 A1111 A1112 P1113 T1114 V1115 S1116 I1117 F1118 P1119 P1120 S1121 S1122 E1123 Q1124 L1125 T1126 S1127

V1133 C1134 F1135 L1136 N1137 N1138 F1139 Y1140 P1141 K1142 D1143 I1144 N1145 V1146 K1147 I1150 D1151 E1154 R1155 N1161 S1162 D1165 Q1166 D1170 S1171 T1172 Y1173 S1174 M1175 S1176 S1177 T1178 L1179 K1183 E1187 R1188 H1189 N1190 S1191 Y1192 T1193 C1194 E1195 A1196 T1197 H1198 K1199 T1200 S1201 P1204 I1205

V1206 K1207 S1208 F1209 N1210 R1211 N1212 E1213

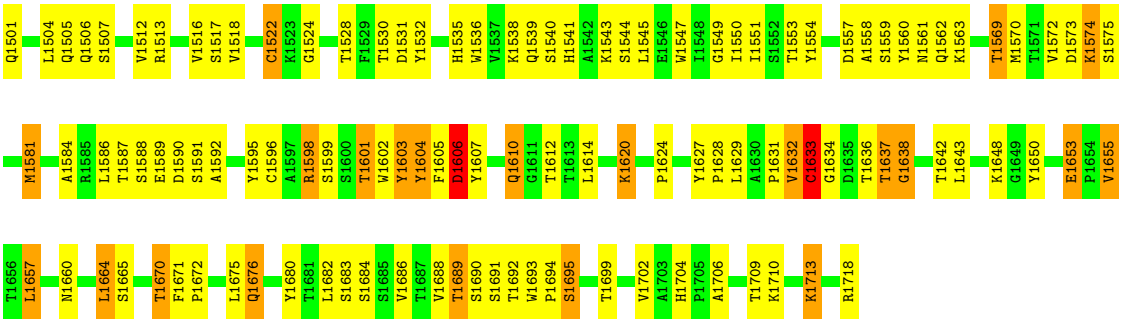
• Molecule 2: 4F11E12 Fab variable heavy chain region

Chain B: 45% 44% 10%



- Molecule 2: 4F11E12 Fab variable heavy chain region

Chain D:

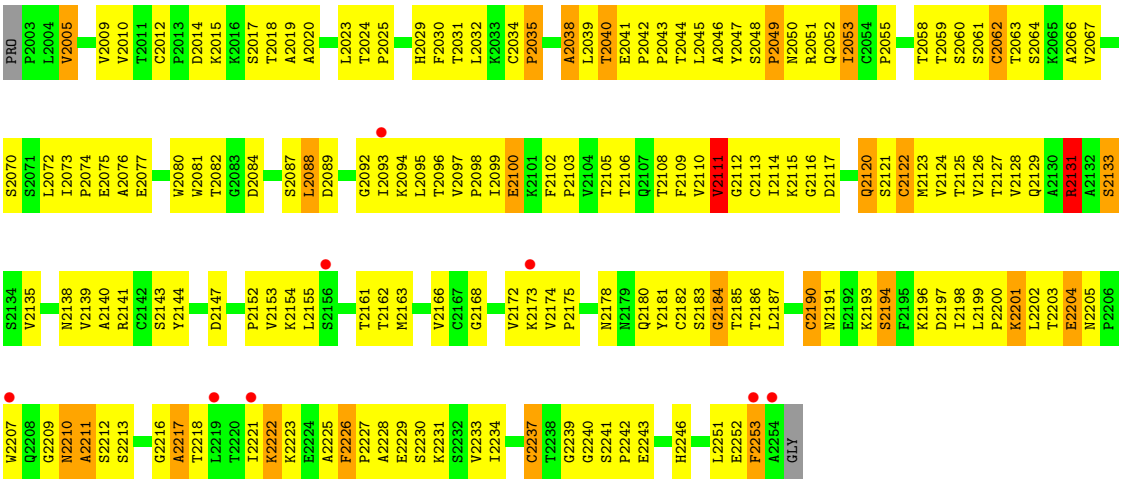


- Molecule 3: protein L

Chain E:

- Molecule 4: Major surface antigen p30

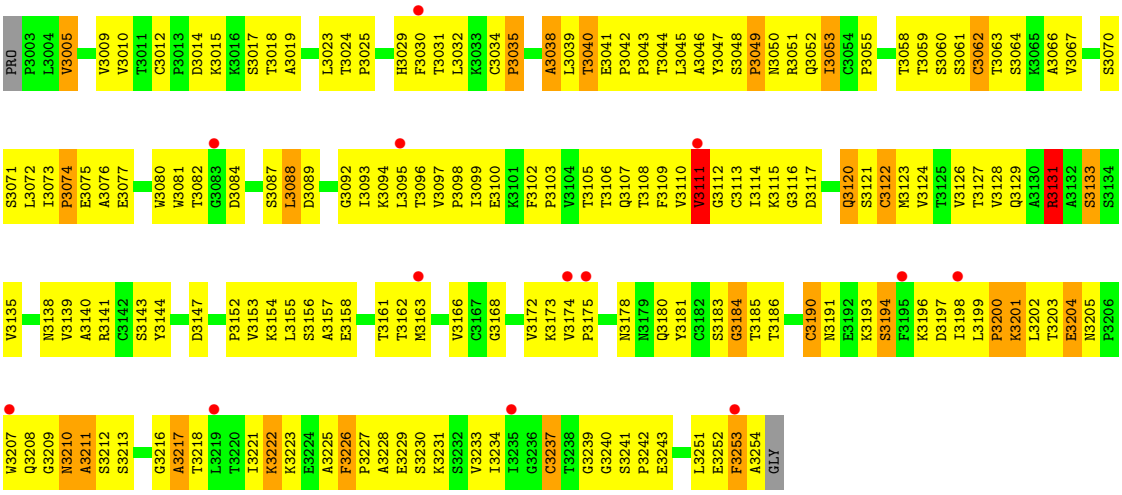
Chain F:



- Molecule 4: Major surface antigen p30

Chain G:

5%
32%
57%
10%


PRO P3003 L3004 V3005 V3009 V3010 T3011 C3012 P3013 D3014 K3015 K3016 S3017 T3018 A3019 L3023 T3024 P3025 H3029 F3030 T3031 L3032 K3033 C3034 P3035 A3038 L3039 T3040 E3041 P3042 P3043 T3044 L3045 A3046 Y3047 S3048 P3049 N3050 R3051 Q3052 I3053 C3054 P3055 T3058 T3059 S3060 S3061 C3062 T3063 S3064 K3065 A3066 V3067 S3070
S3071 L3072 I3073 P3074 E3075 A3076 E3077 W3080 W3081 T3082 G3083 D3084 S3087 L3088 D3089 G3092 I3093 K3094 L3095 T3096 V3097 P3098 I3099 E3100 K3101 F3102 P3103 V3104 T3105 T3106 Q3107 T3108 F3109 V3110 V3111 G3112 C3113 I3114 K3115 G3116 D3117 Q3120 S3121 C3122 M3123 V3124 T3125 V3126 T3127 V3128 Q3129 A3130 R3131 A3132 S3133 S3134
V3135 N3138 V3139 A3140 R3141 C3142 S3143 Y3144 D3147 P3152 V3153 K3154 L3155 S3156 A3157 E3158 T3161 T3162 M3163 V3166 C3167 G3168 V3172 K3173 V3174 P3175 N3178 N3179 Q3180 Y3181 C3182 S3183 G3184 T3185 T3186 C3190 N3191 E3192 K3193 S3194 F3195 K3196 D3197 I3198 L3199 P3200 K3201 L3202 T3203 E3204 N3205 P3206
W3207 Q3208 G3209 N3210 A3211 S3212 S3213 G3216 A3217 T3218 L3219 T3220 I3221 K3222 K3223 E3224 A3225 F3226 P3227 A3228 E3229 S3230 K3231 S3232 V3233 I3234 I3235 G3236 C3237 T3238 G3239 G3240 S3241 P3242 E3243 L3251 E3252 F3253 A3254 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.03Å 198.28Å 128.37Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 39.29 – 3.08	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-3.10) 95.1 (39.29-3.08)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.283 0.237 , 0.275	Depositor DCC
R_{free} test set	1579 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10802	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CD

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	0.48	0/1692	0.74	0/2297
1	C	0.49	0/1692	0.73	0/2297
2	B	0.51	0/1700	0.76	1/2318 (0.0%)
2	D	0.51	0/1700	0.77	1/2318 (0.0%)
3	E	0.46	0/483	0.65	0/649
4	F	0.32	0/1882	0.63	0/2568
4	G	0.32	0/1882	0.63	0/2568
All	All	0.44	0/11031	0.71	2/15015 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	653	GLU	N-CA-C	5.54	125.96	111.00
2	D	1653	GLU	N-CA-C	5.41	125.60	111.00

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	1658	0	1583	137	0
1	C	1658	0	1580	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1657	0	1607	118	0
2	D	1657	0	1607	115	0
3	E	476	0	456	40	0
4	F	1847	0	1844	168	0
4	G	1847	0	1844	176	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10802	0	10521	850	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (850) 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)
4:G:3133:SER:HB3	4:G:3143:SER:H	1.14	1.11
4:F:2133:SER:HB3	4:F:2143:SER:H	1.14	1.08
2:D:1624:PRO:HB3	2:D:1650:TYR:HB3	1.35	1.05
2:B:624:PRO:HB3	2:B:650:TYR:HB3	1.36	1.02
1:C:1002:ILE:HG12	1:C:1002:ILE:O	1.59	1.01
1:A:34:ASN:HD22	1:A:89:GLN:NE2	1.60	0.98
1:A:2:ILE:HG12	1:A:2:ILE:O	1.60	0.98
1:C:1034:ASN:HD22	1:C:1089:GLN:NE2	1.61	0.97
1:A:34:ASN:HD22	1:A:89:GLN:HE22	1.13	0.92
4:G:3183:SER:HB2	4:G:3191:ASN:HD22	1.34	0.92
2:D:1572:VAL:HG22	2:D:1573:ASP:H	1.35	0.92
2:B:572:VAL:HG22	2:B:573:ASP:H	1.33	0.91
2:D:1518:VAL:HG12	2:D:1586:LEU:HD11	1.53	0.91
4:F:2183:SER:HB2	4:F:2191:ASN:HD22	1.36	0.90
1:C:1034:ASN:HD22	1:C:1089:GLN:HE22	1.12	0.88
2:D:1536:TRP:CD2	2:D:1581:MET:HG3	2.08	0.88
1:C:1150:ILE:HD11	1:C:1179:LEU:HD21	1.56	0.87
2:B:536:TRP:CD2	2:B:581:MET:HG3	2.09	0.87
1:C:1205:ILE:HD13	1:C:1205:ILE:H	1.41	0.86
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.57	0.86
1:C:1091:GLY:HA3	2:D:1603:TYR:HB2	1.56	0.86
1:C:1017:ASP:O	1:C:1077:ASN:HA	1.75	0.86
2:B:518:VAL:HG12	2:B:586:LEU:HD11	1.59	0.85
1:A:91:GLY:HA3	2:B:603:TYR:HB2	1.59	0.85
4:G:3041:GLU:O	4:G:3043:PRO:HD3	1.77	0.84
3:E:876:ASN:O	3:E:877:ILE:HG13	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3019:ALA:HB3	4:G:3124:VAL:HG22	1.60	0.83
4:F:2041:GLU:O	4:F:2043:PRO:HD3	1.78	0.83
1:C:1046:LEU:HD12	1:C:1055:HIS:HD2	1.43	0.83
4:G:3010:VAL:HG11	4:G:3124:VAL:HG21	1.60	0.83
2:B:682:LEU:HD23	2:B:683:SER:N	1.94	0.83
1:A:17:ASP:O	1:A:77:ASN:HA	1.77	0.82
1:A:205:ILE:HD13	1:A:205:ILE:H	1.43	0.82
1:C:1085:THR:OG1	1:C:1103:LYS:HG2	1.80	0.82
2:D:1657:LEU:CD2	2:D:1702:VAL:HG22	2.09	0.82
4:F:2183:SER:HB2	4:F:2191:ASN:ND2	1.96	0.81
1:A:36:TYR:CE2	1:A:46:LEU:HD23	2.16	0.81
1:A:46:LEU:HD12	1:A:55:HIS:HD2	1.45	0.81
4:F:2019:ALA:HB3	4:F:2124:VAL:HG22	1.62	0.81
2:B:657:LEU:CD2	2:B:702:VAL:HG22	2.11	0.81
2:D:1682:LEU:HD23	2:D:1683:SER:N	1.95	0.81
4:G:3183:SER:HB2	4:G:3191:ASN:ND2	1.95	0.81
4:F:2010:VAL:HG11	4:F:2124:VAL:HG21	1.61	0.81
4:G:3025:PRO:HA	4:G:3099:ILE:HD12	1.63	0.81
4:F:2133:SER:HB3	4:F:2143:SER:N	1.95	0.80
1:C:1036:TYR:CE2	1:C:1046:LEU:HD23	2.15	0.80
1:C:1046:LEU:HD12	1:C:1055:HIS:CD2	2.16	0.80
4:F:2199:LEU:HD11	4:F:2227:PRO:HD3	1.63	0.80
4:F:2025:PRO:HA	4:F:2099:ILE:HD12	1.64	0.80
4:G:3199:LEU:HD11	4:G:3227:PRO:HD3	1.62	0.80
2:D:1516:VAL:HG12	2:D:1517:SER:N	1.98	0.79
1:A:49:TYR:O	1:A:53:ARG:HB2	1.82	0.79
4:G:3133:SER:HB3	4:G:3143:SER:N	1.95	0.78
1:A:46:LEU:HD12	1:A:55:HIS:CD2	2.16	0.78
1:A:26:SER:O	1:A:27:GLN:HB3	1.84	0.78
1:C:1088:CYS:O	1:C:1099:GLY:N	2.18	0.77
3:E:849:GLU:HG2	3:E:852:ARG:NH1	1.99	0.77
2:B:516:VAL:HG12	2:B:517:SER:N	1.99	0.77
1:C:1026:SER:O	1:C:1027:GLN:HB3	1.83	0.77
1:C:1049:TYR:O	1:C:1053:ARG:HB2	1.84	0.76
4:F:2112:GLY:HA3	4:F:2123:MET:HE2	1.68	0.76
3:E:829:PHE:HZ	3:E:857:LEU:HD13	1.51	0.75
4:G:3112:GLY:HA3	4:G:3123:MET:HE2	1.68	0.75
4:G:3156:SER:HB2	4:G:3254:ALA:HB3	1.67	0.75
1:A:9:SER:OG	3:E:840:LYS:HE2	1.87	0.75
4:G:3009:VAL:HG22	4:G:3031:THR:HB	1.69	0.74
2:D:1624:PRO:CB	2:D:1650:TYR:HB3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:CYS:O	1:A:99:GLY:N	2.20	0.74
2:B:559:SER:HA	4:F:2050:ASN:HD21	1.53	0.73
4:G:3131:ARG:HA	4:G:3131:ARG:NE	2.05	0.72
1:C:1023:CYS:HB2	1:C:1035:TRP:CH2	2.25	0.72
1:A:193:THR:HG23	1:A:208:SER:HB3	1.71	0.71
4:F:2009:VAL:HG22	4:F:2031:THR:HB	1.71	0.71
1:C:1089:GLN:HB2	1:C:1098:PHE:CD1	2.25	0.71
2:B:688:VAL:HG12	2:B:689:THR:H	1.57	0.70
4:F:2201:LYS:HE3	4:F:2202:LEU:N	2.06	0.70
4:G:3201:LYS:HE3	4:G:3202:LEU:N	2.07	0.70
4:F:2131:ARG:HA	4:F:2131:ARG:NE	2.05	0.70
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.26	0.70
1:A:85:THR:OG1	1:A:103:LYS:HG2	1.92	0.70
1:A:89:GLN:HB2	1:A:98:PHE:CD1	2.27	0.70
1:A:41:ASP:OD1	1:A:43:THR:HG23	1.91	0.69
4:G:3034:CYS:HB2	4:G:3088:LEU:HD22	1.74	0.69
4:G:3038:ALA:HB1	4:G:3114:ILE:O	1.92	0.69
2:D:1559:SER:HA	4:G:3050:ASN:HD21	1.56	0.69
2:D:1516:VAL:HG12	2:D:1517:SER:H	1.55	0.69
2:D:1528:THR:HB	2:D:1531:ASP:HB2	1.75	0.69
3:E:849:GLU:HG2	3:E:852:ARG:HH11	1.56	0.69
4:F:2034:CYS:HB2	4:F:2088:LEU:HD22	1.75	0.69
4:F:2038:ALA:HB1	4:F:2114:ILE:O	1.93	0.69
2:B:516:VAL:HG12	2:B:517:SER:H	1.56	0.68
1:C:1034:ASN:ND2	1:C:1089:GLN:HE22	1.88	0.68
4:F:2053:ILE:O	4:F:2053:ILE:HG12	1.94	0.68
1:A:34:ASN:ND2	1:A:89:GLN:HE22	1.88	0.68
2:D:1628:PRO:HG3	2:D:1713:LYS:HG2	1.76	0.68
2:D:1688:VAL:HG12	2:D:1689:THR:H	1.58	0.68
4:F:2135:VAL:HG22	4:F:2140:ALA:HA	1.74	0.68
4:G:3135:VAL:HG22	4:G:3140:ALA:HA	1.75	0.68
4:F:2042:PRO:HG2	4:F:2045:LEU:HB2	1.76	0.68
2:B:624:PRO:CB	2:B:650:TYR:HB3	2.18	0.67
2:B:528:THR:HB	2:B:531:ASP:HB2	1.76	0.67
3:E:829:PHE:CZ	3:E:857:LEU:HD13	2.29	0.67
1:C:1011:LEU:HD21	1:C:1019:VAL:HG12	1.77	0.67
1:C:1108:ARG:HG2	1:C:1171:SER:HB2	1.77	0.67
4:G:3113:CYS:N	4:G:3123:MET:HE2	2.08	0.67
1:A:7:THR:HG21	3:E:849:GLU:OE1	1.94	0.67
2:D:1599:SER:HB2	2:D:1601:THR:O	1.95	0.67
4:G:3042:PRO:HG2	4:G:3045:LEU:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HG2	1:A:171:SER:HB2	1.75	0.67
2:B:551:ILE:HD13	2:B:558:ALA:HB2	1.77	0.67
1:A:205:ILE:HD13	1:A:205:ILE:N	2.11	0.66
1:C:1091:GLY:CA	2:D:1603:TYR:HB2	2.26	0.66
1:A:11:LEU:HD21	1:A:19:VAL:HG12	1.77	0.66
4:G:3087:SER:O	4:G:3088:LEU:HG	1.96	0.66
1:C:1041:ASP:OD1	1:C:1043:THR:HG23	1.94	0.66
4:F:2113:CYS:N	4:F:2123:MET:HE2	2.11	0.66
4:F:2087:SER:O	4:F:2088:LEU:HG	1.96	0.65
4:G:3053:ILE:O	4:G:3053:ILE:HG12	1.96	0.65
2:B:599:SER:HB2	2:B:601:THR:O	1.95	0.65
2:B:506:GLN:N	2:B:610:GLN:OE1	2.21	0.65
4:G:3015:LYS:HA	4:G:3120:GLN:HG3	1.78	0.65
4:F:2038:ALA:HB2	4:F:2115:LYS:HB2	1.78	0.65
4:F:2015:LYS:HA	4:F:2120:GLN:HG3	1.79	0.65
4:F:2180:GLN:HA	4:F:2194:SER:HA	1.79	0.65
4:F:2163:MET:O	4:F:2218:THR:HG23	1.97	0.65
1:C:1205:ILE:HD13	1:C:1205:ILE:N	2.10	0.65
4:G:3241:SER:HA	4:G:3243:GLU:N	2.13	0.64
4:F:2018:THR:HG22	4:F:2019:ALA:H	1.60	0.64
2:B:598:ARG:O	2:B:606:ASP:HB2	1.96	0.64
2:B:572:VAL:HG22	2:B:573:ASP:N	2.10	0.64
1:A:62:PHE:HD2	1:A:73:LEU:HD11	1.63	0.64
1:C:1121:SER:OG	2:D:1627:TYR:HB3	1.98	0.64
1:C:1193:THR:HG23	1:C:1208:SER:HB3	1.79	0.64
1:C:1035:TRP:CZ3	1:C:1088:CYS:HB3	2.32	0.64
2:D:1518:VAL:CG1	2:D:1586:LEU:HD11	2.28	0.64
4:G:3163:MET:O	4:G:3218:THR:HG23	1.98	0.64
1:A:28:ASP:HA	1:A:68:GLY:O	1.98	0.64
1:C:1028:ASP:HA	1:C:1068:GLY:O	1.98	0.64
1:A:91:GLY:CA	2:B:603:TYR:HB2	2.27	0.64
4:F:2241:SER:HA	4:F:2243:GLU:N	2.13	0.64
4:G:3038:ALA:HB2	4:G:3115:LYS:HB2	1.79	0.63
4:G:3025:PRO:CA	4:G:3099:ILE:HD12	2.29	0.63
2:D:1506:GLN:N	2:D:1610:GLN:OE1	2.23	0.63
1:A:66:GLY:HA3	1:A:71:TYR:HA	1.81	0.63
2:D:1602:TRP:CZ2	4:G:3063:THR:HA	2.34	0.63
2:D:1657:LEU:HD22	2:D:1702:VAL:HG22	1.79	0.63
4:G:3018:THR:HG22	4:G:3019:ALA:H	1.62	0.63
4:G:3180:GLN:HA	4:G:3194:SER:HA	1.80	0.62
2:D:1528:THR:HG22	2:D:1531:ASP:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:PRO:HG3	2:B:713:LYS:HG2	1.81	0.62
4:G:3023:LEU:O	4:G:3129:GLN:HG3	2.00	0.62
1:C:1066:GLY:HA3	1:C:1071:TYR:HA	1.82	0.62
3:E:842:THR:CG2	3:E:845:GLU:H	2.13	0.62
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.82	0.62
1:C:1006:GLN:CD	1:C:1100:GLY:H	2.03	0.61
4:F:2025:PRO:CA	4:F:2099:ILE:HD12	2.30	0.61
4:G:3080:TRP:HB3	4:G:3096:THR:O	2.00	0.61
1:A:13:ALA:HA	3:E:835:GLN:HG2	1.82	0.61
1:A:108:ARG:HD3	1:A:109:ALA:O	2.00	0.61
2:B:602:TRP:CZ2	4:F:2063:THR:HA	2.35	0.61
4:F:2023:LEU:O	4:F:2129:GLN:HG3	2.00	0.61
4:G:3233:VAL:C	4:G:3234:ILE:HD12	2.21	0.61
1:C:1037:GLN:HB2	1:C:1047:LEU:HD11	1.81	0.61
2:D:1507:SER:O	2:D:1612:THR:HG23	2.00	0.61
2:D:1598:ARG:O	2:D:1606:ASP:HB2	2.00	0.61
4:F:2030:PHE:CD1	4:F:2095:LEU:HB3	2.36	0.61
2:B:657:LEU:HD22	2:B:702:VAL:HG22	1.81	0.61
3:E:842:THR:HG22	3:E:845:GLU:HB2	1.82	0.61
4:G:3131:ARG:HA	4:G:3131:ARG:HE	1.66	0.61
2:D:1501:GLN:OE1	2:D:1501:GLN:N	2.34	0.61
2:D:1551:ILE:HD13	2:D:1558:ALA:HB2	1.82	0.61
4:F:2172:VAL:O	4:F:2237:CYS:HB3	2.00	0.61
2:B:507:SER:O	2:B:612:THR:HG23	2.01	0.61
4:G:3193:LYS:O	4:G:3194:SER:HB2	1.99	0.61
4:F:2233:VAL:C	4:F:2234:ILE:HD12	2.21	0.60
4:G:3233:VAL:HG22	4:G:3253:PHE:HE1	1.66	0.60
2:B:501:GLN:OE1	2:B:501:GLN:N	2.34	0.60
2:B:518:VAL:CG1	2:B:586:LEU:HD11	2.31	0.60
1:C:1036:TYR:CD2	1:C:1046:LEU:HD23	2.36	0.60
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.36	0.60
1:A:205:ILE:H	1:A:205:ILE:CD1	2.05	0.60
4:F:2080:TRP:CZ3	4:F:2097:VAL:HG13	2.37	0.60
4:F:2193:LYS:O	4:F:2194:SER:HB2	1.99	0.60
1:A:6:GLN:CD	1:A:100:GLY:H	2.04	0.60
4:G:3080:TRP:CZ3	4:G:3097:VAL:HG13	2.36	0.60
1:A:122:SER:HA	1:A:125:LEU:HD12	1.83	0.60
1:A:136:LEU:HD12	1:A:136:LEU:N	2.17	0.59
4:G:3030:PHE:CD1	4:G:3095:LEU:HB3	2.36	0.59
1:A:11:LEU:O	1:A:11:LEU:HG	2.02	0.59
1:A:36:TYR:CD2	1:A:46:LEU:HD23	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:692:THR:HG22	2:B:692:THR:O	2.02	0.59
4:F:2131:ARG:HA	4:F:2131:ARG:HE	1.66	0.59
2:D:1628:PRO:HG3	2:D:1713:LYS:CG	2.33	0.59
4:F:2233:VAL:HG22	4:F:2253:PHE:HE1	1.65	0.59
1:C:1002:ILE:HD11	1:C:1029:ILE:CG2	2.32	0.59
2:D:1675:LEU:HD23	2:D:1680:TYR:CD1	2.37	0.59
4:G:3172:VAL:O	4:G:3237:CYS:HB3	2.03	0.59
2:D:1516:VAL:CG1	2:D:1517:SER:N	2.66	0.59
4:G:3175:PRO:HG2	4:G:3181:TYR:HA	1.85	0.59
2:B:561:ASN:O	2:B:562:GLN:C	2.42	0.58
1:C:1023:CYS:SG	1:C:1033:LEU:HD11	2.43	0.58
4:G:3030:PHE:HD1	4:G:3095:LEU:HB3	1.67	0.58
4:F:2080:TRP:HB3	4:F:2096:THR:O	2.03	0.58
4:F:2154:LYS:C	4:F:2155:LEU:HD22	2.23	0.58
2:D:1624:PRO:HB3	2:D:1650:TYR:CB	2.24	0.58
3:E:845:GLU:HB3	3:E:849:GLU:OE1	2.03	0.58
4:F:2175:PRO:HG2	4:F:2181:TYR:HA	1.85	0.58
3:E:864:TYR:HB2	3:E:878:LYS:O	2.04	0.58
2:B:693:TRP:CD1	2:B:694:PRO:HA	2.37	0.58
1:C:1205:ILE:H	1:C:1205:ILE:CD1	2.04	0.58
2:D:1657:LEU:C	2:D:1657:LEU:HD13	2.24	0.58
4:F:2030:PHE:HD1	4:F:2095:LEU:HB3	1.68	0.58
4:G:3018:THR:HG22	4:G:3019:ALA:N	2.19	0.58
4:G:3141:ARG:HG2	4:G:3166:VAL:HB	1.85	0.58
2:D:1561:ASN:O	2:D:1562:GLN:C	2.42	0.58
4:G:3180:GLN:HG2	4:G:3193:LYS:O	2.03	0.58
2:B:688:VAL:HG11	2:B:692:THR:HG21	1.85	0.57
1:C:1122:SER:HA	1:C:1125:LEU:HD12	1.85	0.57
1:C:1026:SER:O	1:C:1027:GLN:CB	2.51	0.57
1:C:1188:ARG:O	1:C:1189:HIS:ND1	2.37	0.57
2:D:1692:THR:HG22	2:D:1692:THR:O	2.04	0.57
4:F:2018:THR:HG22	4:F:2019:ALA:N	2.18	0.57
4:F:2180:GLN:HG2	4:F:2193:LYS:O	2.03	0.57
1:A:2:ILE:HD11	1:A:29:ILE:CG2	2.34	0.57
2:B:692:THR:O	2:B:692:THR:CG2	2.51	0.57
1:C:1086:TYR:O	1:C:1101:GLY:HA2	2.04	0.57
2:D:1536:TRP:CE3	2:D:1581:MET:HG3	2.40	0.57
2:D:1692:THR:O	2:D:1692:THR:CG2	2.53	0.57
4:F:2178:ASN:HB3	4:F:2207:TRP:CD1	2.39	0.57
2:B:536:TRP:CE3	2:B:581:MET:HG3	2.39	0.57
3:E:858:ALA:O	3:E:860:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3178:ASN:HB3	4:G:3207:TRP:CD1	2.40	0.57
4:G:3199:LEU:HD11	4:G:3227:PRO:CD	2.33	0.57
1:C:1089:GLN:HB2	1:C:1098:PHE:CE1	2.40	0.57
4:F:2062:CYS:SG	4:F:2062:CYS:O	2.62	0.57
1:A:6:GLN:NE2	1:A:101:GLY:H	2.03	0.57
1:A:26:SER:O	1:A:27:GLN:CB	2.52	0.57
1:A:137:ASN:HA	1:A:174:SER:OG	2.05	0.57
2:D:1636:THR:O	2:D:1638:GLY:N	2.31	0.57
1:C:1108:ARG:HD3	1:C:1109:ALA:O	2.05	0.56
4:F:2183:SER:CB	4:F:2191:ASN:HD22	2.14	0.56
2:B:528:THR:HG22	2:B:531:ASP:H	1.69	0.56
2:B:636:THR:C	2:B:638:GLY:H	2.08	0.56
1:A:31:ASN:HA	1:A:51:THR:OG1	2.05	0.56
2:B:535:HIS:O	2:B:596:CYS:HA	2.06	0.56
1:C:1055:HIS:O	1:C:1058:VAL:HG23	2.06	0.56
2:D:1682:LEU:HD23	2:D:1682:LEU:C	2.25	0.56
4:F:2113:CYS:H	4:F:2123:MET:HE2	1.70	0.56
2:B:657:LEU:C	2:B:657:LEU:HD13	2.25	0.56
2:D:1516:VAL:CG1	2:D:1517:SER:H	2.19	0.56
1:C:1137:ASN:HA	1:C:1174:SER:OG	2.06	0.56
2:D:1572:VAL:HG22	2:D:1573:ASP:N	2.12	0.56
4:G:3062:CYS:O	4:G:3062:CYS:SG	2.63	0.56
4:G:3082:THR:HG22	4:G:3082:THR:O	2.04	0.56
1:C:1210:ASN:O	1:C:1212:ASN:N	2.39	0.56
4:G:3034:CYS:H	4:G:3088:LEU:HD22	1.69	0.56
1:C:1004:VAL:HA	1:C:1025:ALA:HA	1.88	0.56
4:F:2082:THR:HG22	4:F:2082:THR:O	2.05	0.56
2:B:682:LEU:HD23	2:B:682:LEU:C	2.26	0.56
1:C:1006:GLN:NE2	1:C:1101:GLY:H	2.03	0.56
1:C:1047:LEU:CD1	1:C:1086:TYR:HE2	2.18	0.56
4:G:3081:TRP:HA	4:G:3094:LYS:O	2.06	0.56
2:B:591:SER:O	2:B:592:ALA:HB2	2.06	0.56
2:B:636:THR:O	2:B:638:GLY:N	2.31	0.55
2:B:506:GLN:HE22	2:B:595:TYR:HA	1.71	0.55
2:B:624:PRO:HB3	2:B:650:TYR:CB	2.25	0.55
1:C:1062:PHE:HD2	1:C:1073:LEU:HD11	1.70	0.55
1:C:1118:PHE:HE1	1:C:1135:PHE:HD2	1.54	0.55
2:D:1693:TRP:CD1	2:D:1694:PRO:HA	2.41	0.55
4:F:2034:CYS:H	4:F:2088:LEU:HD22	1.71	0.55
4:F:2066:ALA:O	4:F:2067:VAL:HG13	2.07	0.55
1:C:1011:LEU:HG	1:C:1011:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2112:GLY:HA3	4:F:2123:MET:CE	2.36	0.55
4:G:3017:SER:O	4:G:3122:CYS:HA	2.06	0.55
1:C:1032:TYR:OH	4:G:3038:ALA:HA	2.06	0.55
2:D:1549:GLY:HA3	2:D:1570:MET:CE	2.36	0.55
4:G:3034:CYS:H	4:G:3088:LEU:CD2	2.20	0.55
1:A:121:SER:OG	2:B:627:TYR:HB3	2.05	0.55
2:B:516:VAL:CG1	2:B:517:SER:H	2.19	0.55
2:B:628:PRO:HG3	2:B:713:LYS:CG	2.36	0.55
2:D:1535:HIS:O	2:D:1596:CYS:HA	2.06	0.55
1:C:1113:PRO:CA	1:C:1139:PHE:HB3	2.37	0.55
2:D:1504:LEU:HD22	2:D:1524:GLY:HA2	1.88	0.55
4:F:2199:LEU:HD11	4:F:2227:PRO:CD	2.34	0.55
1:A:133:VAL:HG12	1:A:134:CYS:N	2.22	0.55
1:C:1093:THR:HA	4:G:3047:TYR:OH	2.07	0.55
2:D:1591:SER:O	2:D:1592:ALA:HB2	2.07	0.55
4:F:2172:VAL:HG12	4:F:2173:LYS:N	2.22	0.55
1:A:209:PHE:HB2	2:B:632:VAL:HG11	1.88	0.54
2:B:516:VAL:CG1	2:B:517:SER:N	2.67	0.54
4:G:3172:VAL:HG12	4:G:3173:LYS:N	2.22	0.54
4:G:3230:SER:C	4:G:3231:LYS:HD2	2.28	0.54
4:F:2017:SER:O	4:F:2122:CYS:HA	2.08	0.54
4:F:2055:PRO:HG2	4:F:2058:THR:CG2	2.37	0.54
1:C:1003:GLN:HG3	1:C:1003:GLN:O	2.08	0.54
2:D:1675:LEU:HD23	2:D:1680:TYR:CE1	2.42	0.54
4:G:3228:ALA:HB3	4:G:3229:GLU:OE1	2.07	0.54
2:B:504:LEU:HD22	2:B:524:GLY:HA2	1.89	0.54
2:B:530:THR:HG22	2:B:554:TYR:HB2	1.88	0.54
2:B:628:PRO:O	2:B:629:LEU:HD23	2.07	0.54
1:A:50:TYR:O	1:A:52:SER:N	2.37	0.54
1:C:1031:ASN:HA	1:C:1051:THR:OG1	2.07	0.54
1:A:89:GLN:HB2	1:A:98:PHE:CE1	2.41	0.54
1:A:86:TYR:O	1:A:101:GLY:HA2	2.07	0.54
2:D:1604:TYR:C	2:D:1604:TYR:CD2	2.81	0.54
4:G:3053:ILE:HD13	4:G:3067:VAL:O	2.08	0.54
1:A:4:VAL:HG23	1:A:99:GLY:HA2	1.89	0.54
2:D:1512:VAL:HG12	2:D:1513:ARG:N	2.23	0.54
2:D:1675:LEU:HD13	2:D:1676:GLN:N	2.22	0.54
4:G:3113:CYS:H	4:G:3123:MET:HE2	1.72	0.54
2:B:512:VAL:HG12	2:B:513:ARG:N	2.23	0.53
2:B:547:TRP:CH2	2:B:549:GLY:HA2	2.43	0.53
2:B:604:TYR:C	2:B:604:TYR:CD2	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3112:GLY:HA3	4:G:3123:MET:CE	2.37	0.53
2:D:1688:VAL:HG11	2:D:1692:THR:HG21	1.90	0.53
4:F:2059:THR:O	4:F:2060:SER:HB3	2.07	0.53
4:F:2230:SER:C	4:F:2231:LYS:HD2	2.29	0.53
4:G:3055:PRO:HG2	4:G:3058:THR:CG2	2.39	0.53
1:A:113:PRO:CA	1:A:139:PHE:HB3	2.38	0.53
1:A:188:ARG:O	1:A:189:HIS:ND1	2.41	0.53
1:C:1038:GLN:HG3	1:C:1044:VAL:HG22	1.88	0.53
2:D:1506:GLN:HE22	2:D:1595:TYR:HA	1.73	0.53
4:F:2034:CYS:H	4:F:2088:LEU:CD2	2.21	0.53
4:F:2044:THR:HG21	4:F:2052:GLN:OE1	2.08	0.53
4:G:3103:PRO:HG2	4:G:3105:THR:O	2.09	0.53
1:C:1004:VAL:HG23	1:C:1099:GLY:HA2	1.91	0.53
4:F:2099:ILE:HA	4:F:2102:PHE:CE1	2.43	0.53
4:F:2216:GLY:O	4:F:2217:ALA:HB2	2.08	0.53
2:B:688:VAL:HG12	2:B:689:THR:N	2.23	0.53
1:C:1089:GLN:OE1	2:D:1603:TYR:O	2.26	0.53
4:F:2121:SER:HB2	4:F:2123:MET:HE3	1.90	0.53
4:G:3154:LYS:C	4:G:3155:LEU:HD22	2.29	0.53
1:A:55:HIS:O	1:A:58:VAL:HG23	2.08	0.53
4:F:2103:PRO:HG2	4:F:2105:THR:O	2.09	0.53
4:G:3059:THR:O	4:G:3060:SER:HB3	2.08	0.53
4:G:3216:GLY:O	4:G:3217:ALA:HB2	2.08	0.53
1:A:4:VAL:HA	1:A:25:ALA:HA	1.89	0.53
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.39	0.53
4:F:2038:ALA:HB2	4:F:2115:LYS:CB	2.38	0.53
4:F:2241:SER:HA	4:F:2243:GLU:H	1.73	0.53
1:A:62:PHE:CD2	1:A:73:LEU:HD11	2.44	0.53
1:C:1050:TYR:O	1:C:1052:SER:N	2.37	0.53
1:A:210:ASN:O	1:A:212:ASN:N	2.41	0.53
2:B:561:ASN:OD1	2:B:563:LYS:HD3	2.09	0.53
1:C:1062:PHE:CE2	1:C:1075:ILE:HG12	2.43	0.53
2:B:549:GLY:HA3	2:B:570:MET:CE	2.39	0.52
2:B:675:LEU:HD13	2:B:676:GLN:N	2.23	0.52
4:F:2228:ALA:HB3	4:F:2229:GLU:OE1	2.09	0.52
4:G:3025:PRO:HA	4:G:3099:ILE:CD1	2.38	0.52
1:A:39:LYS:HB3	1:A:40:PRO:HD2	1.91	0.52
2:D:1670:THR:HA	2:D:1684:SER:HA	1.92	0.52
3:E:876:ASN:C	3:E:877:ILE:HG13	2.29	0.52
4:F:2081:TRP:HA	4:F:2094:LYS:O	2.09	0.52
4:G:3046:ALA:O	4:G:3084:ASP:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1133:VAL:HG12	1:C:1134:CYS:N	2.24	0.52
2:D:1704:HIS:NE2	2:D:1706:ALA:HB3	2.24	0.52
4:F:2203:THR:O	4:F:2205:ASN:N	2.43	0.52
4:G:3203:THR:O	4:G:3205:ASN:N	2.43	0.52
1:A:3:GLN:O	1:A:3:GLN:HG3	2.09	0.52
3:E:853:TYR:HE1	3:E:857:LEU:HD11	1.75	0.52
1:A:32:TYR:OH	4:F:2038:ALA:HA	2.08	0.52
1:A:193:THR:CG2	1:A:208:SER:HB3	2.39	0.52
2:B:559:SER:HA	4:F:2050:ASN:ND2	2.24	0.52
2:B:632:VAL:O	2:B:634:GLY:N	2.43	0.52
4:G:3198:ILE:O	4:G:3199:LEU:HD22	2.10	0.52
1:A:47:LEU:CD1	1:A:86:TYR:HE2	2.23	0.52
1:A:135:PHE:C	1:A:136:LEU:HD12	2.30	0.52
2:D:1530:THR:HG22	2:D:1554:TYR:HB2	1.91	0.52
2:D:1636:THR:C	2:D:1638:GLY:H	2.10	0.52
1:C:1209:PHE:HB2	2:D:1632:VAL:HG11	1.91	0.52
2:D:1561:ASN:OD1	2:D:1563:LYS:HD3	2.10	0.52
4:F:2046:ALA:O	4:F:2084:ASP:HA	2.09	0.52
4:G:3099:ILE:HA	4:G:3102:PHE:CE1	2.45	0.52
4:G:3241:SER:HA	4:G:3243:GLU:H	1.72	0.52
1:A:46:LEU:HD13	1:A:46:LEU:O	2.10	0.52
2:B:670:THR:HA	2:B:684:SER:HA	1.92	0.52
3:E:868:LEU:O	3:E:869:GLU:HG2	2.10	0.52
4:G:3038:ALA:HB2	4:G:3115:LYS:CB	2.39	0.52
3:E:842:THR:HG23	3:E:844:GLU:H	1.75	0.51
1:A:38:GLN:HG3	1:A:44:VAL:HG22	1.92	0.51
1:A:89:GLN:OE1	2:B:603:TYR:O	2.28	0.51
4:G:3112:GLY:CA	4:G:3123:MET:HE2	2.39	0.51
4:G:3199:LEU:HD21	4:G:3227:PRO:HD3	1.93	0.51
1:A:9:SER:CB	3:E:840:LYS:HE2	2.41	0.51
1:C:1037:GLN:HB2	1:C:1047:LEU:CD1	2.40	0.51
1:C:1124:GLN:O	1:C:1124:GLN:HG2	2.09	0.51
2:D:1547:TRP:CH2	2:D:1549:GLY:HA2	2.45	0.51
2:D:1604:TYR:C	2:D:1604:TYR:HD2	2.13	0.51
4:F:2024:THR:HB	4:F:2025:PRO:HD2	1.91	0.51
1:A:6:GLN:CD	1:A:101:GLY:H	2.13	0.51
2:B:530:THR:HG21	2:B:554:TYR:HD1	1.75	0.51
1:C:1065:SER:O	1:C:1072:SER:N	2.41	0.51
1:C:1108:ARG:HH12	1:C:1111:ALA:HB2	1.75	0.51
4:F:2113:CYS:HB2	4:F:2122:CYS:HB3	1.93	0.51
2:B:633:CYS:SG	2:B:634:GLY:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2201:LYS:O	4:F:2225:ALA:HB1	2.11	0.51
4:G:3044:THR:HG21	4:G:3052:GLN:OE1	2.10	0.51
4:F:2141:ARG:HG2	4:F:2166:VAL:HB	1.92	0.51
1:A:65:SER:O	1:A:72:SER:N	2.42	0.51
1:C:1014:SER:O	1:C:1015:LEU:C	2.49	0.51
4:G:3076:ALA:HA	4:G:3080:TRP:CH2	2.46	0.51
2:B:540:SER:O	2:B:544:SER:N	2.44	0.50
4:F:2155:LEU:O	4:F:2226:PHE:HE2	1.94	0.50
4:F:2161:THR:O	4:F:2162:THR:HB	2.11	0.50
4:G:3070:SER:C	4:G:3072:LEU:H	2.14	0.50
4:G:3201:LYS:O	4:G:3225:ALA:HB1	2.10	0.50
4:F:2053:ILE:HD13	4:F:2067:VAL:O	2.12	0.50
4:G:3087:SER:HB3	4:G:3092:GLY:H	1.77	0.50
4:G:3109:PHE:CD1	4:G:3109:PHE:C	2.85	0.50
4:G:3183:SER:CB	4:G:3191:ASN:HD22	2.14	0.50
4:G:3025:PRO:HB3	4:G:3099:ILE:HG23	1.93	0.50
2:B:603:TYR:CD2	2:B:604:TYR:N	2.79	0.50
4:F:2025:PRO:HB3	4:F:2099:ILE:HG23	1.93	0.50
4:G:3045:LEU:HD11	4:G:3081:TRP:CZ3	2.47	0.50
2:B:660:ASN:ND2	2:B:699:THR:H	2.10	0.50
2:B:551:ILE:HD12	2:B:557:ASP:O	2.12	0.50
2:D:1530:THR:HG21	2:D:1554:TYR:HD1	1.76	0.50
4:F:2112:GLY:HA3	4:F:2123:MET:SD	2.52	0.50
4:G:3066:ALA:O	4:G:3067:VAL:HG13	2.11	0.50
4:F:2174:VAL:HG13	4:F:2175:PRO:HA	1.93	0.50
1:A:93:THR:HA	4:F:2047:TYR:OH	2.11	0.50
2:D:1605:PHE:N	2:D:1605:PHE:CD2	2.79	0.50
2:D:1688:VAL:HG12	2:D:1689:THR:N	2.27	0.50
4:F:2045:LEU:HD11	4:F:2081:TRP:CZ3	2.47	0.50
4:F:2209:GLY:O	4:F:2211:ALA:N	2.44	0.50
1:A:34:ASN:ND2	1:A:89:GLN:NE2	2.44	0.49
1:C:1006:GLN:CD	1:C:1101:GLY:H	2.16	0.49
2:D:1603:TYR:CD2	2:D:1604:TYR:N	2.80	0.49
3:E:876:ASN:N	3:E:876:ASN:HD22	2.10	0.49
4:F:2025:PRO:HA	4:F:2099:ILE:CD1	2.39	0.49
4:G:3042:PRO:O	4:G:3043:PRO:C	2.50	0.49
1:C:1083:ILE:HG23	1:C:1104:LEU:O	2.13	0.49
1:C:1113:PRO:HA	1:C:1139:PHE:HB3	1.94	0.49
3:E:853:TYR:CE1	3:E:857:LEU:HD11	2.46	0.49
4:G:3253:PHE:N	4:G:3253:PHE:CD1	2.80	0.49
1:A:62:PHE:CE2	1:A:75:ILE:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:TYR:C	2:B:604:TYR:HD2	2.14	0.49
1:C:1002:ILE:O	1:C:1002:ILE:CG1	2.42	0.49
4:F:2253:PHE:CD1	4:F:2253:PHE:N	2.79	0.49
1:C:1046:LEU:HD13	1:C:1046:LEU:O	2.13	0.49
1:C:1190:ASN:OD1	1:C:1210:ASN:HB3	2.13	0.49
4:F:2199:LEU:HD21	4:F:2227:PRO:HD3	1.94	0.49
4:G:3113:CYS:HB2	4:G:3122:CYS:HB3	1.95	0.49
4:F:2087:SER:HB3	4:F:2092:GLY:H	1.77	0.49
1:A:150:ILE:HG22	1:A:189:HIS:CD2	2.48	0.49
4:G:3108:THR:CG2	4:G:3127:THR:HG23	2.42	0.49
4:G:3209:GLY:O	4:G:3211:ALA:N	2.45	0.49
1:C:1096:TYR:CZ	2:D:1603:TYR:HA	2.48	0.49
4:F:2112:GLY:CA	4:F:2123:MET:HE2	2.41	0.49
4:G:3157:ALA:HB2	4:G:3226:PHE:CD2	2.48	0.49
4:G:3184:GLY:H	4:G:3191:ASN:HB3	1.77	0.49
2:B:591:SER:HA	2:B:614:LEU:O	2.13	0.49
2:B:602:TRP:CG	4:F:2063:THR:HG22	2.48	0.49
1:C:1011:LEU:HA	3:E:866:ALA:O	2.13	0.49
1:C:1136:LEU:HD12	1:C:1136:LEU:N	2.27	0.49
2:D:1602:TRP:CD2	4:G:3063:THR:HG22	2.48	0.49
3:E:829:PHE:HB2	3:E:833:LYS:O	2.12	0.49
4:F:2115:LYS:O	4:F:2117:ASP:N	2.41	0.49
1:A:118:PHE:HE1	1:A:135:PHE:HD2	1.59	0.49
2:B:522:CYS:HB2	2:B:536:TRP:CH2	2.48	0.49
2:B:549:GLY:HA3	2:B:570:MET:HE1	1.95	0.49
2:B:675:LEU:HD23	2:B:680:TYR:CD1	2.47	0.49
3:E:869:GLU:O	3:E:871:GLY:N	2.46	0.49
4:F:2210:ASN:O	4:F:2211:ALA:C	2.51	0.49
4:G:3115:LYS:O	4:G:3117:ASP:N	2.42	0.49
1:A:14:SER:O	1:A:15:LEU:C	2.51	0.48
1:A:23:CYS:SG	1:A:33:LEU:HD11	2.53	0.48
2:B:605:PHE:CD2	2:B:605:PHE:N	2.79	0.48
1:C:1150:ILE:HG22	1:C:1189:HIS:CD2	2.48	0.48
4:F:2076:ALA:HA	4:F:2080:TRP:CH2	2.48	0.48
4:F:2184:GLY:H	4:F:2191:ASN:HB3	1.77	0.48
1:A:170:ASP:OD1	1:A:170:ASP:C	2.52	0.48
1:A:190:ASN:OD1	1:A:210:ASN:HB3	2.13	0.48
4:F:2070:SER:C	4:F:2072:LEU:H	2.15	0.48
4:F:2109:PHE:CD1	4:F:2109:PHE:C	2.87	0.48
4:G:3024:THR:HB	4:G:3025:PRO:HD2	1.93	0.48
1:A:200:THR:O	1:A:201:SER:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:CYS:HB2	1:C:1035:TRP:HH2	1.76	0.48
1:C:1135:PHE:C	1:C:1136:LEU:HD12	2.33	0.48
2:D:1538:LYS:NZ	2:D:1590:ASP:HA	2.28	0.48
1:A:151:ASP:HA	1:A:191:SER:HB2	1.95	0.48
1:C:1154:GLU:HG2	1:C:1155:ARG:H	1.77	0.48
1:A:133:VAL:CG1	1:A:134:CYS:N	2.76	0.48
2:B:553:THR:OG1	4:F:2064:SER:HB2	2.14	0.48
4:F:2110:VAL:HG12	4:F:2111:VAL:N	2.28	0.48
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.95	0.48
1:C:1200:THR:O	1:C:1201:SER:HB2	2.13	0.48
4:F:2041:GLU:HG3	4:F:2042:PRO:HD3	1.96	0.48
4:F:2042:PRO:O	4:F:2043:PRO:C	2.51	0.48
4:G:3050:ASN:O	4:G:3051:ARG:C	2.51	0.48
2:B:602:TRP:CD2	4:F:2063:THR:HG22	2.49	0.48
1:C:1154:GLU:HG2	1:C:1155:ARG:N	2.29	0.48
1:C:1195:GLU:HG3	1:C:1206:VAL:HG13	1.95	0.48
4:F:2198:ILE:O	4:F:2199:LEU:HD22	2.13	0.48
1:C:1039:LYS:HB3	1:C:1040:PRO:HD2	1.95	0.48
4:G:3174:VAL:HG13	4:G:3175:PRO:HA	1.95	0.48
1:C:1151:ASP:HA	1:C:1191:SER:HB2	1.96	0.48
2:D:1540:SER:O	2:D:1544:SER:N	2.47	0.48
1:A:23:CYS:HB2	1:A:35:TRP:HH2	1.77	0.48
1:C:1013:ALA:O	1:C:1107:LYS:N	2.45	0.48
2:D:1657:LEU:C	2:D:1657:LEU:CD1	2.83	0.48
1:C:1006:GLN:OE1	1:C:1099:GLY:HA3	2.14	0.47
4:F:2121:SER:HB2	4:F:2123:MET:CE	2.43	0.47
4:G:3210:ASN:O	4:G:3211:ALA:C	2.52	0.47
2:D:1633:CYS:SG	2:D:1634:GLY:N	2.87	0.47
4:G:3102:PHE:HB3	4:G:3103:PRO:HD2	1.96	0.47
1:C:1118:PHE:CE1	1:C:1135:PHE:HD2	2.30	0.47
1:C:1133:VAL:CG1	1:C:1134:CYS:N	2.77	0.47
1:C:1204:PRO:O	1:C:1206:VAL:HG23	2.14	0.47
2:D:1560:TYR:OH	2:D:1569:THR:HA	2.13	0.47
4:F:2108:THR:CG2	4:F:2127:THR:HG23	2.43	0.47
4:G:3112:GLY:HA3	4:G:3123:MET:HA	1.96	0.47
3:E:823:ILE:HD12	3:E:823:ILE:N	2.29	0.47
1:A:154:GLU:HG2	1:A:155:ARG:N	2.30	0.47
2:D:1559:SER:HA	4:G:3050:ASN:ND2	2.27	0.47
2:B:602:TRP:CD1	2:B:602:TRP:N	2.80	0.47
1:C:1119:PRO:HB3	1:C:1209:PHE:CE1	2.49	0.47
2:D:1591:SER:HA	2:D:1614:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3041:GLU:HG3	4:G:3042:PRO:HD3	1.95	0.47
1:A:195:GLU:HG3	1:A:206:VAL:HG13	1.96	0.47
1:C:1092:ASN:OD1	4:G:3039:LEU:HD11	2.15	0.47
4:F:2042:PRO:HG2	4:F:2045:LEU:CB	2.44	0.47
4:F:2141:ARG:HA	4:F:2166:VAL:HB	1.97	0.47
4:G:3110:VAL:HG12	4:G:3111:VAL:N	2.28	0.47
4:G:3112:GLY:HA3	4:G:3123:MET:SD	2.55	0.47
1:A:83:ILE:HG23	1:A:104:LEU:O	2.15	0.47
1:C:1047:LEU:HD11	1:C:1086:TYR:HE2	1.79	0.47
2:D:1551:ILE:HD12	2:D:1557:ASP:O	2.14	0.47
4:F:2201:LYS:HE3	4:F:2202:LEU:H	1.79	0.47
1:A:193:THR:OG1	1:A:208:SER:HB3	2.14	0.47
2:D:1517:SER:HB2	2:D:1584:ALA:HA	1.97	0.47
2:D:1657:LEU:HD23	2:D:1702:VAL:HG22	1.92	0.47
4:F:2178:ASN:HB3	4:F:2207:TRP:CG	2.50	0.47
4:G:3161:THR:O	4:G:3162:THR:HB	2.15	0.47
1:C:1175:MET:CE	1:C:1177:SER:HB2	2.45	0.47
2:D:1602:TRP:CG	4:G:3063:THR:HG22	2.50	0.47
4:F:2221:ILE:O	4:F:2222:LYS:C	2.54	0.47
1:A:96:TYR:CZ	2:B:603:TYR:HA	2.50	0.46
1:A:108:ARG:HH12	1:A:111:ALA:HB2	1.80	0.46
2:D:1632:VAL:O	2:D:1634:GLY:N	2.48	0.46
3:E:845:GLU:C	3:E:847:THR:N	2.68	0.46
4:F:2099:ILE:HA	4:F:2102:PHE:CD1	2.51	0.46
4:F:2253:PHE:H	4:F:2253:PHE:HD1	1.64	0.46
1:A:24:ARG:NH2	3:E:852:ARG:NH2	2.64	0.46
2:B:538:LYS:NZ	2:B:590:ASP:HA	2.30	0.46
1:C:1170:ASP:OD1	1:C:1170:ASP:C	2.54	0.46
4:F:2098:PRO:HB3	4:F:2100:GLU:OE1	2.15	0.46
1:C:1193:THR:OG1	1:C:1208:SER:HB3	2.16	0.46
4:G:3040:THR:HG21	4:G:3046:ALA:HB2	1.97	0.46
4:G:3121:SER:HB2	4:G:3123:MET:CE	2.45	0.46
1:A:204:PRO:O	1:A:206:VAL:HG23	2.15	0.46
2:B:657:LEU:C	2:B:657:LEU:CD1	2.83	0.46
4:F:2106:THR:HG23	4:F:2128:VAL:O	2.15	0.46
1:C:1002:ILE:HD11	1:C:1029:ILE:HG22	1.97	0.46
1:C:1195:GLU:HG3	1:C:1206:VAL:HG22	1.98	0.46
1:A:124:GLN:O	1:A:124:GLN:HG2	2.15	0.46
1:A:154:GLU:HG2	1:A:155:ARG:H	1.80	0.46
2:B:675:LEU:HD23	2:B:680:TYR:CE1	2.50	0.46
1:C:1035:TRP:CE3	1:C:1088:CYS:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3076:ALA:O	4:G:3077:GLU:HG2	2.15	0.46
4:G:3110:VAL:O	4:G:3111:VAL:HG13	2.16	0.46
2:B:603:TYR:CE2	2:B:604:TYR:CD1	3.04	0.46
4:G:3060:SER:OG	4:G:3061:SER:N	2.47	0.46
4:G:3121:SER:HB2	4:G:3123:MET:HE3	1.97	0.46
1:A:2:ILE:HG21	1:A:93:THR:HB	1.97	0.46
1:C:1001:ASP:N	1:C:1095:PRO:HD2	2.30	0.46
2:D:1671:PHE:HB3	2:D:1672:PRO:HD2	1.97	0.46
4:F:2076:ALA:O	4:F:2077:GLU:HG2	2.16	0.46
4:G:3009:VAL:HG22	4:G:3031:THR:CB	2.42	0.46
4:G:3099:ILE:HA	4:G:3102:PHE:CD1	2.51	0.46
2:B:671:PHE:HB3	2:B:672:PRO:HD2	1.98	0.46
2:D:1549:GLY:HA3	2:D:1570:MET:HE3	1.98	0.46
2:D:1628:PRO:O	2:D:1629:LEU:HD23	2.16	0.46
4:F:2102:PHE:HB3	4:F:2103:PRO:HD2	1.97	0.46
1:A:92:ASN:OD1	4:F:2039:LEU:HD11	2.16	0.45
3:E:845:GLU:C	3:E:847:THR:H	2.18	0.45
4:G:3042:PRO:HG2	4:G:3045:LEU:CB	2.45	0.45
4:G:3233:VAL:HG22	4:G:3251:LEU:HB2	1.97	0.45
2:B:631:PRO:O	2:B:718:ARG:HD2	2.17	0.45
4:G:3178:ASN:HB3	4:G:3207:TRP:CG	2.50	0.45
2:B:539:GLN:HB2	2:B:545:LEU:CD2	2.47	0.45
2:B:602:TRP:CD1	4:F:2063:THR:HG22	2.51	0.45
2:B:709:THR:CG2	2:B:710:LYS:N	2.78	0.45
4:G:3221:ILE:O	4:G:3222:LYS:C	2.54	0.45
1:C:1066:GLY:HA3	1:C:1071:TYR:CD2	2.52	0.45
2:D:1573:ASP:O	2:D:1574:LYS:C	2.54	0.45
4:G:3194:SER:OG	4:G:3196:LYS:HG3	2.15	0.45
3:E:855:ASP:OD1	3:E:864:TYR:HE2	2.00	0.45
4:F:2233:VAL:HG22	4:F:2251:LEU:HB2	1.97	0.45
2:D:1539:GLN:HB2	2:D:1545:LEU:CD2	2.46	0.45
2:D:1603:TYR:CE2	2:D:1604:TYR:CD1	3.05	0.45
4:G:3120:GLN:O	4:G:3120:GLN:HG2	2.17	0.45
4:G:3156:SER:CB	4:G:3254:ALA:HB3	2.43	0.45
3:E:874:HIS:O	3:E:875:MET:HB2	2.17	0.45
2:B:560:TYR:OH	2:B:569:THR:HA	2.16	0.45
4:F:2120:GLN:O	4:F:2120:GLN:HG2	2.16	0.45
4:G:3168:GLY:O	4:G:3213:SER:N	2.50	0.45
4:G:3229:GLU:HB2	4:G:3231:LYS:HE3	1.98	0.45
2:D:1631:PRO:O	2:D:1718:ARG:HD2	2.15	0.45
4:F:2050:ASN:O	4:F:2051:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:ND2	1:A:177:SER:OG	2.48	0.45
1:C:1210:ASN:O	1:C:1211:ARG:C	2.55	0.45
3:E:844:GLU:N	3:E:844:GLU:CD	2.70	0.45
4:F:2012:CYS:HB2	4:F:2034:CYS:HA	1.99	0.45
4:F:2073:ILE:O	4:F:2075:GLU:N	2.50	0.45
4:F:2110:VAL:O	4:F:2111:VAL:HG13	2.17	0.45
4:G:3073:ILE:O	4:G:3075:GLU:N	2.50	0.45
4:F:2005:VAL:HG22	4:F:2005:VAL:O	2.17	0.44
3:E:847:THR:O	3:E:850:ALA:N	2.44	0.44
4:F:2185:THR:HG22	4:F:2186:THR:N	2.32	0.44
4:G:3030:PHE:CZ	4:G:3126:VAL:HG21	2.52	0.44
1:A:118:PHE:CE1	1:A:135:PHE:HD2	2.34	0.44
1:A:144:ILE:HG13	1:A:145:ASN:N	2.33	0.44
4:F:2229:GLU:HB2	4:F:2231:LYS:HE3	1.99	0.44
1:A:175:MET:CE	1:A:177:SER:HB2	2.48	0.44
2:B:620:LYS:HE3	2:B:620:LYS:HA	1.99	0.44
2:B:636:THR:C	2:B:638:GLY:N	2.70	0.44
1:C:1007:THR:OG1	3:E:855:ASP:OD1	2.28	0.44
3:E:824:LYS:C	3:E:825:VAL:HG23	2.38	0.44
2:D:1536:TRP:CE2	2:D:1581:MET:HG3	2.52	0.44
4:G:3253:PHE:H	4:G:3253:PHE:HD1	1.65	0.44
1:C:1183:LYS:O	1:C:1187:GLU:HG3	2.18	0.44
1:C:1195:GLU:CG	1:C:1206:VAL:HG22	2.48	0.44
2:D:1553:THR:OG1	4:G:3064:SER:HB2	2.17	0.44
3:E:829:PHE:HE2	3:E:861:ASN:ND2	2.16	0.44
1:A:6:GLN:CG	1:A:100:GLY:H	2.31	0.44
1:A:15:LEU:HA	1:A:78:LEU:HB3	1.99	0.44
1:A:198:HIS:CD2	1:A:199:LYS:H	2.36	0.44
1:C:1140:TYR:CD2	1:C:1141:PRO:HG3	2.53	0.44
4:F:2040:THR:HG21	4:F:2046:ALA:HB2	1.99	0.44
1:A:13:ALA:O	1:A:107:LYS:N	2.50	0.44
2:B:568:ALA:HB1	2:B:581:MET:CE	2.48	0.44
1:C:1193:THR:CG2	1:C:1208:SER:HB3	2.46	0.44
4:F:2112:GLY:HA3	4:F:2123:MET:HA	1.99	0.44
4:G:3141:ARG:HG2	4:G:3166:VAL:CB	2.48	0.44
4:G:3185:THR:HG22	4:G:3186:THR:N	2.32	0.44
1:A:6:GLN:HG3	1:A:100:GLY:H	1.83	0.43
2:D:1522:CYS:HB2	2:D:1536:TRP:CH2	2.52	0.43
2:D:1572:VAL:CG2	2:D:1573:ASP:H	2.17	0.43
3:E:839:PHE:CD1	3:E:839:PHE:N	2.86	0.43
4:F:2152:PRO:HB2	4:F:2252:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2168:GLY:O	4:F:2213:SER:N	2.51	0.43
4:F:2194:SER:OG	4:F:2196:LYS:HG3	2.17	0.43
4:G:3112:GLY:CA	4:G:3122:CYS:O	2.65	0.43
4:G:3175:PRO:HG3	4:G:3190:CYS:SG	2.57	0.43
1:A:91:GLY:O	2:B:603:TYR:HB2	2.18	0.43
1:A:210:ASN:O	1:A:211:ARG:C	2.56	0.43
2:B:573:ASP:O	2:B:574:LYS:C	2.56	0.43
1:C:1166:GLN:HB2	1:C:1173:TYR:CE1	2.53	0.43
1:C:1198:HIS:CD2	1:C:1199:LYS:H	2.35	0.43
2:D:1694:PRO:O	2:D:1695:SER:C	2.56	0.43
4:F:2144:TYR:HB3	4:F:2239:GLY:O	2.18	0.43
4:G:3097:VAL:HA	4:G:3098:PRO:HD3	1.90	0.43
1:A:35:TRP:CE3	1:A:88:CYS:HB3	2.53	0.43
1:A:162:SER:O	1:A:175:MET:HA	2.18	0.43
1:C:1002:ILE:HG21	1:C:1093:THR:HB	1.99	0.43
2:D:1549:GLY:HA3	2:D:1570:MET:HE1	1.99	0.43
4:G:3106:THR:HG23	4:G:3128:VAL:O	2.19	0.43
4:G:3131:ARG:NE	4:G:3131:ARG:CA	2.78	0.43
1:C:1062:PHE:CD2	1:C:1073:LEU:HD11	2.51	0.43
2:B:637:THR:O	2:B:637:THR:HG22	2.19	0.43
1:C:1089:GLN:HE21	1:C:1089:GLN:HB3	1.59	0.43
4:G:3014:ASP:O	4:G:3015:LYS:HB3	2.18	0.43
1:A:162:SER:OG	2:B:672:PRO:HG2	2.19	0.43
2:D:1642:THR:O	2:D:1643:LEU:HD23	2.18	0.43
4:F:2112:GLY:CA	4:F:2122:CYS:O	2.67	0.43
1:A:11:LEU:HD23	1:A:104:LEU:HD21	2.01	0.43
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.53	0.43
2:D:1636:THR:C	2:D:1638:GLY:N	2.70	0.43
4:F:2182:CYS:HB2	4:F:2234:ILE:HB	2.01	0.43
4:G:3210:ASN:O	4:G:3212:SER:N	2.51	0.43
4:G:3233:VAL:CG2	4:G:3251:LEU:HB2	2.49	0.43
2:B:523:LYS:HG2	2:B:578:THR:OG1	2.18	0.43
2:B:568:ALA:HB1	2:B:581:MET:HE1	2.01	0.43
2:B:694:PRO:O	2:B:695:SER:C	2.56	0.43
1:C:1015:LEU:HA	1:C:1078:LEU:HB3	2.00	0.43
1:A:31:ASN:O	1:A:50:TYR:HA	2.19	0.43
1:A:140:TYR:CD2	1:A:141:PRO:HG3	2.54	0.43
1:A:144:ILE:HG13	1:A:145:ASN:H	1.84	0.43
1:C:1031:ASN:O	1:C:1050:TYR:HA	2.19	0.43
1:C:1098:PHE:O	1:C:1099:GLY:O	2.37	0.43
3:E:843:PHE:HZ	3:E:872:GLY:HA3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3012:CYS:HB2	4:G:3034:CYS:HA	2.01	0.43
1:A:2:ILE:HD11	1:A:29:ILE:HG22	1.99	0.42
1:C:1143:ASP:OD1	3:E:878:LYS:HE2	2.19	0.42
2:D:1664:LEU:HD23	2:D:1686:VAL:HG21	2.00	0.42
4:F:2005:VAL:O	4:F:2005:VAL:HG13	2.18	0.42
4:F:2070:SER:OG	4:F:2076:ALA:HB3	2.19	0.42
4:G:3144:TYR:HB3	4:G:3239:GLY:O	2.19	0.42
1:A:115:VAL:HA	1:A:135:PHE:O	2.19	0.42
2:B:534:MET:O	2:B:550:ILE:HA	2.19	0.42
1:C:1121:SER:C	1:C:1123:GLU:N	2.73	0.42
2:D:1532:TYR:CD1	2:D:1532:TYR:N	2.87	0.42
4:F:2108:THR:HG23	4:F:2127:THR:HG23	2.01	0.42
4:G:3098:PRO:HB3	4:G:3100:GLU:OE1	2.19	0.42
2:B:602:TRP:CE2	4:F:2063:THR:HG22	2.54	0.42
1:C:1049:TYR:CZ	1:C:1053:ARG:HB3	2.53	0.42
1:C:1055:HIS:ND1	1:C:1055:HIS:C	2.72	0.42
1:C:1146:VAL:HG12	1:C:1147:LYS:N	2.35	0.42
2:D:1587:THR:C	2:D:1589:GLU:H	2.23	0.42
4:F:2041:GLU:CB	4:F:2042:PRO:CD	2.97	0.42
4:F:2175:PRO:HG3	4:F:2190:CYS:SG	2.59	0.42
4:F:2210:ASN:O	4:F:2212:SER:N	2.52	0.42
4:G:3005:VAL:O	4:G:3005:VAL:HG22	2.18	0.42
4:G:3041:GLU:O	4:G:3043:PRO:CD	2.59	0.42
4:G:3138:ASN:ND2	4:G:3153:VAL:HG12	2.34	0.42
4:G:3141:ARG:HA	4:G:3166:VAL:HB	2.01	0.42
4:G:3152:PRO:HB2	4:G:3252:GLU:OE2	2.20	0.42
1:A:115:VAL:HG22	1:A:136:LEU:HG	2.02	0.42
2:B:587:THR:O	2:B:589:GLU:N	2.53	0.42
1:C:1135:PHE:CE1	2:D:1671:PHE:HE1	2.37	0.42
1:C:1144:ILE:HG13	1:C:1145:ASN:N	2.35	0.42
4:F:2174:VAL:HA	4:F:2175:PRO:C	2.40	0.42
1:A:12:SER:HA	1:A:105:GLU:O	2.19	0.42
2:B:532:TYR:CD1	2:B:532:TYR:N	2.87	0.42
1:C:1005:THR:HG22	1:C:1006:GLN:N	2.34	0.42
1:C:1015:LEU:HG	1:C:1106:ILE:HD12	2.01	0.42
2:D:1709:THR:CG2	2:D:1710:LYS:N	2.82	0.42
3:E:826:ASN:O	3:E:827:LEU:HD12	2.19	0.42
2:B:587:THR:C	2:B:589:GLU:H	2.23	0.42
4:F:2135:VAL:HG13	4:F:2139:VAL:H	1.84	0.42
4:F:2138:ASN:ND2	4:F:2153:VAL:HG12	2.34	0.42
4:F:2226:PHE:H	4:F:2226:PHE:HD1	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3005:VAL:O	4:G:3005:VAL:HG13	2.19	0.42
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.55	0.42
1:A:161:ASN:HD22	1:A:177:SER:HA	1.85	0.42
1:C:1055:HIS:C	1:C:1055:HIS:HD1	2.23	0.42
1:A:195:GLU:CG	1:A:206:VAL:HG22	2.50	0.42
1:C:1162:SER:OG	2:D:1672:PRO:HG2	2.20	0.42
2:D:1606:ASP:HB3	2:D:1607:TYR:HD1	1.85	0.42
4:F:2131:ARG:NE	4:F:2131:ARG:CA	2.78	0.42
4:G:3108:THR:HG23	4:G:3127:THR:HG23	2.01	0.42
4:G:3226:PHE:H	4:G:3226:PHE:HD1	1.67	0.42
2:B:689:THR:O	2:B:691:SER:N	2.53	0.42
2:B:704:HIS:NE2	2:B:706:ALA:HB3	2.35	0.42
2:D:1539:GLN:O	2:D:1592:ALA:HB1	2.19	0.42
2:D:1547:TRP:CZ2	2:D:1550:ILE:HG22	2.55	0.42
2:D:1602:TRP:CE2	4:G:3063:THR:HG22	2.55	0.42
2:D:1650:TYR:CZ	2:D:1655:VAL:HG11	2.54	0.42
4:F:2030:PHE:HD1	4:F:2095:LEU:HD23	1.85	0.42
4:F:2047:TYR:C	4:F:2049:PRO:CD	2.88	0.42
4:G:3241:SER:HB2	4:G:3242:PRO:HA	2.02	0.42
1:A:55:HIS:C	1:A:55:HIS:ND1	2.73	0.41
2:D:1512:VAL:CG1	2:D:1513:ARG:N	2.83	0.41
2:D:1587:THR:O	2:D:1589:GLU:N	2.53	0.41
4:G:3109:PHE:CD1	4:G:3109:PHE:O	2.73	0.41
4:G:3030:PHE:HD1	4:G:3095:LEU:HD23	1.85	0.41
4:G:3041:GLU:CB	4:G:3042:PRO:CD	2.97	0.41
1:A:5:THR:HG22	1:A:6:GLN:N	2.35	0.41
1:C:1135:PHE:CE1	2:D:1671:PHE:CE1	3.08	0.41
1:C:1144:ILE:HG13	1:C:1145:ASN:H	1.86	0.41
1:A:1:ASP:N	1:A:95:PRO:HD2	2.34	0.41
2:B:537:VAL:HG13	2:B:546:GLU:O	2.20	0.41
2:D:1689:THR:O	2:D:1691:SER:N	2.52	0.41
4:F:2014:ASP:O	4:F:2015:LYS:HB3	2.21	0.41
4:F:2031:THR:HA	4:F:2093:ILE:O	2.20	0.41
4:G:3059:THR:HG22	4:G:3060:SER:N	2.35	0.41
4:G:3133:SER:HB2	4:G:3141:ARG:O	2.20	0.41
4:G:3135:VAL:HG13	4:G:3139:VAL:H	1.85	0.41
4:G:3230:SER:O	4:G:3231:LYS:HD2	2.21	0.41
1:A:39:LYS:HD2	1:A:84:ALA:HB2	2.02	0.41
2:B:522:CYS:HB2	2:B:536:TRP:HH2	1.86	0.41
2:B:606:ASP:HB3	2:B:607:TYR:HD1	1.85	0.41
2:B:632:VAL:O	2:B:633:CYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3107:GLN:HB2	4:G:3128:VAL:CG2	2.50	0.41
2:B:651:PHE:CD2	2:B:651:PHE:C	2.93	0.41
2:B:675:LEU:HD13	2:B:675:LEU:C	2.41	0.41
4:F:2066:ALA:O	4:F:2067:VAL:CG1	2.68	0.41
4:G:3174:VAL:HA	4:G:3175:PRO:C	2.41	0.41
4:G:3175:PRO:HG2	4:G:3181:TYR:CA	2.50	0.41
1:A:15:LEU:HG	1:A:106:ILE:HD12	2.03	0.41
1:A:52:SER:HB3	1:A:64:GLY:O	2.21	0.41
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.59	0.41
1:A:146:VAL:HG12	1:A:147:LYS:N	2.35	0.41
1:A:195:GLU:HG3	1:A:206:VAL:HG22	2.02	0.41
2:B:512:VAL:CG1	2:B:513:ARG:N	2.84	0.41
2:B:627:TYR:HA	2:B:628:PRO:HD3	1.89	0.41
1:C:1039:LYS:HD2	1:C:1084:ALA:HB2	2.03	0.41
1:C:1115:VAL:HG22	1:C:1136:LEU:HG	2.02	0.41
1:C:1118:PHE:CE1	1:C:1135:PHE:CD2	3.08	0.41
2:D:1637:THR:HG22	2:D:1637:THR:O	2.20	0.41
4:F:2020:ALA:HA	4:F:2125:THR:O	2.20	0.41
4:F:2109:PHE:CD1	4:F:2109:PHE:O	2.74	0.41
4:G:3034:CYS:O	4:G:3088:LEU:HB3	2.20	0.41
1:A:2:ILE:O	1:A:2:ILE:CG1	2.44	0.41
1:A:121:SER:C	1:A:123:GLU:N	2.74	0.41
2:B:650:TYR:CZ	2:B:655:VAL:HG11	2.55	0.41
1:C:1035:TRP:HD1	1:C:1048:ILE:HG22	1.85	0.41
2:D:1551:ILE:O	2:D:1551:ILE:HG23	2.21	0.41
2:D:1660:ASN:ND2	2:D:1699:THR:H	2.18	0.41
3:E:842:THR:HG23	3:E:844:GLU:N	2.35	0.41
4:G:3199:LEU:HA	4:G:3200:PRO:HD2	1.90	0.41
1:A:79:GLU:HB2	1:A:82:ASP:OD2	2.21	0.41
2:B:551:ILE:HG23	2:B:551:ILE:O	2.21	0.41
2:B:572:VAL:CG2	2:B:573:ASP:H	2.15	0.41
2:B:637:THR:O	2:B:638:GLY:O	2.39	0.41
2:B:642:THR:O	2:B:643:LEU:HD23	2.20	0.41
1:C:1061:ARG:NH1	1:C:1082:ASP:OD2	2.53	0.41
1:C:1115:VAL:HA	1:C:1135:PHE:O	2.21	0.41
1:C:1136:LEU:HD21	1:C:1196:ALA:HB2	2.02	0.41
1:C:1150:ILE:HD11	1:C:1179:LEU:CD2	2.39	0.41
2:D:1620:LYS:HE3	2:D:1620:LYS:HA	2.02	0.41
4:F:2030:PHE:CZ	4:F:2126:VAL:HG21	2.56	0.41
4:F:2032:LEU:HB3	4:F:2093:ILE:HB	2.03	0.41
4:F:2060:SER:OG	4:F:2061:SER:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2233:VAL:CG2	4:F:2251:LEU:HB2	2.50	0.41
4:G:3034:CYS:O	4:G:3035:PRO:O	2.38	0.41
1:A:15:LEU:HG	1:A:106:ILE:CD1	2.51	0.41
1:A:55:HIS:C	1:A:55:HIS:HD1	2.25	0.41
2:B:657:LEU:HD23	2:B:702:VAL:HG22	1.97	0.41
1:C:1015:LEU:HG	1:C:1106:ILE:CD1	2.51	0.41
1:C:1030:SER:O	1:C:1031:ASN:HB2	2.21	0.41
4:F:2044:THR:OG1	4:F:2052:GLN:HB2	2.21	0.41
4:F:2240:GLY:O	4:F:2241:SER:HB3	2.21	0.41
4:F:2241:SER:HB2	4:F:2242:PRO:HA	2.03	0.41
4:G:3047:TYR:C	4:G:3049:PRO:CD	2.90	0.41
4:G:3181:TYR:CD1	4:G:3181:TYR:C	2.94	0.41
1:C:1006:GLN:CG	1:C:1100:GLY:H	2.32	0.40
2:D:1602:TRP:CD1	4:G:3063:THR:HG22	2.56	0.40
2:D:1675:LEU:HD13	2:D:1675:LEU:C	2.41	0.40
4:G:3044:THR:OG1	4:G:3052:GLN:HB2	2.20	0.40
4:G:3073:ILE:HA	4:G:3074:PRO:HD2	1.81	0.40
4:G:3113:CYS:O	4:G:3121:SER:HA	2.21	0.40
4:G:3201:LYS:HE3	4:G:3202:LEU:H	1.79	0.40
1:C:1006:GLN:HG3	1:C:1100:GLY:H	1.86	0.40
1:C:1161:ASN:ND2	1:C:1177:SER:OG	2.54	0.40
2:D:1602:TRP:CD1	2:D:1602:TRP:N	2.83	0.40
4:F:2034:CYS:O	4:F:2035:PRO:O	2.39	0.40
4:F:2187:LEU:HB2	4:F:2246:HIS:HD2	1.86	0.40
4:G:3032:LEU:HB3	4:G:3093:ILE:HB	2.03	0.40
1:C:1052:SER:HB3	1:C:1064:GLY:O	2.21	0.40
3:E:845:GLU:O	3:E:847:THR:N	2.54	0.40
4:F:2113:CYS:N	4:F:2122:CYS:O	2.52	0.40
4:F:2113:CYS:O	4:F:2121:SER:HA	2.21	0.40
4:F:2154:LYS:HA	4:F:2252:GLU:HB2	2.04	0.40
4:G:3240:GLY:O	4:G:3241:SER:HB3	2.21	0.40
1:A:30:SER:O	1:A:31:ASN:HB2	2.21	0.40
1:A:32:TYR:CE2	1:A:50:TYR:HE1	2.39	0.40
2:B:517:SER:HB2	2:B:584:ALA:HA	2.03	0.40
1:C:1175:MET:HE1	1:C:1177:SER:HB2	2.03	0.40
1:C:1189:HIS:HB3	1:C:1190:ASN:H	1.78	0.40
2:D:1586:LEU:HD23	2:D:1590:ASP:OD2	2.21	0.40
4:F:2141:ARG:HG2	4:F:2166:VAL:CG2	2.51	0.40
4:G:3102:PHE:CB	4:G:3103:PRO:HD2	2.51	0.40
4:G:3208:GLN:O	4:G:3217:ALA:HA	2.21	0.40
1:C:1125:LEU:C	1:C:1127:SER:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2175:PRO:HG2	4:F:2181:TYR:CA	2.49	0.40
4:F:2194:SER:C	4:F:2196:LYS:N	2.75	0.40
4:G:3009:VAL:HG13	4:G:3031:THR:HB	2.03	0.40
4:G:3194:SER:C	4:G:3196:LYS:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	211/213 (99%)	165 (78%)	40 (19%)	6 (3%)	5 25
1	C	211/213 (99%)	166 (79%)	37 (18%)	8 (4%)	3 19
2	B	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1 9
2	D	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1 9
3	E	59/61 (97%)	44 (75%)	9 (15%)	6 (10%)	0 3
4	F	250/254 (98%)	177 (71%)	47 (19%)	26 (10%)	0 3
4	G	250/254 (98%)	173 (69%)	50 (20%)	27 (11%)	0 2
All	All	1413/1431 (99%)	1079 (76%)	235 (17%)	99 (7%)	1 7

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	27	GLN
2	B	575	SER
2	B	633	CYS
1	C	1017	ASP
1	C	1027	GLN
2	D	1574	LYS

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Mol	Chain	Res	Type
2	D	1575	SER
3	E	859	LYS
3	E	870	ASP
4	F	2005	VAL
4	F	2049	PRO
4	F	2089	ASP
4	F	2120	GLN
4	F	2147	ASP
4	F	2200	PRO
4	F	2204	GLU
4	F	2211	ALA
4	G	3005	VAL
4	G	3035	PRO
4	G	3049	PRO
4	G	3089	ASP
4	G	3120	GLN
4	G	3200	PRO
4	G	3204	GLU
4	G	3211	ALA
1	A	211	ARG
2	B	574	LYS
2	B	588	SER
2	B	606	ASP
2	B	637	THR
2	B	638	GLY
2	B	655	VAL
2	B	690	SER
1	C	1099	GLY
1	C	1211	ARG
2	D	1588	SER
2	D	1606	ASP
2	D	1633	CYS
2	D	1637	THR
2	D	1638	GLY
2	D	1655	VAL
2	D	1690	SER
3	E	830	ALA
3	E	873	ASN
4	F	2035	PRO
4	F	2074	PRO
4	F	2111	VAL
4	F	2131	ARG

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Mol	Chain	Res	Type
4	F	2194	SER
4	F	2210	ASN
4	G	3038	ALA
4	G	3074	PRO
4	G	3111	VAL
4	G	3131	ARG
4	G	3147	ASP
4	G	3194	SER
4	G	3210	ASN
1	A	99	GLY
1	A	138	ASN
2	B	522	CYS
1	C	1138	ASN
2	D	1522	CYS
4	F	2038	ALA
4	F	2116	GLY
4	F	2133	SER
4	F	2217	ALA
4	F	2223	LYS
4	G	3116	GLY
4	G	3133	SER
4	G	3217	ALA
4	G	3223	LYS
1	A	81	GLU
2	B	653	GLU
2	B	695	SER
1	C	1191	SER
2	D	1543	LYS
2	D	1695	SER
4	F	2088	LEU
4	F	2197	ASP
4	G	3088	LEU
4	G	3197	ASP
4	G	3222	LYS
2	B	543	LYS
1	C	1015	LEU
1	C	1081	GLU
2	D	1653	GLU
4	F	2184	GLY
4	F	2222	LYS
3	E	875	MET
4	F	2048	SER

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Mol	Chain	Res	Type
4	F	2100	GLU
4	G	3048	SER
4	G	3071	SER
4	G	3158	GLU
4	G	3184	GLY
3	E	832	GLY
4	F	2226	PHE
4	G	3226	PHE

5.3.2 Protein sidechains (i)

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	191/191 (100%)	172 (90%)	19 (10%)	8	29
1	C	191/191 (100%)	174 (91%)	17 (9%)	9	34
2	B	188/188 (100%)	167 (89%)	21 (11%)	6	24
2	D	188/188 (100%)	167 (89%)	21 (11%)	6	24
3	E	47/47 (100%)	43 (92%)	4 (8%)	10	37
4	F	214/215 (100%)	202 (94%)	12 (6%)	21	52
4	G	214/215 (100%)	202 (94%)	12 (6%)	21	52
All	All	1233/1235 (100%)	1127 (91%)	106 (9%)	10	37

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	6	GLN
1	A	7	THR
1	A	19	VAL
1	A	34	ASN
1	A	46	LEU
1	A	69	THR
1	A	70	ASP
1	A	89	GLN

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	108	ARG
1	A	116	SER
1	A	138	ASN
1	A	165	ASP
1	A	171	SER
1	A	175	MET
1	A	176	SER
1	A	197	THR
1	A	205	ILE
2	B	505	GLN
2	B	569	THR
2	B	581	MET
2	B	588	SER
2	B	598	ARG
2	B	601	THR
2	B	603	TYR
2	B	604	TYR
2	B	606	ASP
2	B	610	GLN
2	B	620	LYS
2	B	632	VAL
2	B	633	CYS
2	B	648	LYS
2	B	657	LEU
2	B	664	LEU
2	B	665	SER
2	B	670	THR
2	B	676	GLN
2	B	689	THR
2	B	713	LYS
1	C	1002	ILE
1	C	1007	THR
1	C	1019	VAL
1	C	1046	LEU
1	C	1048	ILE
1	C	1069	THR
1	C	1070	ASP
1	C	1089	GLN
1	C	1094	LEU
1	C	1108	ARG
1	C	1113	PRO

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Mol	Chain	Res	Type
1	C	1116	SER
1	C	1138	ASN
1	C	1165	ASP
1	C	1176	SER
1	C	1197	THR
1	C	1205	ILE
2	D	1505	GLN
2	D	1541	HIS
2	D	1569	THR
2	D	1581	MET
2	D	1598	ARG
2	D	1601	THR
2	D	1603	TYR
2	D	1604	TYR
2	D	1606	ASP
2	D	1610	GLN
2	D	1620	LYS
2	D	1632	VAL
2	D	1633	CYS
2	D	1648	LYS
2	D	1657	LEU
2	D	1664	LEU
2	D	1665	SER
2	D	1670	THR
2	D	1676	GLN
2	D	1689	THR
2	D	1713	LYS
3	E	831	ASP
3	E	842	THR
3	E	865	THR
3	E	876	ASN
4	F	2029	HIS
4	F	2040	THR
4	F	2053	ILE
4	F	2062	CYS
4	F	2111	VAL
4	F	2122	CYS
4	F	2131	ARG
4	F	2190	CYS
4	F	2201	LYS
4	F	2204	GLU
4	F	2237	CYS

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Mol	Chain	Res	Type
4	F	2253	PHE
4	G	3029	HIS
4	G	3040	THR
4	G	3053	ILE
4	G	3062	CYS
4	G	3111	VAL
4	G	3122	CYS
4	G	3131	ARG
4	G	3190	CYS
4	G	3201	LYS
4	G	3204	GLU
4	G	3237	CYS
4	G	3253	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	38	GLN
1	A	89	GLN
1	A	161	ASN
2	B	505	GLN
2	B	539	GLN
2	B	660	ASN
2	B	676	GLN
1	C	1031	ASN
1	C	1038	GLN
1	C	1089	GLN
1	C	1161	ASN
2	D	1501	GLN
2	D	1505	GLN
2	D	1539	GLN
2	D	1660	ASN
2	D	1676	GLN
3	E	861	ASN
3	E	876	ASN
4	F	2050	ASN
4	F	2120	GLN
4	F	2137	ASN
4	F	2138	ASN
4	F	2180	GLN
4	F	2191	ASN

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Mol	Chain	Res	Type
4	G	3050	ASN
4	G	3120	GLN
4	G	3137	ASN
4	G	3138	ASN
4	G	3180	GLN
4	G	3191	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	213/213 (100%)	-0.24	2 (0%) 84 69	24, 54, 77, 89	0
1	C	213/213 (100%)	-0.28	0 100 100	23, 54, 76, 89	0
2	B	218/218 (100%)	-0.31	0 100 100	16, 50, 78, 102	0
2	D	218/218 (100%)	-0.27	0 100 100	16, 50, 78, 102	0
3	E	61/61 (100%)	0.08	0 100 100	48, 76, 95, 103	0
4	F	252/254 (99%)	0.09	8 (3%) 47 25	67, 106, 142, 150	0
4	G	252/254 (99%)	0.18	13 (5%) 27 12	67, 106, 139, 150	0
All	All	1427/1431 (99%)	-0.12	23 (1%) 72 51	16, 68, 134, 150	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	2156	SER	4.3
4	G	3253	PHE	4.3
4	G	3174	VAL	3.8
4	G	3235	ILE	3.7
4	F	2221	ILE	3.5
4	G	3030	PHE	3.2
4	G	3111	VAL	3.0
4	G	3207	TRP	2.8
4	F	2253	PHE	2.7
4	F	2254	ALA	2.6
4	F	2093	ILE	2.5
4	F	2219	LEU	2.5
4	G	3175	PRO	2.4
4	G	3198	ILE	2.4
1	A	148	TRP	2.3
4	F	2207	TRP	2.3
4	G	3095	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	2173	LYS	2.3
1	A	91	GLY	2.3
4	G	3219	LEU	2.3
4	G	3083	GLY	2.2
4	G	3163	MET	2.1
4	G	3195	PHE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CD	B	4001	1/1	0.95	0.10	111,111,111,111	0
5	CD	D	4002	1/1	0.98	0.10	115,115,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.