WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 5, 2022 – 10:39 AM EDT

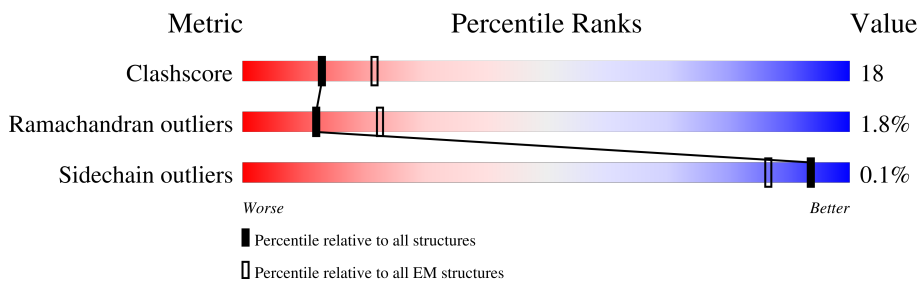|		
PDB ID	:	5VHY
EMDB ID	:	EMD-8687
Title	:	GluA2-2xGSG1L bound to ZK
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	2017-04-13
Resolution	:	4.60 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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

Metric	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		1.8%
Sidechain outliers		0.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1057	10% 46% / 27% / • / 26%
1	B	1057	12% 47% / 26% / 26%
1	C	1057	10% 48% / 25% / • / 26%
1	D	1057	12% 47% / 26% / • / 26%
1	E	1057	8% 8% / 9% / 83%
1	F	1057	8% 9% / 7% / 83%

2　Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 27572 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	E	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		
1	F	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491
F	-588	GLU	ASN	conflict	UNP P19491
F	-447	LEU	VAL	conflict	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	THR	deletion	UNP P19491
F	?	-	GLU	deletion	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	PRO	deletion	UNP P19491
F	?	-	SER	deletion	UNP P19491
F	-445	GLU	GLY	conflict	UNP P19491
F	-444	ASP	ASN	conflict	UNP P19491
F	-437	GLN	ASN	conflict	UNP P19491
F	-2	GLY	-	linker	UNP P19491
F	-1	THR	-	linker	UNP P19491
F	0	GLY	-	linker	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).
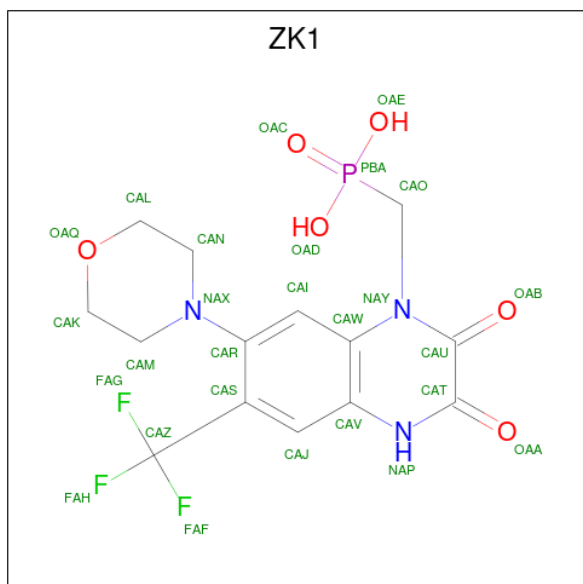
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
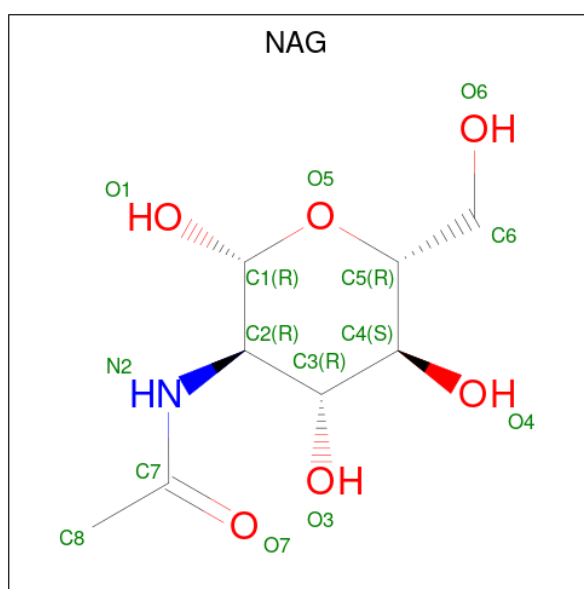
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots ⓘ

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 atom inclusion in map density. Residues are color-coded according to the number of geometric qualit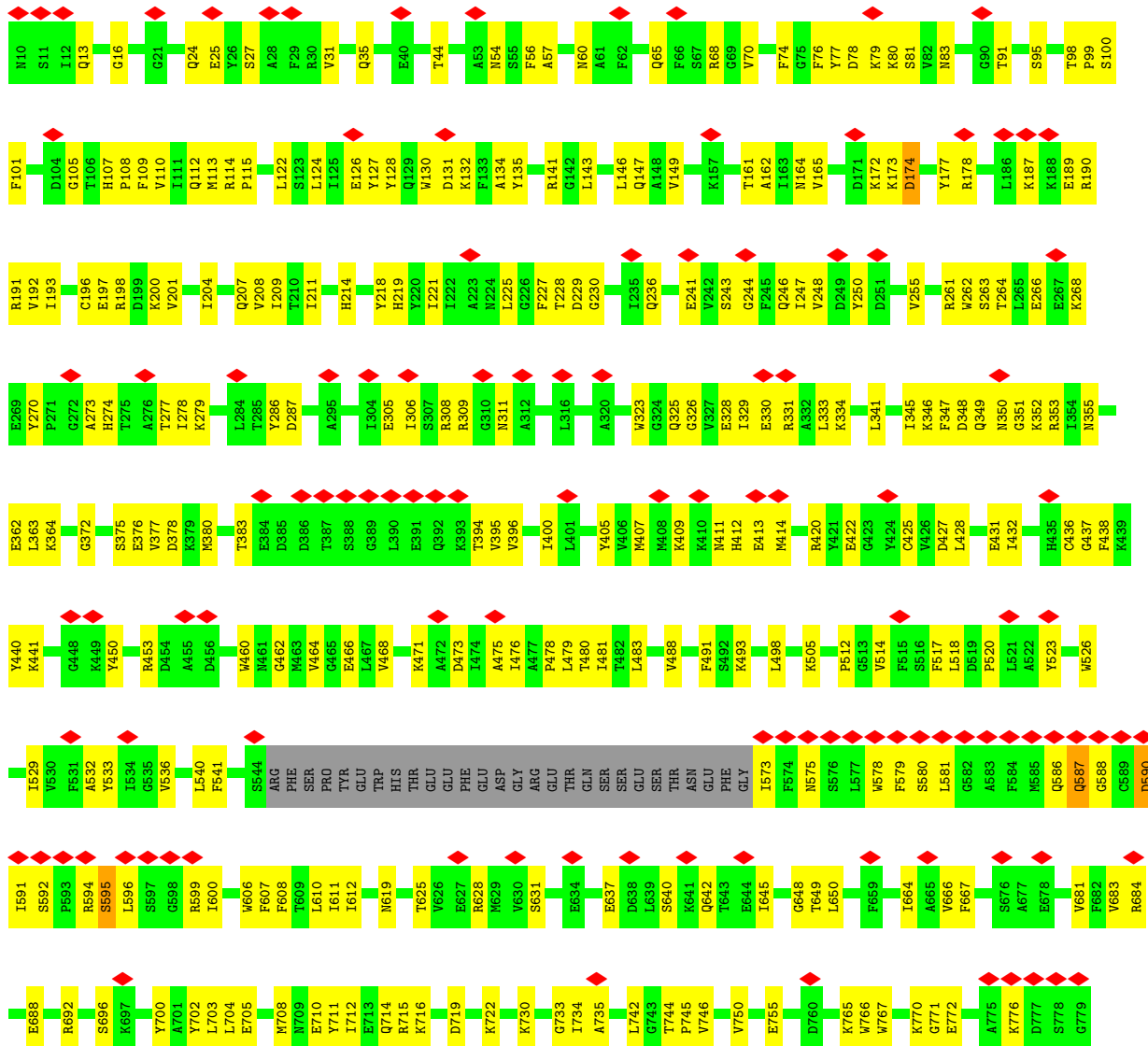y criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
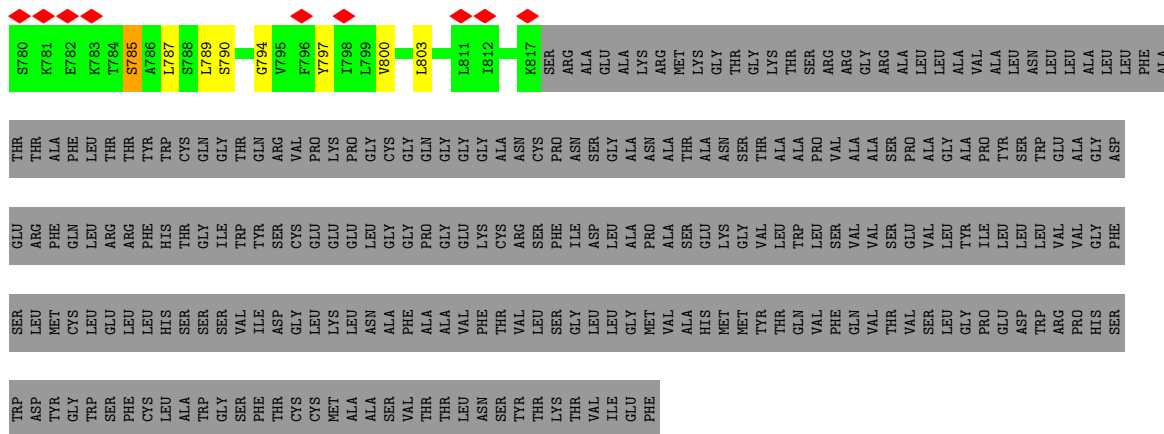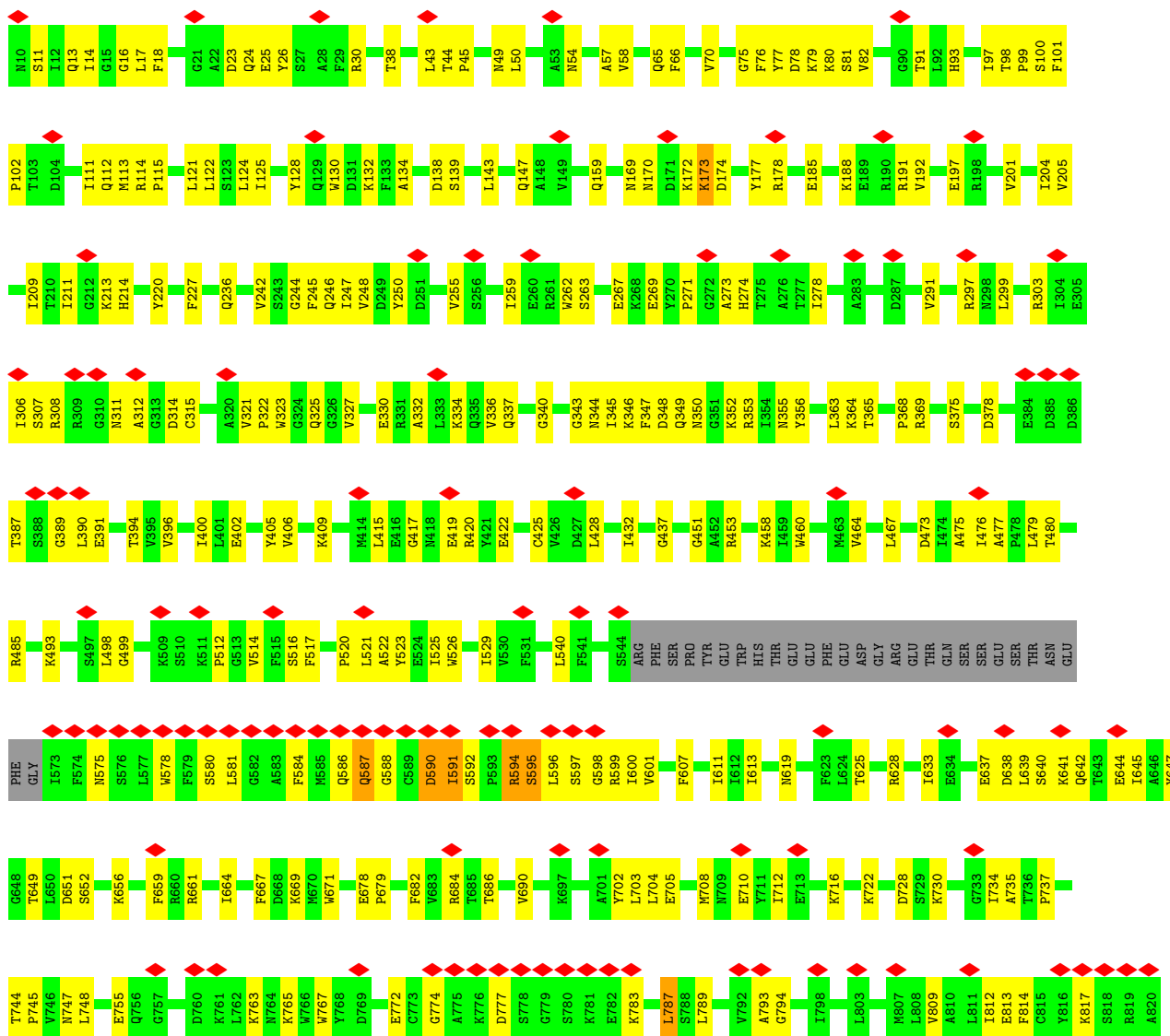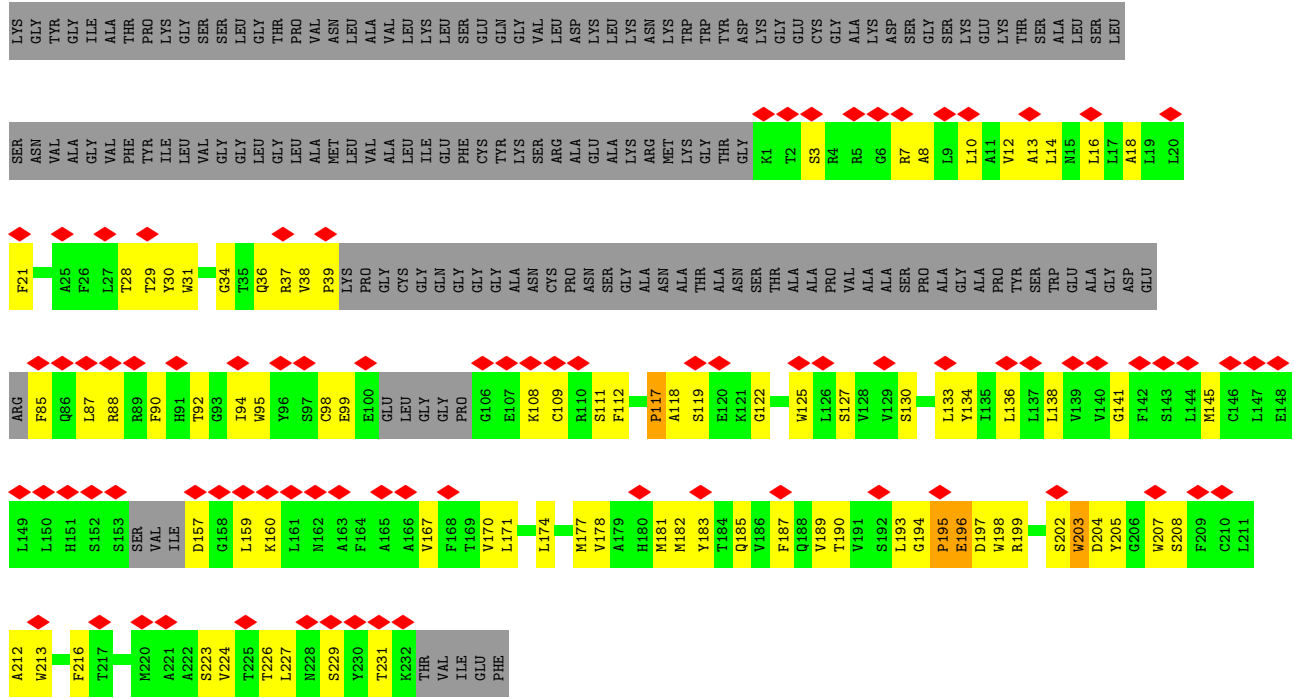
• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain B:

12%

47% 26% 26%

• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain C:

• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain D:

V792 A793 G794 V795 F796 Y797 I798 L799 V800 L803 M807 L811 I812 K817 SER ARG ALA GLU ALA LYS ARG MET LYS THR GLY LYS THR SER ARG ARG GLY ARG ALA LEU LEU ALA VAL LEU ASN LEU LEU ALA LEU PHE ALA THR ALA PHE LEU ARG ARG THR THR TYR

TRP CYS GLN GLY ILE TRP GLN ARG VAL PRO LYS PRO GLY CYS GLY GLN GLY GLY GLY ALA ASN CYS PRO ASN SER GLY ALA ASN ALA THR ALA ASN SER THR ALA ALA PRO VAL ALA SER PRO ALA GLY ALA PRO TYR SER TRP GLU ALA GLY ASP GLU ARG PHE GLN LEU ARG ARG PHE

HIS THR GLY ILE TRP TYR SER CYS GLU GLU LEU GLY PRO GLY GLU LYS CYS ARG SER PHE ILE ASP LEU ALA PRO ALA SER GLU LYS GLY VAL LEU TRP LEU SER VAL SER GLU VAL LEU TYR ILE LEU LEU VAL VAL GLY PHE SER LEU MET CYS LEU GLU LEU

HIS SER SER VAL ILE GLY LEU LEU ASN ALA PHE ALA ALA VAL PHE THR VAL LEU SER LEU LEU GLY MET VAL ALA HIS MET MET TYR THR GLN VAL GLN VAL THR VAL SER LEU PRO GLU ASP TRP ARG PRO HIS SER TRP ASP TYR GLY TRP SER PHE CYS

LEU ALA TRP GLY PHE THR CYS MET ALA ALA SER VAL THR LEU ASN SER TYR THR LYS THR VAL ILE GLU PHE

• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

8%

Chain E: 8% 9% 83%

ASN SER ILE ILE GLN ILE GLY GLY LEU PHE PRO ARG GLY ALA ASP GLN GLU TYR SER ALA PHE ARG VAL GLY MET VAL GLN PHE SER THR SER GLU PHE ARG LEU THR PRO HIS ILE ASP ASN LEU GLU VAL ALA ASN SER PHE ALA VAL THR ASN ALA PHE CYS SER GLN PHE SER ARG GLY

VAL TYR ALA ILE PHE GLY PHE TYR ASP LYS LYS SER VAL ASN THR ILE THR SER PHE CYS GLY THR LEU HIS VAL SER PHE ILE THR PRO SER PHE PRO THR ASP GLY THR HIS PRO PHE VAL ILE GLN MET ARG PRO ASP LEU LYS GLY ALA LEU LEU SER LEU ILE GLU TYR TYR GLN

TRP ASP LYS PHE ALA TYR LEU TYR ASP SER ASP ARG GLY LEU SER THR LEU GLN ALA VAL LEU ASP SER ALA ALA GLU LYS LYS TRP GLN VAL THR ALA ILE ASN VAL GLY ASN ILE ASN ASN ASP LYS LYS ASP GLU THR TYR ARG SER LEU PHE GLN ASP LEU GLU LEU LYS LYS GLU

ARG ARG VAL ILE LEU ASP CYS GLU ARG ASP LYS VAL ASN ASP ILE VAL ASP GLN VAL ILE THR ILE GLY LYS HIS VAL LYS GLY TYR HIS TYR ILE ILE ALA ASN LEU GLY PHE THR ASP GLY ASP LEU LEU LYS ILE GLN PHE GLY GLY ALA GLU VAL SER GLY PHE GLN ILE VAL ASP

TYR ASP ASP SER LEU VAL SER LYS PHE ILE GLU ARG TRP SER THR LEU GLU GLU LYS GLU TYR PRO GLY ALA HIS THR ALA THR ILE LYS TYR THR SER ALA LEU THR TYR ASP ALA VAL MET THR ILE ALA PHE ARG ALA ASN LEU ALA ARG LYS GLN ARG ILE ILE SER ARG ARG

GLY ASN ALA GLY ASP CYS LEU ALA ASN PRO ALA VAL PRO TRP GLY GLN GLY VAL GLU ILE GLU ARG ALA LEU LYS GLN VAL GLN VAL GLU GLY LEU SER GLY ASN ILE LYS PHE ASP GLN ASN GLY LYS ARG ILE ASN TYR THR ILE ASN ILE MET GLU LEU LYS THR ASN GLY PRO ARG

LYS ILE GLY TYR TRP SER GLU VAL ASP LYS MET VAL VAL THR LEU THR GLU LEU PRO SER GLY ASN ASP THR SER GLY LEU GLU ASN LYS THR VAL VAL VAL THR THR ILE LEU GLU SER PRO TYR VAL MET MET LYS LYS ASN HIS GLU MET LEU GLU GLY ASN GLU ARG TYR GLU GLY TYR CYS VAL ASP LEU ALA

ALA GLU ILE ALA LYS HIS CYS GLY PHE LYS TYR LYS LEU THR ILE VAL GLY ASP GLY LYS TYR GLY ALA ARG ASP ALA ASP THR LYS ILE TRP ASN GLY MET VAL GLY GLU LEU VAL TYR GLY LYS ALA ASP ILE ALA ILE ALA PRO LEU THR ILE THR LEU VAL ARG GLU GLU VAL ILE

ASP PHE SER LYS PRO PHE MET SER LEU GLY ILE SER ILE MET ILE LYS LYS PRO GLN LYS SER LYS PRO GLY VAL PHE SER PHE LEU ASP PRO LEU ALA TYR GLU ILE TRP MET CYS ILE VAL PHE ALA TYR ILE GLY VAL SER VAL VAL LEU PHE LEU VAL SER ARG PHE SER PRO TYR

GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR ASN GLU PHE GLY ILE PHE ASN SER LEU TRP PHE SER LEU GLY ALA PHE MET GLN GLN GLY CYS ASP ILE SER PRO ARG SER LEU SER GLY ARG ILE VAL GLY GLY VAL TRP TRP PHE PHE THR

LEU ILE ILE ILE SER SER TYR THR ALA ASN LEU ALA ALA PHE LEU THR VAL GLU ARG MET VAL SER PRO ILE GLU SER ALA GLU ASP LEU SER LYS GLN THR GLU ILE ALA TYR GLY THR LEU ASP SER GLY SER THR LYS GLU PHE PHE ARG ARG SER LYS ILE ALA VAL PHE ASP LYS

MET TRP THR TYR MET ARG SER ALA GLU PRO SER VAL PHE VAL ARG THR THR ALA GLU GLY VAL ALA ARG VAL ARG LYS SER LYS GLY LYS TYR ALA TYR LEU LEU GLU SER THR MET ASN GLU TYR ILE GLU GLN ARG LYS PRO CYS ASP THR MET LYS VAL GLY GLY ASN LEU ASP SER

LYS GLY TYR GLY ILE ALA THR PRO LYS GLY SER SER LEU GLY THR PRO VAL ASN LEU ALA VAL LEU LYS LEU SER GLU GLN GLY VAL LEU ASP LYS LEU LYS ASN LYS TRP TRP TYR ASP LYS GLY GLU CYS GLY ALA LYS ASP SER GLY SER LYS GLU LYS THR SER ALA LEU SER LEU

SER ASN VAL ALA GLY VAL PHE TYR ILE LEU LEU VAL GLY GLY LEU GLY LEU ALA MET LEU VAL ALA LEU ILE GLU PHE CYS TYR LYS SER ARG GLU ALA GLU ALA LYS ARG MET LYS GLY THR GLY K1 T2 S3 R4 R5 G6 R7 A8 L9 L10 A11 V12 A13 L14 N15 L16 L17 A18 L19 L20

F21 T24 A25 F26 L27 T28 T29 Y30 W31 C32 Q33 G34 T35 Q36 R37 V38 P39 LYS PRO GLY CYS GLY GLN GLY GLY ALA ASN CYS PRO ASN SER GLY ALA ASN ALA THR ALA ASN SER THR ALA ALA PRO VAL ALA ALA SER PRO ALA GLY ALA PRO TYR SER TRP GLU ALA GLY

ASP GLU ARG F85 Q86 L87 R88 R89 F90 H91 T92 G93 I94 W95 Y96 S97 C98 E99 E100 GLU LEU GLY GLY PRO G106 E107 K108 C109 R110 S111 A116 P117 A118 S119 E120 K121 G122 W125 L126 S127 V128 V129 S130 L133 Y134 I135 L136 L137 L138 V139 V140 G141 F142 S143 L144 M145 C146

L147 E148 L149 L150 H151 S152 S153 SER VAL ILE D157 G158 L159 K160 L161 N162 A163 A166 V167 F168 T169 V170 L171 L174 M177 V178 A179 H180 M181 M182 Y183 T184 Q185 V186 F187 Q188 V189 T190 V191 S192 L193 G194 P195 E196 D197 W198 R199 S202 W203 D204 Y205 G206 W207 S208 F209 C210

L211 A212 W213 G214 S215 F216 T217 C218 C219 M220 A221 A222 S223 V224 T225 T226 L227 N228 S229 Y230 T231 K232 THR VAL ILE GLU PHE

- Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

8%

Chain F: 9%   7%   83%

ASN SER ILE GLN ILE GLY GLY LEU PHE PRO ARG GLY ALA ASP GLN GLU TYR SER ALA PHE ARG VAL GLY MET VAL GLN PHE SER THR SER GLU PHE ARG LEU THR PRO HIS ILE ASP ASN LEU GLU VAL ALA ASN SER PHE ALA VAL THR ASN ALA PHE CYS SER GLN PHE SER ARG GLY

VAL TYR ALA ILE PHE GLY PHE TYR ASP LYS LYS SER VAL ASN THR ILE THR SER PHE CYS GLY THR LEU HIS VAL SER PHE ILE THR PRO SER PHE PRO THR ASP GLY THR HIS PRO PHE VAL ILE GLN MET ARG PRO ASP LEU LYS GLY ALA LEU LEU SER LEU ILE GLU TYR TYR GLN

TRP ASP LYS PHE ALA TYR LEU TYR ASP SER ASP ARG GLY LEU SER THR LEU GLN ALA VAL LEU ASP SER ALA ALA GLU LYS LYS TRP GLN VAL THR ALA ILE ASN VAL GLY ASN ILE ASN ASN ASP LYS LYS ASP GLU THR TYR ARG SER LEU PHE GLN ASP LEU GLU LEU LYS LYS GLU

ARG ARG VAL ILE LEU ASP CYS GLU ARG ASP LYS VAL ASN ASP ILE VAL ASP GLN VAL ILE THR ILE GLY LYS HIS VAL LYS GLY TYR HIS TYR ILE ILE ALA ASN LEU GLY PHE THR ASP GLY ASP LEU LEU LYS ILE GLN PHE GLY GLY ALA GLU VAL SER GLY PHE GLN ILE VAL ASP

TYR ASP ASP SER LEU VAL SER LYS PHE ILE GLU ARG TRP SER THR LEU GLU GLU LYS GLU TYR PRO GLY ALA HIS THR ALA THR ILE LYS TYR THR SER ALA LEU THR TYR ASP ALA VAL GLN VAL MET THR GLU ALA PHE ARG ASN LEU ARG LYS GLN ARG ILE GLU ILE SER ARG ARG

GLY ASN ALA GLY ASP CYS LEU ALA ASN PRO ALA VAL PRO TRP GLY GLN GLY VAL GLU ILE GLU ARG ALA LEU LYS GLN VAL GLN VAL GLU GLY LEU SER GLY ASN ILE LYS PHE ASP GLN ASN GLY LYS ARG ILE ASN TYR THR ILE ASN ILE MET GLU LEU LYS THR ASN GLY PRO ARG

LYS ILE GLY TYR TRP SER GLU VAL ASP LYS MET VAL LEU THR GLU ASP ASP THR SER GLY LEU GLU GLN LYS THR VAL VAL VAL THR THR ILE LEU GLU SER PRO TYR VAL MET MET LYS LYS ASN HIS GLU MET LEU GLU GLY ASN GLU ARG TYR GLU GLY TYR CYS VAL ASP LEU ALA

ALA GLU ILE ALA LYS HIS CYS GLY PHE LYS TYR LYS LEU THR ILE VAL GLY ASP GLY LYS TYR GLY ALA ARG ASP ALA ASP THR LYS ILE TRP ASN GLY MET VAL GLY GLU LEU VAL TYR GLY LYS ALA ASP ILE ALA ILE ALA PRO LEU THR ILE THR LEU VAL ARG GLU GLU VAL ILE

ASP PHE SER LYS PRO PHE MET SER LEU GLY ILE SER ILE MET ILE LYS LYS PRO GLN LYS SER LYS PRO GLY VAL PHE SER PHE LEU ASP PRO LEU ALA TYR GLU ILE TRP MET CYS ILE VAL PHE ALA TYR ILE GLY VAL SER VAL VAL LEU PHE LEU VAL SER ARG PHE SER PRO TYR

GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR ASN GLU PHE GLY ILE PHE ASN SER LEU TRP PHE SER LEU GLY ALA PHE MET GLN GLN GLY CYS ASP ILE SER PRO ARG SER LEU SER GLY ARG ILE VAL GLY GLY VAL TRP TRP PHE PHE THR

LEU ILE ILE ILE SER SER TYR THR ALA ASN LEU ALA ALA PHE LEU THR VAL GLU ARG MET VAL SER PRO ILE GLU SER ALA GLU ASP LEU SER LYS GLN THR GLU ILE ALA TYR GLY THR LEU ASP SER GLY SER THR LYS GLU PHE PHE ARG ARG SER LYS ILE ALA VAL PHE ASP LYS

MET TRP THR TYR MET ARG SER ALA GLU PRO SER VAL PHE ARG THR ALA GLU GLY VAL ALA GLU THR ALA GLU GLY VAL ALA ALA GLU PHE LEU ARG THR ALA GLU GLY VAL VAL SER SER THR MET ALA GLU ASN TYR THR ALA TYR LEU GLU GLY LYS LYS SER ASP CYS ASP THR MET LYS VAL ASP GLY VAL ASN LEU ASP SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42637	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, NAG

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	0.32	0/6287	0.46	0/8493
1	B	0.32	0/6265	0.44	0/8464
1	C	0.32	0/6287	0.45	0/8493
1	D	0.32	0/6265	0.44	0/8464
1	E	0.29	0/1443	0.48	0/1959
1	F	0.29	0/1443	0.48	0/1959
All	All	0.32	0/27990	0.45	0/37832

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 ⓘ

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	6159	0	6155	250	0
1	B	6137	0	6132	224	0
1	C	6159	0	6155	203	0
1	D	6137	0	6132	217	0
1	E	1408	0	1406	168	0
1	F	1408	0	1406	53	0
2	A	27	0	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	13	5	0
2	C	27	0	13	2	0
2	D	27	0	13	4	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	3	0
All	All	27572	0	27490	1011	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 18.

All (1011) 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:541:PHE:CD2	1:E:227:LEU:HB3	1.41	1.55
1:A:541:PHE:CE2	1:E:227:LEU:CB	1.87	1.51
1:E:18:ALA:HB2	1:E:218:CYS:CB	1.42	1.47
1:A:541:PHE:CE2	1:E:227:LEU:HB3	0.94	1.46
1:E:187:PHE:HE2	1:E:203:TRP:NE1	1.24	1.31
1:A:541:PHE:HE2	1:E:227:LEU:CB	1.34	1.29
1:E:223:SER:O	1:E:227:LEU:HD23	1.33	1.25
1:E:31:TRP:HZ2	1:E:209:PHE:CD1	1.58	1.20
1:E:18:ALA:CB	1:E:218:CYS:HB2	1.75	1.16
1:A:542:LEU:CD2	1:E:227:LEU:HD11	1.81	1.10
1:A:541:PHE:HE2	1:E:227:LEU:CA	1.65	1.09
1:E:31:TRP:CZ2	1:E:209:PHE:HB2	1.88	1.07
1:E:31:TRP:CZ2	1:E:209:PHE:CD1	2.42	1.07
1:A:541:PHE:CD2	1:E:227:LEU:CB	2.21	1.06
1:E:24:THR:HG21	1:E:211:LEU:CD1	1.85	1.05
1:A:542:LEU:HD23	1:E:227:LEU:CD1	1.85	1.04
1:A:542:LEU:HD23	1:E:227:LEU:HD11	1.09	1.04
1:A:541:PHE:CZ	1:E:231:THR:HG23	1.93	1.02
1:E:15:ASN:HD21	1:E:222:ALA:HB1	1.17	1.02
1:E:18:ALA:HB2	1:E:218:CYS:HB2	1.02	1.01
1:E:31:TRP:CZ2	1:E:209:PHE:HD1	1.79	1.01
1:E:32:CYS:SG	1:E:204:ASP:O	2.19	1.01
1:A:541:PHE:CZ	1:E:231:THR:CG2	2.44	1.00
1:E:187:PHE:CE2	1:E:203:TRP:NE1	2.10	0.99
1:A:541:PHE:CE1	1:E:231:THR:HG21	1.97	0.99
1:E:18:ALA:CB	1:E:218:CYS:CB	2.38	0.98

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:TRP:O	1:E:206:GLY:O	1.83	0.97
1:E:18:ALA:HB2	1:E:218:CYS:HB3	1.44	0.96
1:E:223:SER:O	1:E:227:LEU:CD2	2.12	0.96
1:E:7:ARG:HH22	1:E:228:ASN:ND2	1.65	0.94
1:E:7:ARG:HH22	1:E:228:ASN:HD22	0.96	0.94
1:F:31:TRP:HE1	1:F:208:SER:HG	1.15	0.93
1:E:15:ASN:HD21	1:E:222:ALA:CB	1.81	0.93
1:E:24:THR:HG21	1:E:211:LEU:HD13	1.51	0.91
1:E:7:ARG:NH2	1:E:228:ASN:HD22	1.67	0.91
1:E:180:HIS:HB3	1:E:209:PHE:CE1	2.06	0.90
1:E:24:THR:HG21	1:E:211:LEU:HD12	1.53	0.90
1:D:595:SER:HA	1:D:599:ARG:HB3	1.53	0.89
1:A:541:PHE:HD2	1:E:227:LEU:HG	1.37	0.89
1:A:541:PHE:CE2	1:E:227:LEU:C	2.46	0.87
1:A:541:PHE:HD2	1:E:227:LEU:CG	1.89	0.86
1:E:15:ASN:OD1	1:E:222:ALA:HB2	1.76	0.85
1:E:180:HIS:CE1	1:E:212:ALA:HB1	2.13	0.83
1:A:541:PHE:CD2	1:E:227:LEU:CG	2.61	0.83
1:A:531:PHE:HE2	1:E:213:TRP:CE3	1.97	0.82
1:E:21:PHE:CD1	1:E:211:LEU:HD22	2.14	0.81
1:E:31:TRP:CZ2	1:E:209:PHE:CB	2.64	0.80
1:E:21:PHE:HB2	1:E:215:SER:HB3	1.64	0.79
1:C:337:GLN:HE21	1:C:346:LYS:HE2	1.47	0.79
1:A:188:LYS:HD2	1:A:190:ARG:HH22	1.46	0.79
1:C:595:SER:H	1:C:599:ARG:HE	1.28	0.79
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.66	0.78
1:A:16:GLY:H	1:A:65:GLN:HE22	1.30	0.78
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.65	0.78
1:D:134:ALA:HB3	1:D:192:VAL:HG22	1.66	0.77
1:E:21:PHE:CE1	1:E:211:LEU:HD22	2.19	0.77
1:A:541:PHE:CE1	1:E:231:THR:CG2	2.66	0.77
1:A:77:TYR:HE2	1:A:98:THR:HG21	1.49	0.77
1:B:595:SER:HA	1:B:599:ARG:HB2	1.65	0.77
1:B:247:ILE:HG23	1:B:248:VAL:HG23	1.67	0.77
1:E:21:PHE:HB3	1:E:211:LEU:O	1.85	0.76
1:E:15:ASN:ND2	1:E:222:ALA:CB	2.48	0.76
1:E:31:TRP:HZ2	1:E:209:PHE:HD1	1.11	0.76
1:C:16:GLY:H	1:C:65:GLN:HE22	1.33	0.76
1:A:541:PHE:HZ	1:E:231:THR:HG23	1.49	0.75
1:D:355:ASN:N	1:D:376:GLU:OE2	2.19	0.75
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.51	0.75
1:B:77:TYR:OH	1:B:101:PHE:O	2.06	0.74
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.53	0.74
1:E:15:ASN:ND2	1:E:222:ALA:HB1	1.98	0.74
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.52	0.74
1:A:541:PHE:CZ	1:E:231:THR:HG21	2.18	0.73
1:E:18:ALA:O	1:E:215:SER:HB3	1.89	0.73
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.69	0.73
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.68	0.73
1:A:451:GLY:O	1:A:485:ARG:NH2	2.22	0.73
1:E:180:HIS:CE1	1:E:212:ALA:CB	2.72	0.73
1:A:599:ARG:HH22	1:B:581:LEU:HB3	1.53	0.73
1:E:214:GLY:O	1:E:218:CYS:SG	2.45	0.72
1:A:594:ARG:HD3	1:B:575:ASN:HB2	1.71	0.72
1:D:247:ILE:HG23	1:D:248:VAL:HG23	1.71	0.72
1:A:531:PHE:CE2	1:E:213:TRP:CE3	2.78	0.72
1:D:308:ARG:NH2	1:D:325:GLN:OE1	2.22	0.72
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.71	0.72
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.69	0.72
1:E:180:HIS:NE2	1:E:212:ALA:HB1	2.05	0.72
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.72	0.72
1:E:221:ALA:HA	1:E:224:VAL:HG22	1.69	0.72
1:E:18:ALA:O	1:E:215:SER:CB	2.38	0.72
1:E:187:PHE:HE2	1:E:203:TRP:CD1	2.07	0.71
1:A:661:ARG:NH1	1:D:755:GLU:O	2.23	0.71
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.73	0.71
1:D:77:TYR:OH	1:D:101:PHE:O	2.08	0.71
1:A:541:PHE:CZ	1:E:227:LEU:O	2.44	0.71
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.71	0.71
1:A:541:PHE:HE2	1:E:227:LEU:C	1.86	0.70
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.73	0.70
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.56	0.70
1:B:246:GLN:HE21	1:B:248:VAL:H	1.37	0.70
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.55	0.70
1:F:98:CYS:HA	1:F:109:CYS:HA	1.74	0.70
1:A:595:SER:H	1:A:599:ARG:HE	1.39	0.70
1:A:586:GLN:HA	1:D:587:GLN:HE21	1.57	0.69
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.74	0.69
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.72	0.69
1:B:376:GLU:HG2	1:B:377:VAL:HG13	1.73	0.69
1:E:98:CYS:HA	1:E:109:CYS:HA	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.75	0.69
1:B:13:GLN:HA	1:B:44:THR:HB	1.74	0.69
1:E:180:HIS:HB3	1:E:209:PHE:HE1	1.53	0.69
1:A:355:ASN:ND2	3:A:1102:NAG:O6	2.26	0.69
1:A:541:PHE:CZ	1:E:227:LEU:C	2.66	0.69
1:D:590:ASP:O	1:D:592:SER:N	2.24	0.69
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.75	0.69
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.58	0.69
1:B:263:SER:O	1:B:274:HIS:ND1	2.25	0.68
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.27	0.68
1:C:344:ASN:HD21	1:C:346:LYS:HE3	1.57	0.68
1:D:309:ARG:HG2	1:D:311:ASN:H	1.58	0.68
1:A:637:GLU:OE1	1:D:776:LYS:NZ	2.25	0.68
1:B:16:GLY:H	1:B:65:GLN:HE22	1.41	0.68
1:C:451:GLY:O	1:C:485:ARG:NH2	2.21	0.68
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.75	0.68
1:D:24:GLN:HE21	1:D:278:ILE:HG13	1.58	0.68
1:B:710:GLU:OE2	1:B:722:LYS:NZ	2.24	0.68
1:C:307:SER:O	1:C:308:ARG:NH1	2.25	0.67
1:D:372:GLY:HA2	1:D:383:THR:HG23	1.75	0.67
1:D:246:GLN:HE21	1:D:248:VAL:H	1.40	0.67
1:C:246:GLN:HE21	1:C:248:VAL:H	1.42	0.67
1:C:476:ILE:HG12	1:C:734:ILE:HD12	1.77	0.66
1:B:790:SER:OG	1:E:185:GLN:NE2	2.25	0.66
1:A:541:PHE:HE1	1:E:231:THR:HG21	1.58	0.66
1:D:13:GLN:HA	1:D:44:THR:HB	1.76	0.66
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.26	0.66
1:D:592:SER:O	1:D:599:ARG:NH2	2.28	0.66
1:E:180:HIS:HB3	1:E:209:PHE:CZ	2.29	0.66
1:B:346:LYS:HD3	1:B:355:ASN:HD22	1.60	0.66
1:E:209:PHE:HE2	1:E:213:TRP:CZ2	2.12	0.66
1:D:710:GLU:OE2	1:D:722:LYS:NZ	2.24	0.66
1:E:31:TRP:CZ2	1:E:209:PHE:CG	2.83	0.66
1:B:520:PRO:O	1:B:619:ASN:ND2	2.29	0.66
1:D:592:SER:HB3	1:D:599:ARG:HB2	1.78	0.66
1:A:512:PRO:HB2	1:A:516:SER:HB3	1.77	0.66
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.61	0.66
1:B:628:ARG:HG2	1:C:628:ARG:HH12	1.61	0.65
1:A:206:ASP:HA	1:A:209:ILE:HD12	1.77	0.65
1:A:246:GLN:HE21	1:A:248:VAL:H	1.44	0.65
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HG2	1:B:311:ASN:H	1.60	0.65
1:A:247:ILE:HG23	1:A:248:VAL:HG23	1.79	0.65
1:D:161:THR:OG1	1:D:187:LYS:NZ	2.28	0.65
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.62	0.65
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.32	0.65
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.61	0.65
1:D:51:GLU:HG3	1:D:53:ALA:H	1.61	0.65
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.62	0.65
1:B:305:GLU:O	1:B:325:GLN:NE2	2.29	0.64
1:D:348:ASP:OD1	1:D:352:LYS:N	2.30	0.64
1:C:11:SER:OG	1:C:44:THR:OG1	2.15	0.64
1:D:78:ASP:OD1	1:D:79:LYS:N	2.30	0.64
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.27	0.64
1:B:579:PHE:HZ	1:B:590:ASP:H	1.45	0.64
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.80	0.64
1:C:13:GLN:HA	1:C:44:THR:HB	1.79	0.64
1:D:16:GLY:H	1:D:65:GLN:HE22	1.45	0.64
1:A:236:GLN:NE2	1:A:365:THR:O	2.29	0.64
1:A:531:PHE:HE2	1:E:213:TRP:CD2	2.15	0.64
1:D:480:THR:O	1:D:485:ARG:NH1	2.31	0.64
1:A:541:PHE:HZ	1:E:227:LEU:O	1.81	0.63
1:B:78:ASP:OD1	1:B:79:LYS:N	2.31	0.63
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.81	0.63
1:A:11:SER:OG	1:A:44:THR:OG1	2.16	0.63
1:C:78:ASP:OD1	1:C:79:LYS:N	2.32	0.63
1:E:18:ALA:HB2	1:E:218:CYS:SG	2.38	0.63
1:A:520:PRO:O	1:A:619:ASN:ND2	2.32	0.63
1:B:348:ASP:OD1	1:B:352:LYS:N	2.31	0.63
1:D:692:ARG:O	1:D:696:SER:OG	2.12	0.63
1:E:18:ALA:CB	1:E:215:SER:HA	2.29	0.63
1:E:24:THR:CG2	1:E:211:LEU:HD12	2.27	0.63
1:D:263:SER:O	1:D:274:HIS:ND1	2.31	0.63
1:A:628:ARG:NH1	1:D:622:ALA:O	2.32	0.63
1:C:595:SER:N	1:C:599:ARG:HE	1.96	0.63
1:F:31:TRP:N	1:F:92:THR:O	2.32	0.62
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.64	0.62
1:A:541:PHE:CE2	1:E:227:LEU:CA	2.53	0.62
1:A:13:GLN:HA	1:A:44:THR:HB	1.81	0.62
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.34	0.62
1:E:221:ALA:O	1:E:224:VAL:HG22	1.99	0.62
1:C:716:LYS:N	1:C:772:GLU:OE1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ASP:O	1:C:592:SER:N	2.30	0.62
1:E:37:ARG:HD2	1:E:87:LEU:HD22	1.82	0.62
1:A:541:PHE:HZ	1:E:231:THR:CG2	2.08	0.62
1:C:337:GLN:HG3	1:C:346:LYS:HG2	1.81	0.62
1:D:513:GLY:O	1:D:515:PHE:N	2.32	0.62
1:B:334:LYS:NZ	1:B:349:GLN:O	2.26	0.61
1:E:31:TRP:N	1:E:92:THR:O	2.32	0.61
1:C:259:ILE:HA	1:C:262:TRP:HB3	1.82	0.61
1:A:476:ILE:HG12	1:A:734:ILE:HD12	1.81	0.61
1:F:37:ARG:HD2	1:F:87:LEU:HD22	1.81	0.61
1:C:334:LYS:HD3	1:C:349:GLN:HA	1.82	0.61
1:A:623:PHE:HE1	1:B:785:SER:HB2	1.66	0.61
1:B:164:ASN:OD1	1:B:165:VAL:N	2.34	0.61
1:A:594:ARG:HB3	1:B:578:TRP:HE3	1.66	0.61
1:A:78:ASP:OD1	1:A:79:LYS:N	2.33	0.61
1:E:18:ALA:HA	1:E:215:SER:HA	1.83	0.61
1:B:161:THR:OG1	1:B:187:LYS:NZ	2.33	0.60
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.36	0.60
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.65	0.60
1:C:262:TRP:CZ2	1:C:273:ALA:HA	2.37	0.60
1:B:776:LYS:NZ	1:C:637:GLU:OE1	2.27	0.60
1:C:38:THR:HG21	1:C:297:ARG:HH21	1.67	0.60
1:E:221:ALA:HA	1:E:224:VAL:CG2	2.31	0.60
1:A:623:PHE:CE1	1:B:785:SER:HB2	2.36	0.60
1:A:514:VAL:HA	1:A:794:GLY:HA3	1.83	0.60
1:B:483:LEU:N	1:C:755:GLU:OE2	2.28	0.60
1:E:31:TRP:CE2	1:E:209:PHE:HB2	2.34	0.60
1:A:30:ARG:NH1	1:A:269:GLU:O	2.35	0.60
1:D:583:ALA:HA	1:D:589:CYS:H	1.67	0.60
1:A:308:ARG:HB3	1:A:311:ASN:HD22	1.67	0.60
1:B:755:GLU:O	1:C:661:ARG:NH1	2.35	0.60
1:E:209:PHE:CE2	1:E:213:TRP:CZ2	2.90	0.60
1:D:579:PHE:HZ	1:D:590:ASP:H	1.50	0.59
1:D:411:ASN:HB2	1:D:414:MET:HB2	1.84	0.59
1:D:597:SER:O	1:D:600:ILE:HG12	2.02	0.59
1:B:436:CYS:HB2	1:B:438:PHE:HE2	1.67	0.59
1:E:15:ASN:OD1	1:E:222:ALA:CB	2.48	0.59
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.67	0.59
1:C:308:ARG:HB3	1:C:311:ASN:HD22	1.68	0.59
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.85	0.59
1:B:493:LYS:HD3	1:C:493:LYS:HD3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ALA:CA	1:E:224:VAL:HG22	2.32	0.59
1:A:78:ASP:N	1:A:81:SER:OG	2.34	0.59
1:B:705:GLU:OE1	2:B:1101:ZK1:FAF	2.11	0.59
1:A:595:SER:N	1:A:599:ARG:HE	2.01	0.59
1:A:787:LEU:HD12	1:D:521:LEU:HA	1.85	0.59
1:E:177:MET:HE3	1:E:213:TRP:CD1	2.38	0.59
1:A:355:ASN:N	1:A:376:GLU:OE2	2.22	0.59
1:E:15:ASN:CG	1:E:222:ALA:HB2	2.23	0.59
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.67	0.58
1:D:594:ARG:O	1:D:596:LEU:N	2.36	0.58
1:B:625:THR:HG21	1:C:625:THR:HG23	1.84	0.58
1:D:586:GLN:O	1:D:588:GLY:N	2.36	0.58
1:A:25:GLU:N	1:A:25:GLU:OE1	2.36	0.58
1:F:18:ALA:HA	1:F:21:PHE:HD2	1.67	0.58
1:C:236:GLN:NE2	1:C:365:THR:O	2.35	0.58
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.85	0.58
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.84	0.58
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.86	0.58
1:E:36:GLN:NE2	1:E:197:ASP:O	2.35	0.58
1:B:25:GLU:HG2	1:B:76:PHE:HZ	1.68	0.57
1:B:587:GLN:HE21	1:C:586:GLN:HA	1.69	0.57
1:E:18:ALA:HA	1:E:21:PHE:HD2	1.69	0.57
1:B:35:GLN:OE1	1:B:261:ARG:NH2	2.36	0.57
1:B:716:LYS:HG3	1:B:772:GLU:HB3	1.87	0.57
1:A:77:TYR:OH	1:A:101:PHE:O	2.13	0.57
1:A:493:LYS:HD3	1:D:493:LYS:HD3	1.85	0.57
1:E:18:ALA:HB1	1:E:215:SER:HA	1.86	0.57
1:E:31:TRP:CH2	1:E:209:PHE:HB2	2.38	0.57
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.35	0.57
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.69	0.57
1:B:308:ARG:HH21	1:B:325:GLN:H	1.52	0.57
1:C:520:PRO:O	1:C:619:ASN:ND2	2.38	0.57
1:D:684:ARG:N	1:D:688:GLU:OE1	2.38	0.57
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.87	0.57
1:B:250:TYR:HA	1:B:255:VAL:HG11	1.87	0.57
1:F:195:PRO:HD2	1:F:199:ARG:HB3	1.87	0.57
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.86	0.57
1:C:347:PHE:HE1	1:C:353:ARG:HG2	1.70	0.56
1:E:37:ARG:HA	1:E:87:LEU:HA	1.85	0.56
1:D:25:GLU:HG2	1:D:76:PHE:HZ	1.69	0.56
1:C:594:ARG:HB3	1:D:578:TRP:HE3	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:VAL:HG23	1:E:225:THR:N	2.21	0.56
1:C:594:ARG:HD3	1:D:575:ASN:HB2	1.87	0.56
1:D:705:GLU:OE1	2:D:1101:ZK1:FAF	2.13	0.56
1:E:177:MET:CE	1:E:213:TRP:CD1	2.88	0.56
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.88	0.56
1:A:334:LYS:HD3	1:A:349:GLN:HA	1.86	0.56
1:B:328:GLU:OE2	1:B:331:ARG:NH1	2.34	0.56
1:B:600:ILE:HG22	1:C:581:LEU:HD11	1.87	0.56
1:B:631:SER:O	1:C:783:LYS:NZ	2.38	0.56
1:A:640:SER:HB2	1:A:669:LYS:HD2	1.87	0.56
1:C:345:ILE:HG12	1:C:353:ARG:NH2	2.21	0.56
1:A:578:TRP:CG	1:D:595:SER:HB3	2.41	0.56
1:C:586:GLN:O	1:C:588:GLY:N	2.39	0.56
1:C:633:ILE:HG23	1:C:638:ASP:HB2	1.86	0.56
1:D:236:GLN:NE2	1:D:364:LYS:O	2.38	0.56
1:F:37:ARG:HA	1:F:87:LEU:HA	1.86	0.56
1:B:586:GLN:O	1:B:588:GLY:N	2.38	0.55
1:E:122:GLY:HA2	1:E:125:TRP:HD1	1.71	0.55
1:D:396:VAL:N	1:D:473:ASP:OD2	2.35	0.55
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.89	0.55
1:A:262:TRP:CZ2	1:A:273:ALA:HA	2.41	0.55
1:A:266:GLU:HG2	1:A:268:LYS:H	1.70	0.55
1:A:453:ARG:HH21	1:A:458:LYS:HB3	1.70	0.55
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.89	0.55
1:F:13:ALA:HA	1:F:16:LEU:HD12	1.89	0.55
1:F:122:GLY:HA2	1:F:125:TRP:HD1	1.72	0.55
1:A:628:ARG:HH21	1:D:628:ARG:HG2	1.70	0.55
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.88	0.55
1:C:25:GLU:OE1	1:C:25:GLU:N	2.34	0.55
1:C:78:ASP:N	1:C:81:SER:OG	2.39	0.55
1:D:409:LYS:NZ	1:D:419:GLU:OE1	2.39	0.55
1:E:31:TRP:CH2	1:E:209:PHE:HD1	2.24	0.55
1:A:584:PHE:CZ	1:D:606:TRP:HZ3	2.25	0.55
1:B:692:ARG:O	1:B:696:SER:N	2.40	0.55
1:C:453:ARG:HH21	1:C:458:LYS:HB3	1.72	0.55
1:D:711:TYR:HB2	1:D:767:TRP:HE1	1.69	0.55
1:E:21:PHE:HD1	1:E:211:LEU:HD22	1.68	0.55
1:E:191:VAL:HA	1:E:195:PRO:HG3	1.89	0.55
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.42	0.55
1:A:307:SER:O	1:A:308:ARG:NH1	2.39	0.55
1:A:396:VAL:HB	1:A:473:ASP:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ARG:O	1:D:264:THR:OG1	2.18	0.55
1:E:18:ALA:O	1:E:215:SER:HB2	2.07	0.55
1:A:587:GLN:NE2	1:B:587:GLN:OE1	2.40	0.54
1:D:225:LEU:HD22	1:D:247:ILE:HB	1.89	0.54
1:E:195:PRO:HD2	1:E:199:ARG:HB3	1.88	0.54
1:A:452:ALA:N	1:A:461:ASN:OD1	2.30	0.54
1:C:396:VAL:HB	1:C:473:ASP:H	1.73	0.54
1:A:66:PHE:CZ	1:A:312:ALA:HB1	2.42	0.54
1:A:541:PHE:CD2	1:E:227:LEU:HG	2.27	0.54
1:A:633:ILE:HG23	1:A:638:ASP:HB2	1.88	0.54
1:B:177:TYR:CD2	1:B:207:GLN:HG3	2.42	0.54
1:B:608:PHE:CZ	1:B:612:ILE:HD11	2.43	0.54
1:B:711:TYR:HB2	1:B:767:TRP:HE1	1.72	0.54
1:C:405:TYR:HB3	1:C:425:CYS:SG	2.47	0.54
1:D:355:ASN:ND2	3:D:1102:NAG:O5	2.33	0.54
1:D:800:VAL:HA	1:D:803:LEU:HD12	1.89	0.54
1:A:625:THR:HG23	1:D:625:THR:HG21	1.89	0.54
1:C:66:PHE:CZ	1:C:312:ALA:HB1	2.43	0.54
1:E:18:ALA:CA	1:E:215:SER:HA	2.38	0.54
1:C:705:GLU:OE1	2:C:1101:ZK1:FAF	2.15	0.54
1:C:402:GLU:H	1:C:406:VAL:HB	1.72	0.54
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.42	0.54
1:B:261:ARG:O	1:B:264:THR:OG1	2.21	0.54
1:D:337:GLN:OE1	1:D:346:LYS:NZ	2.33	0.54
1:D:436:CYS:HB2	1:D:438:PHE:HE2	1.73	0.54
1:A:355:ASN:ND2	3:A:1102:NAG:O5	2.40	0.54
1:B:592:SER:O	1:B:599:ARG:NH2	2.41	0.54
1:C:587:GLN:NE2	1:D:587:GLN:OE1	2.40	0.53
1:A:586:GLN:O	1:A:588:GLY:N	2.41	0.53
1:D:791:ASN:OD1	1:D:792:VAL:HG23	2.09	0.53
1:E:11:ALA:HB2	1:E:225:THR:HG21	1.90	0.53
1:A:79:LYS:NZ	1:A:140:ASP:HA	2.23	0.53
1:A:409:LYS:HG2	1:A:422:GLU:CD	2.29	0.53
1:A:716:LYS:N	1:A:772:GLU:OE1	2.40	0.53
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.89	0.53
1:E:29:THR:HG23	1:E:30:TYR:CD2	2.44	0.53
1:C:402:GLU:O	1:C:406:VAL:N	2.36	0.53
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.89	0.53
1:E:34:GLY:O	1:E:90:PHE:N	2.42	0.53
1:A:405:TYR:HB3	1:A:425:CYS:SG	2.49	0.53
1:C:112:GLN:HE21	1:C:352:LYS:HA	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:LEU:HA	1:C:368:PRO:HA	1.91	0.53
1:E:133:LEU:HD23	1:E:136:LEU:HD12	1.91	0.53
1:A:402:GLU:O	1:A:406:VAL:N	2.35	0.53
1:C:138:ASP:OD1	1:C:139:SER:N	2.41	0.53
1:F:29:THR:HG23	1:F:30:TYR:CD2	2.43	0.53
1:A:402:GLU:H	1:A:406:VAL:HB	1.74	0.53
1:A:705:GLU:OE1	2:A:1101:ZK1:FAF	2.17	0.53
1:B:579:PHE:CZ	1:B:591:ILE:HG22	2.44	0.53
1:D:642:GLN:NE2	1:D:645:ILE:HB	2.24	0.53
1:A:263:SER:O	1:A:274:HIS:ND1	2.42	0.53
1:B:219:HIS:HD2	1:B:241:GLU:HB2	1.73	0.53
1:D:76:PHE:HE1	1:D:99:PRO:HG2	1.73	0.53
1:E:13:ALA:HA	1:E:16:LEU:HD12	1.91	0.53
1:E:221:ALA:C	1:E:224:VAL:HG22	2.29	0.53
1:D:452:ALA:N	1:D:461:ASN:OD1	2.42	0.53
1:B:453:ARG:HB2	1:B:460:TRP:CD2	2.45	0.52
1:C:409:LYS:HG3	1:C:415:LEU:HD12	1.91	0.52
1:C:477:ALA:O	1:C:479:LEU:N	2.42	0.52
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.91	0.52
1:F:39:PRO:O	1:F:85:PHE:N	2.42	0.52
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.89	0.52
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.91	0.52
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.74	0.52
1:E:39:PRO:O	1:E:85:PHE:N	2.43	0.52
1:F:34:GLY:O	1:F:90:PHE:N	2.42	0.52
1:B:480:THR:N	2:B:1101:ZK1:OAA	2.37	0.52
1:C:211:ILE:HG13	1:C:213:LYS:H	1.73	0.52
1:C:247:ILE:HG23	1:C:248:VAL:HG23	1.90	0.52
1:C:637:GLU:O	1:C:640:SER:OG	2.21	0.52
1:B:642:GLN:NE2	1:B:645:ILE:HB	2.25	0.52
1:D:608:PHE:CZ	1:D:612:ILE:HD11	2.45	0.52
1:B:498:LEU:N	1:B:730:LYS:O	2.40	0.52
1:D:794:GLY:HA2	1:D:797:TYR:CD2	2.45	0.52
1:E:127:SER:O	1:E:130:SER:OG	2.22	0.52
1:A:590:ASP:OD1	1:A:591:ILE:N	2.37	0.52
1:B:76:PHE:HE1	1:B:99:PRO:HG2	1.73	0.52
1:C:77:TYR:CE2	1:C:100:SER:HB2	2.45	0.52
1:C:346:LYS:NZ	3:C:1102:NAG:H4	2.25	0.52
1:C:590:ASP:CG	1:C:591:ILE:H	2.13	0.52
1:D:348:ASP:OD1	1:D:351:GLY:N	2.43	0.52
1:A:542:LEU:HD21	1:E:227:LEU:HD21	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASP:O	1:B:599:ARG:NE	2.43	0.52
1:C:710:GLU:OE2	1:C:722:LYS:NZ	2.43	0.52
1:B:532:ALA:O	1:B:536:VAL:HG23	2.10	0.52
1:B:606:TRP:HZ3	1:C:584:PHE:CZ	2.28	0.52
1:A:581:LEU:HD21	1:D:600:ILE:HA	1.92	0.51
1:B:219:HIS:CD2	1:B:241:GLU:HB2	2.45	0.51
1:D:330:GLU:HA	1:D:333:LEU:HD12	1.91	0.51
1:A:539:VAL:HA	1:A:542:LEU:HD12	1.92	0.51
1:B:396:VAL:N	1:B:473:ASP:OD2	2.36	0.51
1:D:716:LYS:HE3	1:D:772:GLU:HB3	1.91	0.51
1:F:127:SER:O	1:F:130:SER:OG	2.23	0.51
1:B:236:GLN:HA	1:B:363:LEU:HD21	1.91	0.51
1:B:684:ARG:N	1:B:688:GLU:OE1	2.42	0.51
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.45	0.51
1:A:317:ALA:O	1:A:320:ALA:N	2.44	0.51
1:A:259:ILE:HA	1:A:262:TRP:HB3	1.93	0.51
1:B:174:ASP:CG	1:B:178:ARG:HH12	2.14	0.51
1:C:121:LEU:HA	1:C:245:PHE:CZ	2.46	0.51
1:C:263:SER:O	1:C:274:HIS:ND1	2.44	0.51
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.51	0.51
1:C:789:LEU:HG	1:C:793:ALA:HB2	1.93	0.51
1:E:32:CYS:HG	1:E:204:ASP:C	2.08	0.51
1:B:130:TRP:CD2	1:B:191:ARG:HD3	2.45	0.51
1:D:219:HIS:HD2	1:D:241:GLU:HB2	1.75	0.51
1:D:412:HIS:CE1	1:D:413:GLU:HG3	2.46	0.51
1:D:637:GLU:HG2	1:D:666:VAL:HG21	1.92	0.51
1:A:247:ILE:HG13	1:A:342:SER:HB2	1.93	0.51
1:A:581:LEU:HD11	1:D:600:ILE:HG22	1.93	0.51
1:B:326:GLY:HA2	1:B:329:ILE:HD12	1.93	0.51
1:C:512:PRO:HB2	1:C:516:SER:HB3	1.93	0.51
1:C:521:LEU:O	1:C:526:TRP:NE1	2.44	0.51
1:D:130:TRP:CD2	1:D:191:ARG:HD3	2.46	0.51
1:D:396:VAL:O	1:D:473:ASP:HB2	2.11	0.51
1:E:157:ASP:HB3	1:E:160:LYS:HB2	1.93	0.51
1:A:415:LEU:HD13	1:A:419:GLU:HB3	1.93	0.50
1:A:477:ALA:O	1:A:479:LEU:N	2.43	0.50
1:D:309:ARG:HD3	1:D:311:ASN:HB2	1.93	0.50
1:D:346:LYS:HD3	1:D:355:ASN:HD22	1.76	0.50
1:A:657:GLU:HA	1:A:660:ARG:HG2	1.93	0.50
1:B:594:ARG:O	1:B:596:LEU:N	2.42	0.50
1:D:246:GLN:HE21	1:D:248:VAL:N	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.46	0.50
1:F:133:LEU:HD23	1:F:136:LEU:HD12	1.92	0.50
1:F:157:ASP:HB3	1:F:160:LYS:HB2	1.94	0.50
1:D:99:PRO:HA	1:D:113:MET:HB2	1.93	0.50
1:A:664:ILE:HA	1:D:761:LYS:HZ3	1.77	0.50
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.93	0.50
1:A:77:TYR:CE2	1:A:100:SER:HB2	2.47	0.50
1:B:190:ARG:HD3	1:B:218:TYR:CE1	2.46	0.50
1:B:348:ASP:OD1	1:B:351:GLY:N	2.45	0.50
1:B:619:ASN:ND2	1:C:787:LEU:HB2	2.27	0.50
1:C:642:GLN:NE2	1:C:645:ILE:HB	2.26	0.50
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.47	0.50
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.46	0.50
1:A:584:PHE:HD1	1:A:605:TRP:HZ2	1.59	0.50
1:A:619:ASN:HD21	1:B:787:LEU:HB2	1.77	0.50
1:C:607:PHE:O	1:C:611:ILE:HG12	2.11	0.50
1:D:803:LEU:O	1:D:807:MET:HG2	2.12	0.50
1:E:187:PHE:CE2	1:E:203:TRP:CD1	2.89	0.50
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.93	0.49
1:A:347:PHE:HE1	1:A:353:ARG:HG2	1.77	0.49
1:C:619:ASN:ND2	1:D:787:LEU:HB2	2.26	0.49
1:D:190:ARG:HD3	1:D:218:TYR:CE1	2.47	0.49
1:E:177:MET:O	1:E:181:MET:HG2	2.11	0.49
1:A:17:LEU:HB2	1:A:75:GLY:HA3	1.93	0.49
1:A:188:LYS:HD2	1:A:190:ARG:NH2	2.22	0.49
1:A:369:ARG:HH12	1:A:386:ASP:C	2.15	0.49
1:B:702:TYR:CD2	1:B:704:LEU:HD23	2.46	0.49
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.77	0.49
1:D:77:TYR:CE2	1:D:100:SER:HB2	2.47	0.49
1:D:466:GLU:HA	1:D:471:LYS:HB2	1.94	0.49
1:D:593:PRO:HD2	1:D:596:LEU:HD23	1.93	0.49
1:D:595:SER:O	1:D:597:SER:N	2.44	0.49
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.44	0.49
1:B:329:ILE:O	1:B:333:LEU:HG	2.13	0.49
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.94	0.49
1:D:532:ALA:O	1:D:536:VAL:HG23	2.12	0.49
1:A:101:PHE:HA	1:A:114:ARG:HH11	1.77	0.49
1:E:205:TYR:CD1	1:E:205:TYR:C	2.86	0.49
1:C:267:GLU:HG3	1:C:271:PRO:HA	1.94	0.49
1:D:209:ILE:HA	1:D:214:HIS:HD2	1.77	0.49
1:D:453:ARG:HB2	1:D:460:TRP:CE3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PHE:CE2	1:E:227:LEU:O	2.62	0.49
1:C:178:ARG:NH1	1:C:211:ILE:HG22	2.27	0.49
1:F:170:VAL:O	1:F:174:LEU:HG	2.13	0.49
1:A:708:MET:O	1:A:712:ILE:HG12	2.13	0.49
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.52	0.49
1:B:794:GLY:HA2	1:B:797:TYR:CD2	2.47	0.49
1:C:211:ILE:HD12	1:C:213:LYS:HD2	1.94	0.49
1:D:435:HIS:CD2	1:D:753:LEU:HD21	2.48	0.49
1:B:476:ILE:HG12	1:B:734:ILE:HD12	1.94	0.49
1:B:800:VAL:HA	1:B:803:LEU:HD12	1.94	0.49
1:C:115:PRO:HB3	1:C:356:TYR:CG	2.48	0.49
1:D:592:SER:OG	1:D:596:LEU:HB3	2.12	0.49
1:A:138:ASP:OD1	1:A:139:SER:N	2.46	0.49
1:B:436:CYS:HB2	1:B:438:PHE:CE2	2.46	0.49
1:C:619:ASN:HD21	1:D:787:LEU:HB2	1.78	0.49
1:D:453:ARG:HB2	1:D:460:TRP:CD2	2.47	0.49
1:A:124:LEU:HD11	1:A:128:TYR:HE2	1.77	0.48
1:A:348:ASP:OD1	1:A:352:LYS:N	2.46	0.48
1:B:306:ILE:HA	1:B:325:GLN:HE21	1.78	0.48
1:B:428:LEU:O	1:B:432:ILE:HG12	2.13	0.48
1:C:597:SER:O	1:C:600:ILE:HG12	2.12	0.48
1:D:595:SER:HA	1:D:599:ARG:CB	2.35	0.48
1:A:23:ASP:HB3	1:A:271:PRO:HG2	1.95	0.48
1:B:35:GLN:HG2	1:B:286:TYR:OH	2.13	0.48
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.48	0.48
1:C:480:THR:N	2:C:1101:ZK1:OAA	2.45	0.48
1:B:400:ILE:HG21	1:B:450:TYR:HE1	1.78	0.48
1:A:14:ILE:HG13	1:A:45:PRO:HA	1.95	0.48
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.96	0.48
1:C:525:ILE:HG12	1:D:789:LEU:HB2	1.94	0.48
1:B:77:TYR:CE2	1:B:100:SER:HB2	2.48	0.48
1:C:77:TYR:OH	1:C:101:PHE:O	2.16	0.48
1:C:299:LEU:O	1:C:303:ARG:N	2.45	0.48
1:D:243:SER:OG	1:D:362:GLU:HG2	2.13	0.48
1:D:250:TYR:HA	1:D:255:VAL:HG11	1.94	0.48
1:D:451:GLY:HA2	1:D:461:ASN:O	2.12	0.48
1:E:221:ALA:O	1:E:224:VAL:CG2	2.61	0.48
1:F:28:THR:HG23	1:F:207:TRP:CD1	2.49	0.48
1:F:159:LEU:HD12	1:F:229:SER:HB3	1.95	0.48
1:B:396:VAL:O	1:B:473:ASP:HB2	2.13	0.48
1:C:337:GLN:NE2	1:C:346:LYS:HE2	2.23	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ALA:HB1	1:E:215:SER:CA	2.43	0.48
1:D:35:GLN:HG2	1:D:286:TYR:OH	2.14	0.48
1:D:174:ASP:CG	1:D:178:ARG:HH12	2.16	0.48
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.47	0.48
1:D:498:LEU:N	1:D:730:LYS:O	2.46	0.48
1:F:7:ARG:HH21	1:F:224:VAL:HG13	1.79	0.48
1:A:255:VAL:O	1:A:259:ILE:HG12	2.13	0.48
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.78	0.48
1:B:412:HIS:CE1	1:B:413:GLU:HG3	2.49	0.48
1:B:746:VAL:O	1:B:750:VAL:HG23	2.13	0.48
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.95	0.48
1:D:702:TYR:CD2	1:D:704:LEU:HD23	2.49	0.48
1:A:256:SER:O	1:A:260:GLU:HG3	2.14	0.47
1:A:619:ASN:HD22	1:B:787:LEU:HD22	1.79	0.47
1:A:642:GLN:NE2	1:A:645:ILE:HB	2.29	0.47
1:C:14:ILE:HG13	1:C:45:PRO:HA	1.96	0.47
1:C:291:VAL:HG13	1:C:336:VAL:HG11	1.95	0.47
1:A:459:ILE:HG23	1:A:469:TYR:OH	2.14	0.47
1:A:607:PHE:O	1:A:611:ILE:HG12	2.14	0.47
1:B:308:ARG:NH2	1:B:325:GLN:HG2	2.29	0.47
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.96	0.47
1:D:534:ILE:O	1:D:537:SER:OG	2.27	0.47
1:A:522:ALA:H	1:A:525:ILE:HD12	1.80	0.47
1:A:744:THR:HB	1:A:745:PRO:HD3	1.97	0.47
1:C:80:LYS:HA	1:D:83:ASN:ND2	2.30	0.47
1:D:24:GLN:HE22	1:D:279:LYS:H	1.62	0.47
1:D:708:MET:O	1:D:712:ILE:HG12	2.15	0.47
1:F:36:GLN:NE2	1:F:199:ARG:H	2.11	0.47
1:B:24:GLN:NE2	1:B:278:ILE:HG13	2.27	0.47
1:B:309:ARG:HD3	1:B:311:ASN:HB2	1.96	0.47
1:E:227:LEU:O	1:E:231:THR:HG23	2.14	0.47
1:C:364:LYS:HG3	1:C:369:ARG:NH2	2.29	0.47
1:C:595:SER:H	1:C:599:ARG:NE	2.05	0.47
1:E:38:VAL:HG11	1:E:85:PHE:HD2	1.79	0.47
1:A:639:LEU:HA	1:A:642:GLN:HG2	1.96	0.47
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.78	0.47
1:C:744:THR:HB	1:C:745:PRO:HD3	1.96	0.47
1:A:236:GLN:HA	1:A:363:LEU:HD21	1.97	0.47
1:A:619:ASN:ND2	1:B:787:LEU:HB2	2.30	0.47
1:A:774:GLY:N	1:A:777:ASP:OD2	2.41	0.47
1:B:25:GLU:OE1	1:B:25:GLU:N	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:OG	1:B:362:GLU:HG2	2.14	0.47
1:C:122:LEU:HA	1:C:125:ILE:HD12	1.97	0.47
1:C:340:GLY:N	1:C:343:GLY:O	2.43	0.47
1:C:389:GLY:O	1:C:391:GLU:N	2.48	0.47
1:D:428:LEU:O	1:D:432:ILE:HG12	2.14	0.47
1:A:585:MET:HG3	1:D:603:GLY:HA2	1.97	0.47
1:B:78:ASP:N	1:B:81:SER:OG	2.48	0.47
1:B:579:PHE:CE1	1:B:591:ILE:HG22	2.49	0.47
1:D:498:LEU:O	1:D:730:LYS:N	2.48	0.47
1:B:711:TYR:HB2	1:B:767:TRP:NE1	2.29	0.47
1:C:323:TRP:CE3	1:C:325:GLN:HB2	2.50	0.47
1:C:639:LEU:HD13	1:C:647:TYR:CG	2.50	0.47
1:C:716:LYS:HG3	1:C:772:GLU:OE1	2.15	0.47
1:A:172:LYS:O	1:A:174:ASP:N	2.48	0.47
1:A:613:ILE:HG21	1:D:610:LEU:HD21	1.95	0.47
1:B:95:SER:HA	1:B:109:PHE:HB3	1.97	0.47
1:B:637:GLU:O	1:B:640:SER:OG	2.21	0.47
1:B:714:GLN:HB3	1:B:771:GLY:HA2	1.96	0.47
1:D:746:VAL:O	1:D:750:VAL:HG23	2.15	0.47
1:F:141:GLY:O	1:F:145:MET:HG3	2.15	0.47
1:C:346:LYS:HD2	1:C:355:ASN:HD22	1.80	0.46
1:D:25:GLU:OE1	1:D:25:GLU:N	2.44	0.46
1:E:196:GLU:OE1	1:E:198:TRP:NE1	2.48	0.46
1:F:94:ILE:HG12	1:F:95:TRP:CD1	2.50	0.46
1:A:526:TRP:HA	1:A:529:ILE:HG22	1.98	0.46
1:B:24:GLN:HE22	1:B:279:LYS:H	1.61	0.46
1:D:711:TYR:O	1:D:715:ARG:HG2	2.15	0.46
1:D:714:GLN:NE2	1:D:768:TYR:HA	2.31	0.46
1:F:187:PHE:HE2	1:F:203:TRP:CD1	2.32	0.46
1:A:594:ARG:O	1:A:596:LEU:N	2.49	0.46
1:A:651:ASP:HA	1:A:682:PHE:HB3	1.97	0.46
1:B:24:GLN:NE2	1:B:279:LYS:H	2.13	0.46
1:C:185:GLU:HA	1:C:188:LYS:HA	1.97	0.46
1:D:197:GLU:O	1:D:201:VAL:HG23	2.15	0.46
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.97	0.46
1:D:744:THR:HB	1:D:745:PRO:HD3	1.98	0.46
1:B:411:ASN:HB2	1:B:414:MET:HB2	1.96	0.46
1:C:197:GLU:O	1:C:201:VAL:HG23	2.15	0.46
1:F:189:VAL:O	1:F:193:LEU:HD13	2.15	0.46
1:A:521:LEU:O	1:A:526:TRP:NE1	2.49	0.46
1:B:526:TRP:HA	1:B:529:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLN:NE2	1:E:199:ARG:H	2.13	0.46
1:F:36:GLN:NE2	1:F:197:ASP:O	2.38	0.46
1:D:95:SER:HA	1:D:109:PHE:HB3	1.97	0.46
1:E:18:ALA:HB1	1:E:218:CYS:HB2	1.86	0.46
1:E:21:PHE:HD1	1:E:211:LEU:HB3	1.80	0.46
1:F:38:VAL:HG11	1:F:85:PHE:HD2	1.79	0.46
1:B:696:SER:OG	1:B:700:TYR:HB3	2.15	0.46
1:D:344:ASN:ND2	3:D:1102:NAG:H4	2.31	0.46
1:D:529:ILE:HD12	1:D:612:ILE:HD13	1.98	0.46
1:F:213:TRP:O	1:F:216:PHE:HB3	2.16	0.46
1:B:330:GLU:HA	1:B:333:LEU:HD12	1.97	0.46
1:B:498:LEU:O	1:B:730:LYS:N	2.47	0.46
1:C:18:PHE:O	1:C:49:ASN:HA	2.16	0.46
1:C:409:LYS:HG2	1:C:420:ARG:O	2.16	0.46
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.97	0.46
1:B:744:THR:HB	1:B:745:PRO:HD3	1.98	0.46
1:D:16:GLY:H	1:D:65:GLN:NE2	2.13	0.46
1:D:329:ILE:O	1:D:333:LEU:HG	2.16	0.46
1:E:15:ASN:CG	1:E:222:ALA:CB	2.81	0.46
1:B:146:LEU:HA	1:B:149:VAL:HG22	1.98	0.46
1:B:236:GLN:NE2	1:B:364:LYS:O	2.47	0.46
1:B:466:GLU:O	1:B:471:LYS:N	2.49	0.46
1:B:481:ILE:HG12	1:B:491:PHE:CD1	2.50	0.46
1:B:595:SER:HB3	1:C:578:TRP:CG	2.51	0.46
1:C:132:LYS:HD3	1:C:159:GLN:OE1	2.16	0.46
1:E:180:HIS:CB	1:E:209:PHE:HE1	2.27	0.46
1:A:113:MET:HB3	1:A:284:LEU:HD22	1.98	0.45
1:B:250:TYR:OH	1:B:277:THR:HB	2.16	0.45
1:B:453:ARG:HA	1:B:460:TRP:HA	1.97	0.45
1:C:112:GLN:NE2	1:C:352:LYS:HG2	2.31	0.45
1:C:121:LEU:HA	1:C:245:PHE:HZ	1.81	0.45
1:C:255:VAL:O	1:C:259:ILE:HG12	2.16	0.45
1:C:428:LEU:O	1:C:432:ILE:HG12	2.16	0.45
1:D:204:ILE:O	1:D:208:VAL:HG23	2.16	0.45
1:B:708:MET:O	1:B:712:ILE:HG12	2.16	0.45
1:D:436:CYS:HB2	1:D:438:PHE:CE2	2.50	0.45
1:D:696:SER:OG	1:D:700:TYR:HB3	2.15	0.45
1:D:765:LYS:O	1:D:770:LYS:HG2	2.16	0.45
1:E:94:ILE:HG12	1:E:95:TRP:CD1	2.51	0.45
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.51	0.45
1:A:597:SER:O	1:A:600:ILE:HG12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:PHE:O	1:B:611:ILE:HG12	2.16	0.45
1:D:124:LEU:HD11	1:D:128:TYR:HE2	1.80	0.45
1:D:215:VAL:HA	1:D:238:GLY:O	2.16	0.45
1:D:481:ILE:HG12	1:D:491:PHE:CD1	2.51	0.45
1:D:592:SER:N	1:D:599:ARG:HH21	2.14	0.45
1:F:178:VAL:O	1:F:181:MET:HB2	2.17	0.45
1:A:330:GLU:HG2	1:A:334:LYS:HE3	1.98	0.45
1:B:345:ILE:HG12	1:B:353:ARG:NH2	2.31	0.45
1:B:347:PHE:HE1	1:B:353:ARG:HG2	1.82	0.45
1:C:169:ASN:HD21	1:C:172:LYS:HE3	1.82	0.45
1:D:345:ILE:HG12	1:D:353:ARG:NH2	2.31	0.45
1:D:526:TRP:HA	1:D:529:ILE:HG22	1.98	0.45
1:E:195:PRO:HB2	1:E:198:TRP:O	2.16	0.45
1:A:77:TYR:CE2	1:A:98:THR:HG21	2.40	0.45
1:A:480:THR:N	2:A:1101:ZK1:OAA	2.44	0.45
1:A:598:GLY:O	1:A:601:VAL:HB	2.16	0.45
1:C:100:SER:C	1:C:114:ARG:HD3	2.37	0.45
1:C:177:TYR:HE1	1:C:204:ILE:HG12	1.82	0.45
1:C:498:LEU:O	1:C:730:LYS:N	2.48	0.45
1:C:652:SER:HA	1:C:656:LYS:HD3	1.99	0.45
1:C:708:MET:O	1:C:712:ILE:HG12	2.16	0.45
1:C:813:GLU:O	1:C:817:LYS:HG3	2.16	0.45
1:D:122:LEU:O	1:D:126:GLU:HG3	2.16	0.45
1:D:714:GLN:HE21	1:D:768:TYR:HA	1.81	0.45
1:E:34:GLY:HA3	1:E:90:PHE:HB2	1.99	0.45
1:E:181:MET:O	1:E:185:GLN:N	2.41	0.45
1:A:362:GLU:O	1:A:369:ARG:N	2.49	0.45
1:A:628:ARG:NH1	1:D:623:PHE:HA	2.31	0.45
1:B:124:LEU:HD11	1:B:128:TYR:HE2	1.82	0.45
1:B:198:ARG:CZ	1:B:230:GLY:HA2	2.47	0.45
1:E:170:VAL:O	1:E:174:LEU:HG	2.15	0.45
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.51	0.45
1:A:261:ARG:O	1:A:265:LEU:HG	2.16	0.45
1:A:664:ILE:HA	1:D:761:LYS:NZ	2.32	0.45
1:B:427:ASP:O	1:B:431:GLU:HG2	2.16	0.45
1:C:308:ARG:HB3	1:C:311:ASN:ND2	2.29	0.45
1:C:598:GLY:O	1:C:601:VAL:HB	2.16	0.45
1:D:598:GLY:O	1:D:601:VAL:HB	2.17	0.45
1:E:141:GLY:O	1:E:145:MET:HG3	2.16	0.45
1:B:540:LEU:HD12	1:B:580:SER:HB3	1.99	0.45
1:E:213:TRP:O	1:E:216:PHE:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:O	1:B:126:GLU:HG3	2.17	0.45
1:C:594:ARG:O	1:C:596:LEU:N	2.48	0.45
1:E:4:ARG:HB3	1:E:232:LYS:NZ	2.32	0.45
1:E:178:VAL:O	1:E:182:MET:HG2	2.17	0.45
1:F:195:PRO:HB2	1:F:198:TRP:O	2.17	0.45
1:A:428:LEU:O	1:A:432:ILE:HG12	2.17	0.45
1:A:534:ILE:O	1:A:537:SER:OG	2.24	0.45
1:C:124:LEU:HD11	1:C:128:TYR:HE2	1.82	0.45
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.98	0.45
1:D:116:ASP:OD1	1:D:118:LYS:HG2	2.17	0.45
1:E:8:ALA:O	1:E:12:VAL:HG23	2.16	0.45
1:F:117:PRO:O	1:F:119:SER:N	2.49	0.45
1:F:195:PRO:O	1:F:197:ASP:N	2.49	0.45
1:A:18:PHE:O	1:A:49:ASN:HA	2.17	0.44
1:B:131:ASP:OD1	1:B:132:LYS:N	2.50	0.44
1:B:309:ARG:HG2	1:B:311:ASN:N	2.30	0.44
1:B:453:ARG:HB2	1:B:460:TRP:CE3	2.52	0.44
1:C:54:ASN:O	1:C:58:VAL:HG23	2.18	0.44
1:C:267:GLU:CG	1:C:271:PRO:HA	2.48	0.44
1:E:180:HIS:CB	1:E:209:PHE:CE1	2.91	0.44
1:A:400:ILE:HG12	1:A:402:GLU:HG2	1.99	0.44
1:B:99:PRO:HA	1:B:113:MET:HB2	1.99	0.44
1:B:628:ARG:HG2	1:C:628:ARG:NH1	2.28	0.44
1:D:403:SER:HA	1:D:404:PRO:HA	1.80	0.44
1:D:607:PHE:O	1:D:611:ILE:HG12	2.16	0.44
1:A:83:ASN:ND2	1:B:80:LYS:HA	2.32	0.44
1:A:502:ILE:O	1:A:722:LYS:HA	2.17	0.44
1:A:595:SER:HB2	1:B:578:TRP:CG	2.52	0.44
1:B:204:ILE:O	1:B:208:VAL:HG23	2.18	0.44
1:B:595:SER:H	1:B:599:ARG:HG3	1.81	0.44
1:C:702:TYR:CD2	1:C:704:LEU:HD23	2.53	0.44
1:D:24:GLN:NE2	1:D:279:LYS:H	2.16	0.44
1:E:209:PHE:CE2	1:E:213:TRP:CE2	3.05	0.44
1:F:31:TRP:CE2	1:F:183:TYR:HE2	2.36	0.44
1:A:174:ASP:OD2	1:A:178:ARG:NH2	2.45	0.44
1:A:246:GLN:HE21	1:A:248:VAL:N	2.13	0.44
1:A:702:TYR:CD2	1:A:704:LEU:HD23	2.53	0.44
1:C:76:PHE:CD1	1:C:99:PRO:HD2	2.52	0.44
1:C:521:LEU:HA	1:D:787:LEU:HD23	2.00	0.44
1:C:599:ARG:HH22	1:D:581:LEU:HB3	1.83	0.44
1:E:189:VAL:O	1:E:193:LEU:HD13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:SER:HA	1:A:593:PRO:HD3	1.88	0.44
1:B:68:ARG:HB3	1:B:70:VAL:HG13	1.99	0.44
1:C:651:ASP:HA	1:C:682:PHE:HB3	1.99	0.44
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.99	0.44
1:D:24:GLN:NE2	1:D:278:ILE:HG13	2.28	0.44
1:D:711:TYR:HB2	1:D:767:TRP:NE1	2.33	0.44
1:D:714:GLN:HB3	1:D:771:GLY:HA2	1.99	0.44
1:A:54:ASN:O	1:A:58:VAL:HG23	2.18	0.44
1:B:308:ARG:NE	1:B:323:TRP:HB2	2.33	0.44
1:D:464:VAL:O	1:D:468:VAL:HG23	2.18	0.44
1:E:138:LEU:CD2	1:E:219:CYS:SG	3.06	0.44
1:A:384:GLU:O	1:A:386:ASP:N	2.50	0.44
1:C:306:ILE:HA	1:C:325:GLN:HE21	1.82	0.44
1:C:637:GLU:O	1:C:641:LYS:HG2	2.17	0.44
1:A:314:ASP:OD1	1:A:315:CYS:N	2.50	0.44
1:A:716:LYS:HG3	1:A:772:GLU:OE1	2.18	0.44
1:B:323:TRP:CE3	1:B:325:GLN:HB2	2.53	0.44
1:C:651:ASP:OD1	1:C:652:SER:N	2.51	0.44
1:D:477:ALA:O	1:D:479:LEU:N	2.50	0.44
1:F:8:ALA:O	1:F:12:VAL:HG23	2.17	0.44
1:A:628:ARG:NH2	1:D:628:ARG:H	2.16	0.44
1:B:541:PHE:CD1	1:B:573:ILE:HA	2.53	0.44
1:C:130:TRP:CZ3	1:C:191:ARG:HB3	2.52	0.44
1:C:314:ASP:OD1	1:C:315:CYS:N	2.51	0.44
1:D:99:PRO:O	1:D:114:ARG:HB2	2.18	0.44
1:D:135:TYR:O	1:D:162:ALA:HA	2.18	0.44
1:D:541:PHE:CD1	1:D:573:ILE:HA	2.53	0.44
1:F:37:ARG:HG2	1:F:88:ARG:H	1.82	0.44
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.43
1:A:800:VAL:HA	1:A:803:LEU:HD12	2.00	0.43
1:B:27:SER:O	1:B:31:VAL:HG23	2.17	0.43
1:B:197:GLU:O	1:B:201:VAL:HG23	2.18	0.43
1:C:24:GLN:HE22	1:C:278:ILE:HA	1.83	0.43
1:C:522:ALA:H	1:C:525:ILE:HD12	1.83	0.43
1:C:526:TRP:HA	1:C:529:ILE:HG22	1.99	0.43
1:C:814:PHE:HA	1:C:817:LYS:HD2	2.00	0.43
1:D:523:TYR:HA	1:D:526:TRP:CD1	2.43	0.43
1:D:651:ASP:HA	1:D:682:PHE:CD1	2.53	0.43
1:E:37:ARG:HG2	1:E:88:ARG:H	1.83	0.43
1:F:177:MET:HE3	1:F:212:ALA:HA	1.99	0.43
1:F:204:ASP:OD1	1:F:205:TYR:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD3	1:A:218:TYR:CE1	2.53	0.43
1:B:57:ALA:HA	1:B:60:ASN:ND2	2.33	0.43
1:C:348:ASP:OD1	1:C:352:LYS:N	2.50	0.43
1:E:21:PHE:CB	1:E:211:LEU:O	2.63	0.43
1:E:38:VAL:HB	1:E:85:PHE:HB2	2.00	0.43
1:F:34:GLY:HA3	1:F:90:PHE:HB2	2.00	0.43
1:A:813:GLU:O	1:A:817:LYS:HG3	2.19	0.43
1:B:394:THR:O	1:B:440:TYR:HA	2.19	0.43
1:B:409:LYS:HG2	1:B:420:ARG:O	2.17	0.43
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.53	0.43
1:D:540:LEU:HD12	1:D:580:SER:HB3	2.00	0.43
1:A:117:LEU:HD11	1:A:245:PHE:CG	2.53	0.43
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.00	0.43
1:B:266:GLU:HG2	1:B:268:LYS:H	1.83	0.43
1:B:400:ILE:HG21	1:B:450:TYR:CE1	2.53	0.43
1:C:453:ARG:HB2	1:C:460:TRP:CE2	2.53	0.43
1:D:27:SER:O	1:D:31:VAL:HG23	2.18	0.43
1:D:685:THR:OG1	1:D:688:GLU:HG3	2.18	0.43
2:D:1101:ZK1:HAI	2:D:1101:ZK1:HAOA	1.73	0.43
1:E:117:PRO:O	1:E:119:SER:N	2.51	0.43
1:E:177:MET:HE1	1:E:213:TRP:CD1	2.53	0.43
1:F:195:PRO:O	1:F:198:TRP:N	2.51	0.43
1:A:79:LYS:O	1:A:82:VAL:HG12	2.18	0.43
1:A:93:HIS:ND1	1:A:322:PRO:HG2	2.34	0.43
1:A:637:GLU:HG2	1:A:666:VAL:HG11	1.99	0.43
1:B:460:TRP:HE1	1:B:488:VAL:HG11	1.84	0.43
1:C:246:GLN:HE21	1:C:248:VAL:N	2.13	0.43
1:C:250:TYR:HA	1:C:255:VAL:HG11	1.99	0.43
1:E:167:VAL:O	1:E:171:LEU:HG	2.18	0.43
1:E:177:MET:HG3	1:E:216:PHE:CE1	2.53	0.43
1:F:227:LEU:O	1:F:231:THR:HG23	2.18	0.43
1:A:481:ILE:HG12	1:A:491:PHE:CD1	2.54	0.43
1:A:702:TYR:CE2	1:A:704:LEU:HD23	2.54	0.43
1:B:198:ARG:HG2	1:B:279:LYS:NZ	2.33	0.43
1:B:481:ILE:HD11	1:B:733:GLY:HA3	2.00	0.43
1:B:637:GLU:HG2	1:B:666:VAL:HG11	2.00	0.43
1:C:417:GLY:O	1:C:420:ARG:NE	2.37	0.43
1:C:644:GLU:HG2	1:D:781:LYS:HG3	2.01	0.43
1:D:332:ALA:O	1:D:336:VAL:HG23	2.19	0.43
1:D:374:TRP:CH2	1:D:376:GLU:HA	2.54	0.43
1:D:427:ASP:O	1:D:431:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:O	1:A:486:GLU:N	2.52	0.43
1:A:595:SER:HA	1:A:599:ARG:HE	1.84	0.43
1:C:115:PRO:HB3	1:C:356:TYR:CD1	2.54	0.43
1:C:514:VAL:HG22	1:C:794:GLY:HA2	2.00	0.43
1:D:137:TYR:CE1	1:D:164:ASN:HB2	2.54	0.43
1:D:146:LEU:HA	1:D:149:VAL:HG22	1.99	0.43
1:D:325:GLN:O	1:D:329:ILE:HG13	2.17	0.43
1:F:196:GLU:OE1	1:F:198:TRP:NE1	2.50	0.43
1:C:526:TRP:O	1:C:529:ILE:HG22	2.19	0.43
1:A:101:PHE:HA	1:A:114:ARG:HD3	2.00	0.43
1:A:500:ILE:HB	1:A:727:LEU:HB2	2.00	0.43
1:B:112:GLN:HE21	1:B:352:LYS:HA	1.82	0.43
1:B:592:SER:HB3	1:B:599:ARG:HG2	2.01	0.43
1:B:765:LYS:O	1:B:770:LYS:HG2	2.18	0.43
1:D:480:THR:N	2:D:1101:ZK1:OAA	2.35	0.43
1:E:223:SER:HA	1:E:226:THR:HG22	2.01	0.43
1:B:464:VAL:O	1:B:468:VAL:HG23	2.19	0.43
1:B:505:LYS:HG3	1:B:719:ASP:HB2	2.00	0.43
1:C:17:LEU:HB2	1:C:75:GLY:HA3	1.99	0.43
1:C:220:TYR:HB2	1:C:242:VAL:HG22	2.01	0.43
1:C:415:LEU:HD13	1:C:419:GLU:HB3	2.00	0.43
1:D:790:SER:OG	1:F:185:GLN:NE2	2.39	0.43
1:E:18:ALA:HB1	1:E:215:SER:O	2.18	0.43
1:A:198:ARG:HA	1:A:201:VAL:HB	2.01	0.42
1:A:220:TYR:HB2	1:A:242:VAL:HG22	2.01	0.42
1:A:308:ARG:HB3	1:A:311:ASN:ND2	2.33	0.42
1:A:678:GLU:HA	1:A:679:PRO:C	2.39	0.42
1:B:100:SER:HA	1:B:114:ARG:NH2	2.33	0.42
1:B:650:LEU:HD12	1:B:683:VAL:O	2.19	0.42
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.42
1:D:305:GLU:OE2	1:D:307:SER:N	2.52	0.42
1:D:445:VAL:HG13	1:D:448:GLY:HA2	1.99	0.42
1:A:478:PRO:HB3	1:A:732:TYR:CE2	2.54	0.42
1:B:198:ARG:NH2	1:B:229:ASP:O	2.52	0.42
1:B:533:TYR:OH	1:B:581:LEU:HA	2.19	0.42
1:E:116:ALA:HA	1:E:117:PRO:HA	1.81	0.42
1:A:763:LYS:O	1:A:767:TRP:HB2	2.18	0.42
1:B:462:GLY:O	1:B:466:GLU:HG3	2.19	0.42
1:E:28:THR:OG1	1:E:208:SER:OG	2.23	0.42
1:E:195:PRO:O	1:E:198:TRP:N	2.52	0.42
1:A:107:HIS:HA	1:A:108:PRO:HD3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HB2	1:B:460:TRP:CE2	2.54	0.42
1:B:600:ILE:HA	1:C:581:LEU:HD21	2.02	0.42
1:C:26:TYR:CE2	1:C:30:ARG:HD2	2.54	0.42
1:C:113:MET:O	1:C:115:PRO:HD3	2.19	0.42
1:C:651:ASP:OD2	1:C:684:ARG:HA	2.20	0.42
1:D:704:LEU:HD12	1:D:705:GLU:O	2.19	0.42
1:A:784:THR:OG1	1:A:785:SER:N	2.50	0.42
1:B:262:TRP:CZ2	1:B:273:ALA:HA	2.54	0.42
1:D:10:ASN:N	1:D:41:PHE:HA	2.35	0.42
1:D:100:SER:HA	1:D:114:ARG:NH2	2.35	0.42
1:D:344:ASN:HD22	3:D:1102:NAG:H4	1.84	0.42
1:D:505:LYS:NZ	1:D:697:LYS:HA	2.34	0.42
1:E:195:PRO:O	1:E:197:ASP:N	2.53	0.42
1:F:182:MET:O	1:F:185:GLN:HB3	2.20	0.42
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.85	0.42
1:B:105:GLY:O	1:B:107:HIS:ND1	2.53	0.42
1:B:514:VAL:O	1:B:517:PHE:HB3	2.19	0.42
1:C:364:LYS:HG3	1:C:369:ARG:HH21	1.85	0.42
1:D:131:ASP:OD1	1:D:132:LYS:N	2.53	0.42
1:D:742:LEU:O	1:D:746:VAL:HG23	2.20	0.42
1:A:369:ARG:NH1	1:A:385:ASP:O	2.53	0.42
1:C:348:ASP:OD2	1:C:350:ASN:HB2	2.19	0.42
1:C:774:GLY:N	1:C:777:ASP:OD2	2.42	0.42
1:D:462:GLY:O	1:D:466:GLU:HG3	2.19	0.42
1:E:182:MET:O	1:E:185:GLN:HB3	2.20	0.42
1:A:595:SER:CA	1:A:599:ARG:HE	2.32	0.42
1:B:308:ARG:HE	1:B:323:TRP:HE3	1.67	0.42
1:A:197:GLU:O	1:A:201:VAL:HG23	2.20	0.42
1:A:247:ILE:HD13	1:A:358:ILE:HG12	2.02	0.42
1:C:387:THR:C	1:C:389:GLY:H	2.23	0.42
1:D:299:LEU:HD23	1:D:306:ILE:HG21	2.01	0.42
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.84	0.42
1:E:134:TYR:O	1:E:138:LEU:HG	2.20	0.42
1:F:223:SER:HA	1:F:226:THR:HG22	2.01	0.42
1:A:267:GLU:HB2	1:A:274:HIS:HB3	2.02	0.42
1:A:372:GLY:HA2	1:A:383:THR:OG1	2.20	0.42
1:B:518:LEU:HD22	1:B:526:TRP:CE2	2.55	0.42
1:B:607:PHE:HZ	1:C:517:PHE:HZ	1.67	0.42
1:C:344:ASN:HD21	1:C:346:LYS:CE	2.29	0.42
1:C:763:LYS:O	1:C:767:TRP:HB2	2.20	0.42
1:F:117:PRO:HG3	1:F:193:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:HE22	1:A:278:ILE:HA	1.84	0.41
1:A:348:ASP:OD1	1:A:351:GLY:N	2.53	0.41
2:B:1101:ZK1:HAI	2:B:1101:ZK1:HAOA	1.73	0.41
1:C:460:TRP:CE3	1:C:464:VAL:HG11	2.55	0.41
1:E:3:SER:O	1:E:7:ARG:HG2	2.20	0.41
1:A:41:PHE:CE2	1:A:297:ARG:HD2	2.55	0.41
1:A:79:LYS:HB3	1:A:101:PHE:HZ	1.85	0.41
1:B:127:TYR:HB2	1:B:380:MET:SD	2.60	0.41
1:B:135:TYR:O	1:B:162:ALA:HA	2.19	0.41
1:B:141:ARG:HH22	1:B:196:CYS:N	2.18	0.41
1:C:409:LYS:HD2	1:C:422:GLU:CD	2.41	0.41
1:C:575:ASN:O	1:C:578:TRP:HB2	2.20	0.41
1:D:57:ALA:HA	1:D:60:ASN:ND2	2.35	0.41
1:D:347:PHE:HE1	1:D:353:ARG:HG2	1.85	0.41
1:F:34:GLY:HA2	1:F:202:SER:HB2	2.03	0.41
1:A:101:PHE:HA	1:A:102:PRO:HD3	1.80	0.41
1:A:506:LYS:HA	1:A:507:PRO:HD3	1.68	0.41
1:A:714:GLN:HG3	1:A:767:TRP:O	2.20	0.41
1:B:607:PHE:CZ	1:C:517:PHE:HZ	2.37	0.41
1:C:678:GLU:HA	1:C:679:PRO:C	2.41	0.41
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.55	0.41
1:E:10:LEU:O	1:E:14:LEU:HG	2.20	0.41
1:A:56:PHE:CE2	1:B:91:THR:HG21	2.55	0.41
1:A:453:ARG:HB2	1:A:460:TRP:CD2	2.56	0.41
1:C:321:VAL:HA	1:C:322:PRO:HD3	1.87	0.41
1:C:332:ALA:O	1:C:336:VAL:HG23	2.20	0.41
1:C:639:LEU:HA	1:C:642:GLN:HG2	2.02	0.41
1:D:511:LYS:HA	1:D:512:PRO:HD3	1.77	0.41
1:E:194:GLY:O	1:E:196:GLU:N	2.53	0.41
1:F:178:VAL:O	1:F:182:MET:HG2	2.19	0.41
1:A:345:ILE:HG12	1:A:353:ARG:NH2	2.35	0.41
1:A:764:ASN:HA	1:A:768:TYR:HD2	1.85	0.41
1:B:228:THR:OG1	1:B:246:GLN:OE1	2.20	0.41
1:B:348:ASP:OD2	1:B:350:ASN:HB2	2.20	0.41
1:B:704:LEU:HD12	1:B:705:GLU:O	2.20	0.41
1:C:400:ILE:HG12	1:C:402:GLU:HG2	2.02	0.41
1:A:711:TYR:HB2	1:A:767:TRP:HE1	1.85	0.41
1:B:479:LEU:HD12	2:B:1101:ZK1:OAA	2.21	0.41
1:B:591:ILE:HG23	1:B:591:ILE:O	2.21	0.41
1:B:702:TYR:HD2	1:B:704:LEU:HD23	1.84	0.41
1:C:599:ARG:NH1	1:D:578:TRP:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:VAL:O	1:F:171:LEU:HG	2.21	0.41
1:A:113:MET:O	1:A:115:PRO:HD3	2.20	0.41
1:A:383:THR:HG22	1:A:385:ASP:H	1.86	0.41
1:B:27:SER:HB3	1:B:270:TYR:HB3	2.03	0.41
1:B:648:GLY:HA3	1:B:681:VAL:HB	2.01	0.41
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.53	0.41
1:C:323:TRP:CZ3	1:C:325:GLN:HB2	2.55	0.41
1:D:451:GLY:HA3	1:D:464:VAL:HG23	2.02	0.41
1:D:479:LEU:HD12	2:D:1101:ZK1:OAA	2.20	0.41
1:F:99:GLU:OE2	1:F:108:LYS:HD2	2.21	0.41
1:A:39:SER:HA	1:A:42:ARG:NH2	2.36	0.41
1:A:535:GLY:HA2	1:E:220:MET:CE	2.50	0.41
1:B:98:THR:HA	1:B:99:PRO:HD3	1.79	0.41
1:B:99:PRO:O	1:B:114:ARG:HB2	2.20	0.41
1:C:209:ILE:HA	1:C:214:HIS:HD2	1.86	0.41
1:C:745:PRO:HA	1:C:748:LEU:HD12	2.03	0.41
1:D:309:ARG:HG2	1:D:311:ASN:N	2.31	0.41
1:A:26:TYR:CE2	1:A:30:ARG:HD2	2.56	0.41
1:A:80:LYS:HA	1:B:83:ASN:ND2	2.36	0.41
1:A:209:ILE:HA	1:A:214:HIS:HD2	1.86	0.41
1:A:479:LEU:HD12	2:A:1101:ZK1:OAA	2.21	0.41
1:A:532:ALA:O	1:A:536:VAL:HG23	2.21	0.41
1:A:575:ASN:O	1:A:578:TRP:HB2	2.20	0.41
1:B:54:ASN:OD1	1:B:56:PHE:HB3	2.21	0.41
1:B:172:LYS:O	1:B:174:ASP:N	2.54	0.41
1:B:400:ILE:HD13	1:B:450:TYR:CE1	2.56	0.41
1:B:742:LEU:O	1:B:746:VAL:HG23	2.20	0.41
1:C:93:HIS:HB3	1:C:327:VAL:HG22	2.03	0.41
1:C:201:VAL:O	1:C:205:VAL:HG23	2.21	0.41
1:C:453:ARG:HB2	1:C:460:TRP:CD2	2.55	0.41
1:C:540:LEU:HD12	1:C:580:SER:HB3	2.02	0.41
1:D:250:TYR:OH	1:D:277:THR:HB	2.21	0.41
1:D:255:VAL:O	1:D:259:ILE:HG12	2.21	0.41
1:D:334:LYS:HA	1:D:347:PHE:HD2	1.84	0.41
1:D:648:GLY:HA3	1:D:681:VAL:HB	2.02	0.41
1:E:190:THR:O	1:E:195:PRO:HG3	2.20	0.41
1:F:3:SER:O	1:F:7:ARG:HG2	2.21	0.41
1:F:10:LEU:O	1:F:14:LEU:HG	2.21	0.41
1:F:134:TYR:O	1:F:138:LEU:HG	2.21	0.41
1:A:91:THR:HG21	1:B:56:PHE:CD2	2.56	0.41
1:A:577:LEU:O	1:A:580:SER:OG	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PRO:O	1:B:110:VAL:HG23	2.21	0.41
1:B:460:TRP:CE3	1:B:464:VAL:HG11	2.56	0.41
1:B:711:TYR:O	1:B:715:ARG:HG2	2.21	0.41
1:D:231:ASP:HB3	1:D:234:LYS:HE3	2.02	0.41
1:D:402:GLU:O	1:D:405:TYR:N	2.54	0.41
1:E:174:LEU:O	1:E:178:VAL:HG23	2.21	0.41
1:A:246:GLN:HB2	1:A:361:MET:HG3	2.03	0.40
1:A:483:LEU:N	1:D:755:GLU:OE2	2.35	0.40
1:B:207:GLN:O	1:B:211:ILE:HG12	2.21	0.40
1:C:79:LYS:O	1:C:82:VAL:HG12	2.21	0.40
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.77	0.40
1:A:78:ASP:N	1:A:81:SER:HG	2.18	0.40
1:A:112:GLN:NE2	1:A:352:LYS:HG2	2.36	0.40
1:A:318:ASN:HA	1:A:319:PRO:HA	1.95	0.40
1:A:599:ARG:NH2	1:B:581:LEU:HB3	2.29	0.40
1:B:74:PHE:CE1	1:B:99:PRO:HD3	2.57	0.40
1:B:196:CYS:HB3	1:B:200:LYS:HB2	2.04	0.40
1:B:480:THR:H	2:B:1101:ZK1:CAT	2.34	0.40
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.87	0.40
1:C:686:THR:O	1:C:690:VAL:HG23	2.22	0.40
1:D:445:VAL:HG23	1:D:466:GLU:OE2	2.21	0.40
1:E:187:PHE:O	1:E:190:THR:OG1	2.27	0.40
1:F:187:PHE:O	1:F:190:THR:OG1	2.26	0.40
1:A:76:PHE:CD1	1:A:99:PRO:HD2	2.56	0.40
1:B:190:ARG:HA	1:B:218:TYR:CD1	2.56	0.40
1:B:394:THR:HG21	1:B:441:LYS:HD2	2.02	0.40
1:B:523:TYR:HA	1:B:526:TRP:CD1	2.46	0.40
1:C:330:GLU:HG2	1:C:334:LYS:HE3	2.02	0.40
1:D:405:TYR:CD2	1:D:478:PRO:HG2	2.57	0.40
1:D:650:LEU:HD12	1:D:683:VAL:O	2.22	0.40
1:A:435:HIS:CD2	1:A:752:LYS:HD3	2.56	0.40
1:B:76:PHE:CE1	1:B:99:PRO:HG2	2.54	0.40
1:B:115:PRO:HG3	1:B:353:ARG:CZ	2.51	0.40
1:B:287:ASP:CG	1:B:341:LEU:H	2.24	0.40
1:C:499:GLY:HA3	1:C:728:ASP:O	2.21	0.40
1:E:99:GLU:OE2	1:E:108:LYS:HD2	2.21	0.40
1:E:138:LEU:HD21	1:E:219:CYS:SG	2.61	0.40
1:A:16:GLY:H	1:A:65:GLN:NE2	2.09	0.40
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.03	0.40
1:B:407:MET:N	1:B:422:GLU:O	2.53	0.40
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:807:MET:HE3	1:F:167:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	779/1057 (74%)	726 (93%)	41 (5%)	12 (2%)	10	46
1	B	776/1057 (73%)	726 (94%)	40 (5%)	10 (1%)	12	48
1	C	779/1057 (74%)	724 (93%)	43 (6%)	12 (2%)	10	46
1	D	776/1057 (73%)	725 (93%)	38 (5%)	13 (2%)	9	43
1	E	171/1057 (16%)	153 (90%)	12 (7%)	6 (4%)	3	28
1	F	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	2	24
All	All	3452/6342 (54%)	3210 (93%)	181 (5%)	61 (2%)	12	42

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	B	395	VAL
1	B	512	PRO
1	C	591	ILE
1	D	395	VAL
1	D	590	ASP
1	D	591	ILE
1	A	389	GLY
1	A	394	THR
1	A	591	ILE
1	B	587	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	595	SER
1	B	785	SER
1	C	174	ASP
1	C	587	GLN
1	D	520	PRO
1	D	587	GLN
1	D	595	SER
1	D	596	LEU
1	E	111	SER
1	E	117	PRO
1	E	118	ALA
1	E	196	GLU
1	F	111	SER
1	F	118	ALA
1	F	196	GLU
1	F	203	TRP
1	A	587	GLN
1	A	594	ARG
1	A	595	SER
1	B	173	LYS
1	B	174	ASP
1	B	590	ASP
1	C	173	LYS
1	C	390	LEU
1	C	594	ARG
1	C	595	SER
1	D	785	SER
1	F	117	PRO
1	A	174	ASP
1	A	437	GLY
1	B	437	GLY
1	C	394	THR
1	C	437	GLY
1	C	590	ASP
1	C	787	LEU
1	D	512	PRO
1	D	594	ARG
1	A	765	LYS
1	A	787	LEU
1	C	765	LYS
1	D	514	VAL
1	F	112	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	478	PRO
1	E	194	GLY
1	F	194	GLY
1	E	195	PRO
1	F	195	PRO
1	A	478	PRO
1	D	437	GLY
1	D	593	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 PDB entries followed by that with respect to all EM entries.

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	666/888 (75%)	666 (100%)	0	100	100
1	B	664/888 (75%)	664 (100%)	0	100	100
1	C	666/888 (75%)	666 (100%)	0	100	100
1	D	664/888 (75%)	664 (100%)	0	100	100
1	E	152/888 (17%)	150 (99%)	2 (1%)	69	82
1	F	152/888 (17%)	152 (100%)	0	100	100
All	All	2964/5328 (56%)	2962 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	202	SER
1	E	205	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	46	HIS
1	A	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	147	GLN
1	A	246	GLN
1	A	311	ASN
1	A	355	ASN
1	A	587	GLN
1	A	619	ASN
1	A	642	GLN
1	A	756	GLN
1	B	24	GLN
1	B	65	GLN
1	B	83	ASN
1	B	147	GLN
1	B	214	HIS
1	B	325	GLN
1	B	355	ASN
1	B	412	HIS
1	B	587	GLN
1	B	619	ASN
1	B	642	GLN
1	C	24	GLN
1	C	46	HIS
1	C	65	GLN
1	C	112	GLN
1	C	147	GLN
1	C	246	GLN
1	C	311	ASN
1	C	325	GLN
1	C	337	GLN
1	C	344	ASN
1	C	355	ASN
1	C	587	GLN
1	C	619	ASN
1	C	642	GLN
1	D	24	GLN
1	D	65	GLN
1	D	147	GLN
1	D	412	HIS
1	D	435	HIS
1	D	587	GLN
1	D	642	GLN
1	D	714	GLN
1	E	15	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	228	ASN
1	F	15	ASN
1	F	180	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	D	1102	-	14,14,15	0.18	0	17,19,21	0.45	0
3	NAG	C	1102	-	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	B	1102	-	14,14,15	0.22	0	17,19,21	0.42	0
2	ZK1	D	1101	-	28,29,29	3.39	9 (32%)	42,45,45	1.63	9 (21%)
2	ZK1	C	1101	-	28,29,29	3.37	8 (28%)	42,45,45	1.67	10 (23%)
2	ZK1	A	1101	-	28,29,29	3.36	8 (28%)	42,45,45	1.66	10 (23%)
3	NAG	A	1102	-	14,14,15	0.23	0	17,19,21	0.36	0
2	ZK1	B	1101	-	28,29,29	3.39	9 (32%)	42,45,45	1.60	8 (19%)

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
3	NAG	D	1102	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1102	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1102	-	-	2/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	5/13/23/23	0/3/3/3
2	ZK1	C	1101	-	-	5/13/23/23	0/3/3/3
2	ZK1	A	1101	-	-	5/13/23/23	0/3/3/3
3	NAG	A	1102	-	-	2/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	5/13/23/23	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ZK1	OAA-CAT	9.22	1.41	1.23
2	C	1101	ZK1	OAA-CAT	9.20	1.41	1.23
2	A	1101	ZK1	OAA-CAT	9.16	1.41	1.23
2	D	1101	ZK1	OAA-CAT	9.14	1.41	1.23
2	B	1101	ZK1	OAB-CAU	8.33	1.40	1.23
2	D	1101	ZK1	OAB-CAU	8.33	1.40	1.23
2	C	1101	ZK1	OAB-CAU	8.30	1.40	1.23
2	A	1101	ZK1	OAB-CAU	8.28	1.40	1.23
2	A	1101	ZK1	PBA-OAC	7.10	1.65	1.50
2	B	1101	ZK1	PBA-OAC	7.09	1.65	1.50
2	D	1101	ZK1	PBA-OAC	7.08	1.65	1.50
2	C	1101	ZK1	PBA-OAC	7.08	1.65	1.50
2	B	1101	ZK1	CAT-NAP	5.86	1.43	1.35
2	D	1101	ZK1	CAT-NAP	5.78	1.43	1.35
2	C	1101	ZK1	CAT-NAP	5.66	1.43	1.35
2	A	1101	ZK1	CAT-NAP	5.61	1.43	1.35
2	A	1101	ZK1	PBA-OAE	4.55	1.65	1.54
2	C	1101	ZK1	PBA-OAE	4.52	1.65	1.54
2	D	1101	ZK1	PBA-OAE	4.51	1.65	1.54
2	B	1101	ZK1	PBA-OAE	4.45	1.65	1.54
2	A	1101	ZK1	PBA-OAD	-3.82	1.46	1.54
2	C	1101	ZK1	PBA-OAD	-3.78	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.74	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.73	1.46	1.54
2	D	1101	ZK1	CAJ-CAS	3.14	1.44	1.39
2	C	1101	ZK1	CAJ-CAS	3.12	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ZK1	CAJ-CAS	3.10	1.44	1.39
2	B	1101	ZK1	CAJ-CAS	3.09	1.44	1.39
2	D	1101	ZK1	CAW-NAY	2.84	1.46	1.41
2	B	1101	ZK1	CAW-NAY	2.77	1.46	1.41
2	C	1101	ZK1	CAW-NAY	2.68	1.45	1.41
2	A	1101	ZK1	CAW-NAY	2.65	1.45	1.41
2	D	1101	ZK1	CAR-NAX	2.11	1.45	1.41
2	B	1101	ZK1	CAR-NAX	2.04	1.45	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	ZK1	CAO-NAY-CAU	4.74	121.12	116.51
2	A	1101	ZK1	CAO-NAY-CAU	4.72	121.11	116.51
2	D	1101	ZK1	CAV-NAP-CAT	-4.32	119.30	124.80
2	B	1101	ZK1	CAV-NAP-CAT	-4.15	119.52	124.80
2	B	1101	ZK1	CAO-NAY-CAU	3.99	120.40	116.51
2	A	1101	ZK1	CAV-NAP-CAT	-3.99	119.73	124.80
2	C	1101	ZK1	CAV-NAP-CAT	-3.98	119.73	124.80
2	D	1101	ZK1	CAO-NAY-CAU	3.95	120.36	116.51
2	A	1101	ZK1	CAN-NAX-CAM	3.72	119.72	111.52
2	C	1101	ZK1	CAN-NAX-CAM	3.63	119.54	111.52
2	B	1101	ZK1	CAN-NAX-CAM	3.57	119.41	111.52
2	D	1101	ZK1	CAN-NAX-CAM	3.51	119.27	111.52
2	D	1101	ZK1	CAU-CAT-NAP	2.88	120.46	117.49
2	D	1101	ZK1	CAI-CAR-NAX	-2.78	118.41	122.52
2	C	1101	ZK1	CAI-CAR-NAX	-2.72	118.50	122.52
2	B	1101	ZK1	CAI-CAR-NAX	-2.70	118.53	122.52
2	A	1101	ZK1	CAI-CAR-NAX	-2.70	118.53	122.52
2	B	1101	ZK1	CAU-CAT-NAP	2.64	120.20	117.49
2	A	1101	ZK1	CAU-CAT-NAP	2.57	120.14	117.49
2	C	1101	ZK1	FAG-CAZ-CAS	-2.55	108.26	112.70
2	D	1101	ZK1	FAG-CAZ-CAS	-2.54	108.27	112.70
2	A	1101	ZK1	FAG-CAZ-CAS	-2.53	108.30	112.70
2	B	1101	ZK1	FAG-CAZ-CAS	-2.50	108.34	112.70
2	C	1101	ZK1	CAT-CAU-NAY	2.45	120.13	117.32
2	C	1101	ZK1	CAU-CAT-NAP	2.43	119.99	117.49
2	C	1101	ZK1	CAW-NAY-CAU	-2.35	119.88	122.79
2	A	1101	ZK1	CAW-NAY-CAU	-2.34	119.89	122.79
2	A	1101	ZK1	CAT-CAU-NAY	2.33	119.99	117.32
2	D	1101	ZK1	CAW-NAY-CAU	-2.30	119.94	122.79
2	B	1101	ZK1	CAT-CAU-NAY	2.26	119.91	117.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	ZK1	CAW-NAY-CAU	-2.24	120.02	122.79
2	D	1101	ZK1	CAT-CAU-NAY	2.19	119.83	117.32
2	C	1101	ZK1	CAM-NAX-CAR	2.15	121.37	116.27
2	A	1101	ZK1	CAM-NAX-CAR	2.09	121.22	116.27
2	D	1101	ZK1	CAM-NAX-CAR	2.09	121.22	116.27
2	C	1101	ZK1	CAI-CAW-NAY	-2.07	119.03	121.84
2	A	1101	ZK1	CAI-CAW-NAY	-2.01	119.11	121.84

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ZK1	NAY-CAO-PBA-OAC
2	A	1101	ZK1	NAY-CAO-PBA-OAE
2	B	1101	ZK1	NAY-CAO-PBA-OAD
2	B	1101	ZK1	NAY-CAO-PBA-OAE
2	C	1101	ZK1	NAY-CAO-PBA-OAE
2	D	1101	ZK1	NAY-CAO-PBA-OAD
2	D	1101	ZK1	NAY-CAO-PBA-OAE
3	A	1102	NAG	O5-C5-C6-O6
3	B	1102	NAG	C4-C5-C6-O6
3	A	1102	NAG	C4-C5-C6-O6
3	B	1102	NAG	O5-C5-C6-O6
2	D	1101	ZK1	CAI-CAR-NAX-CAN
2	A	1101	ZK1	CAI-CAR-NAX-CAN
2	C	1101	ZK1	CAI-CAR-NAX-CAN
2	B	1101	ZK1	CAI-CAR-NAX-CAN
2	B	1101	ZK1	CAS-CAR-NAX-CAN
2	D	1101	ZK1	CAS-CAR-NAX-CAN
2	A	1101	ZK1	NAY-CAO-PBA-OAD
2	C	1101	ZK1	NAY-CAO-PBA-OAD
2	C	1101	ZK1	NAY-CAO-PBA-OAC
2	A	1101	ZK1	CAS-CAR-NAX-CAN
2	C	1101	ZK1	CAS-CAR-NAX-CAN
2	B	1101	ZK1	NAY-CAO-PBA-OAC
2	D	1101	ZK1	NAY-CAO-PBA-OAC

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1102	NAG	3	0
3	C	1102	NAG	1	0
2	D	1101	ZK1	4	0
2	C	1101	ZK1	2	0
2	A	1101	ZK1	3	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ZK1 D 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 C 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 A 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 B 1101

Bond lengths

Bond angles

Torsions

Rings
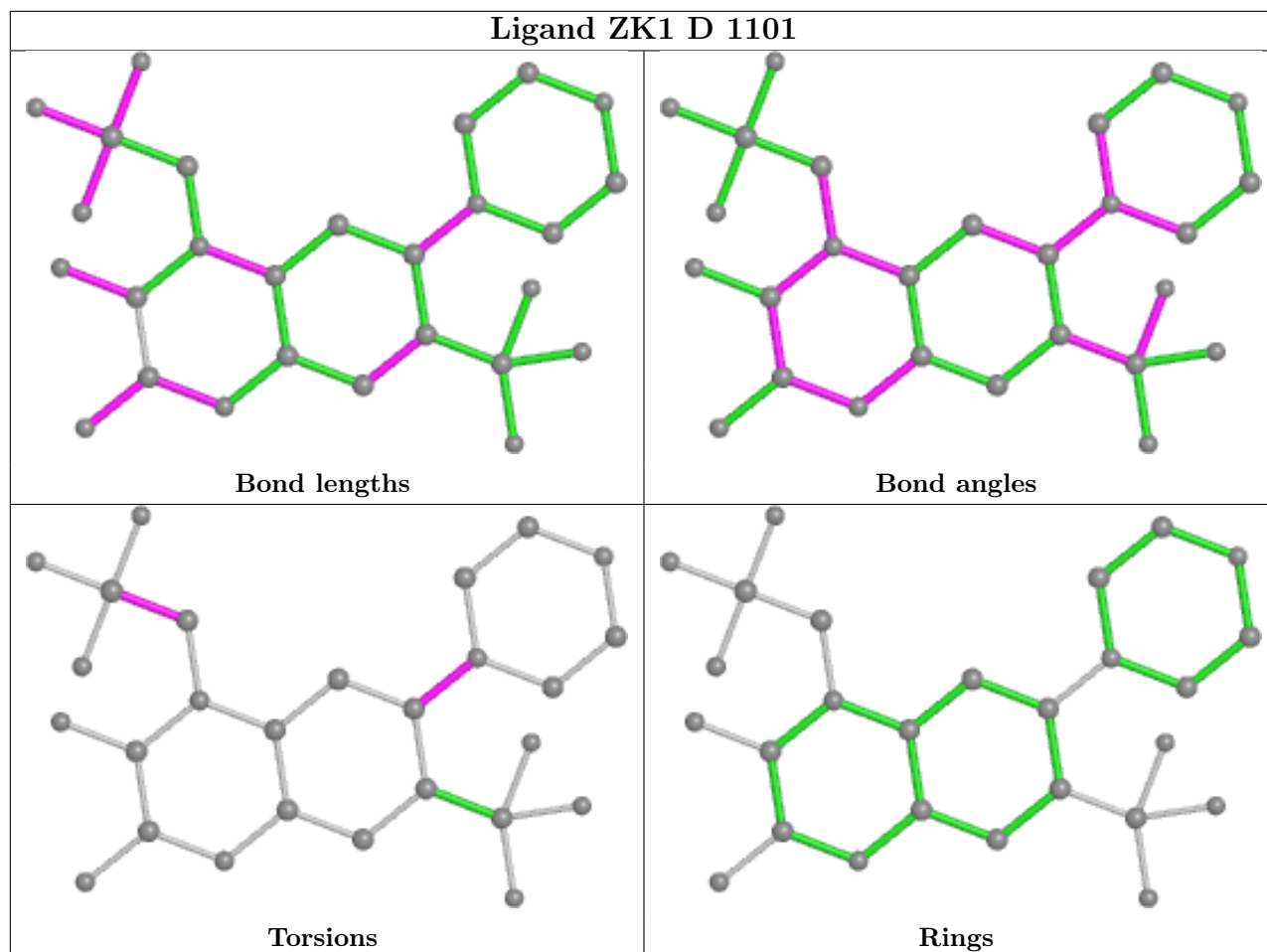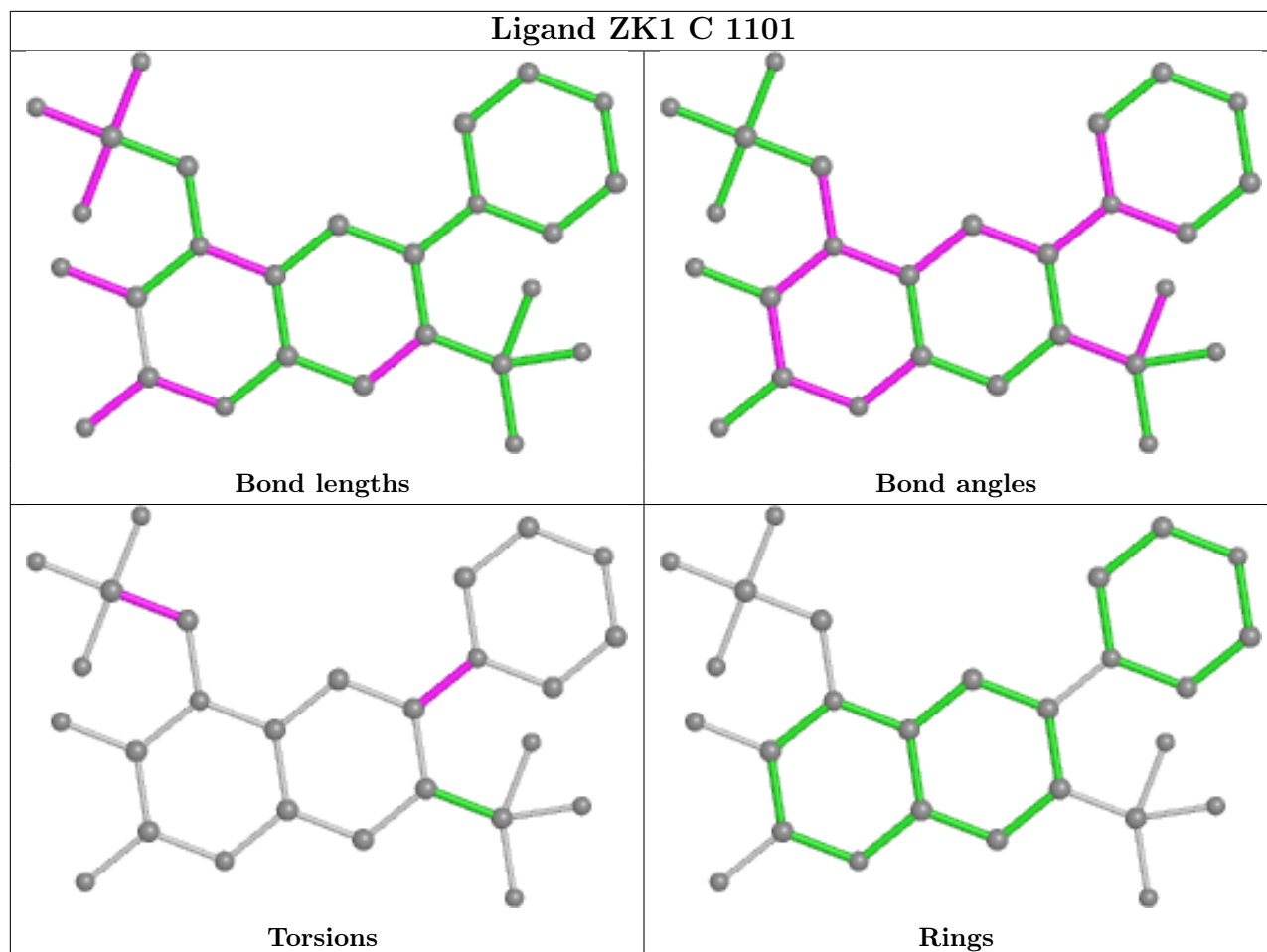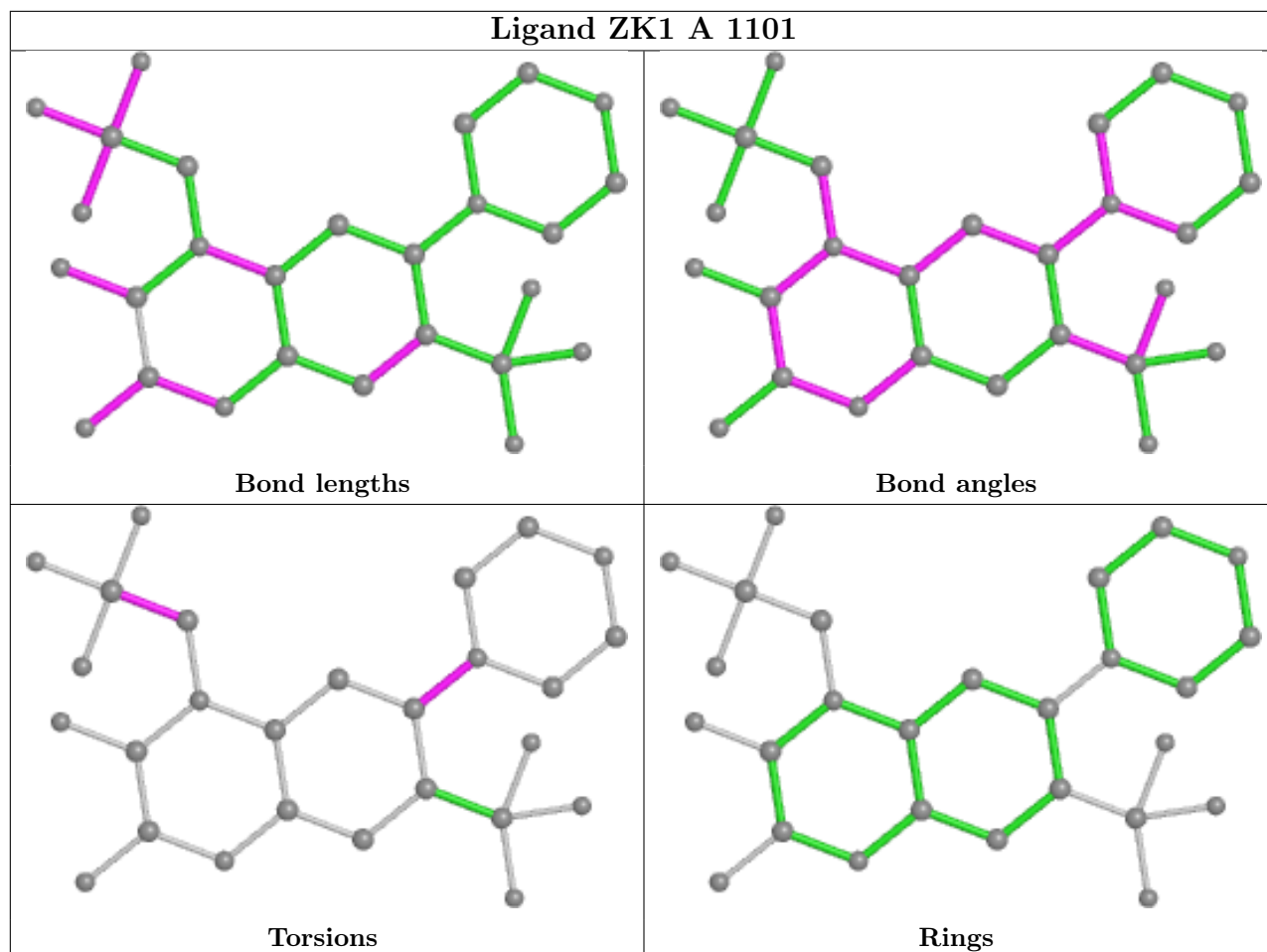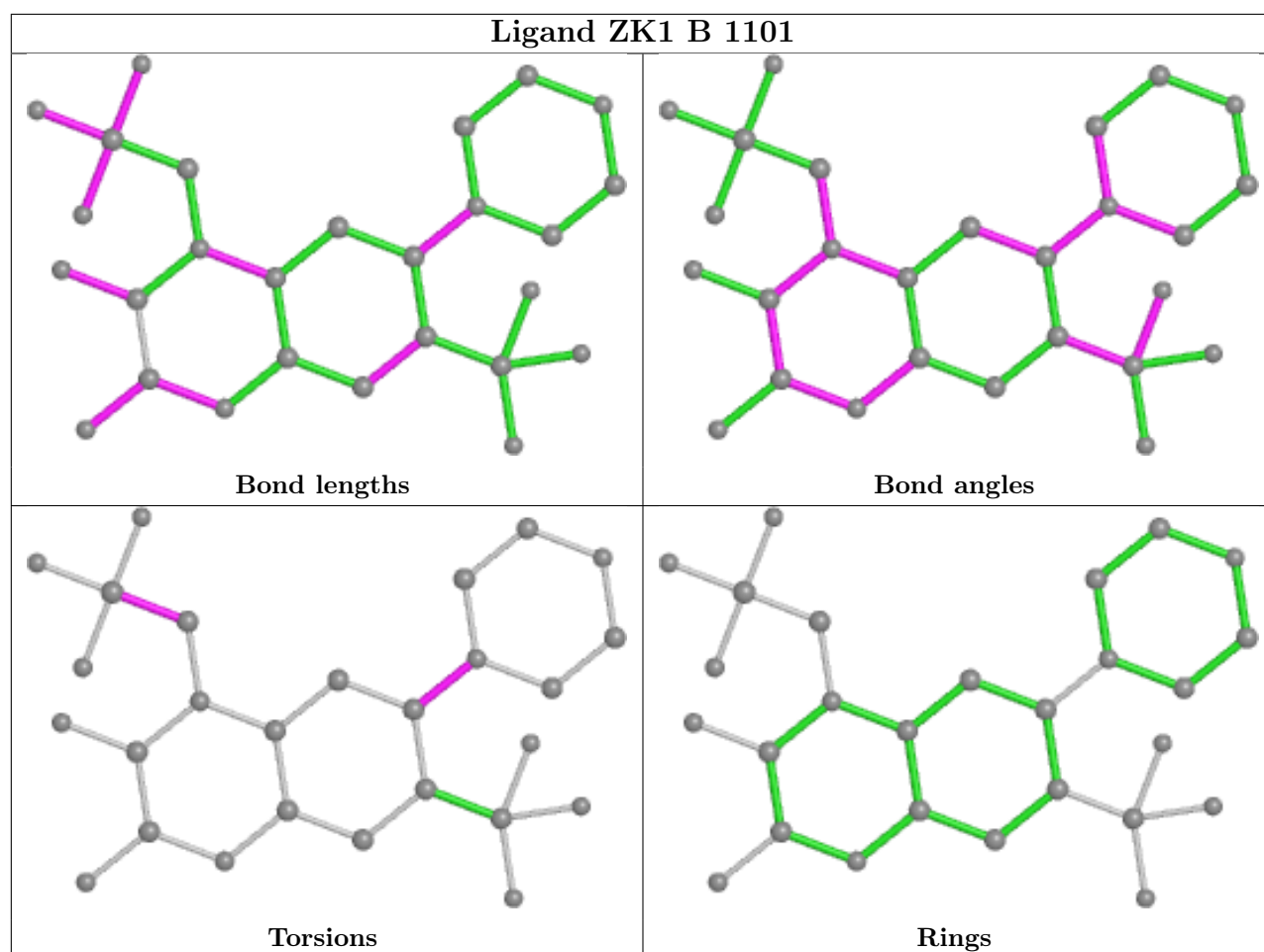
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-8687. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
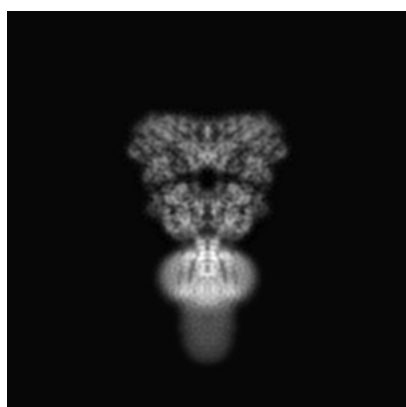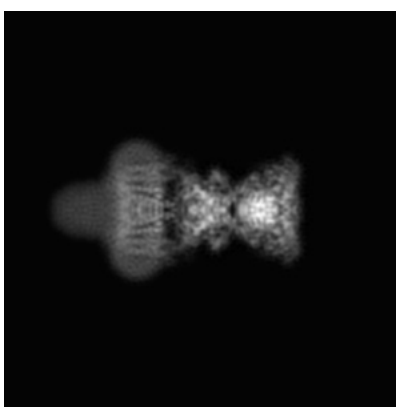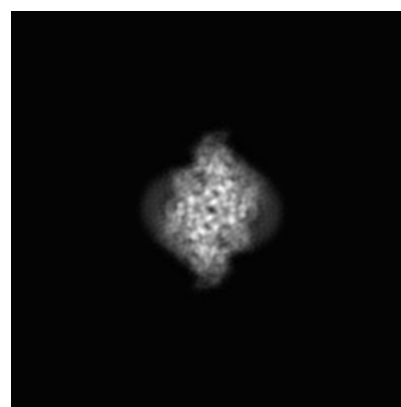
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
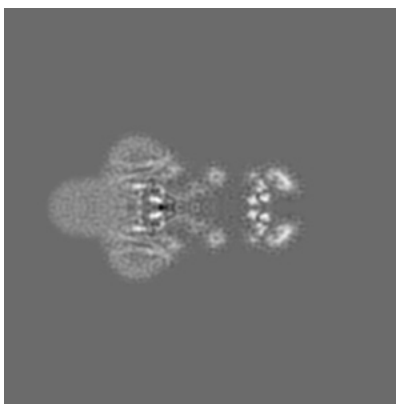
| X Index: 180 | Y Index: 180 | Z Index: 180 |
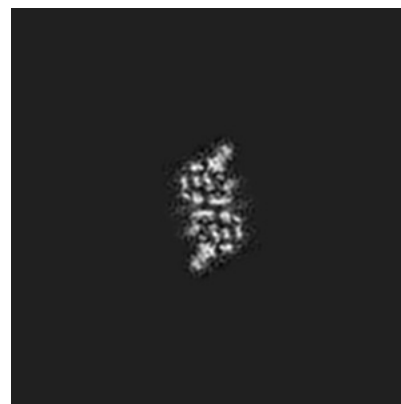
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
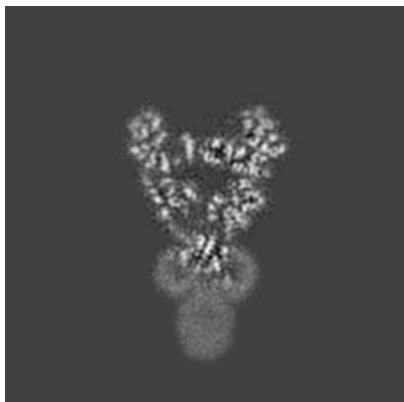
6.3.1 Primary map
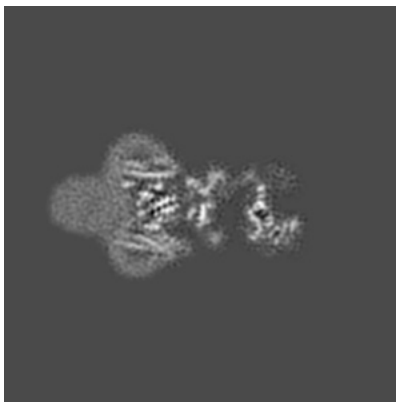
| X Index: 185 | Y Index: 175 | Z Index: 226 |
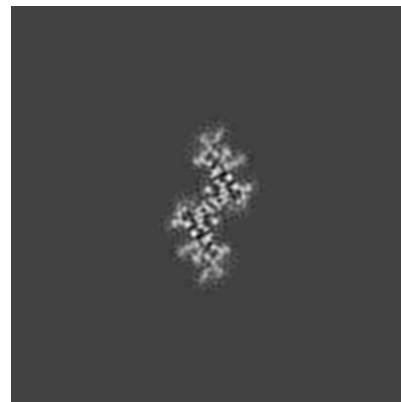
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ
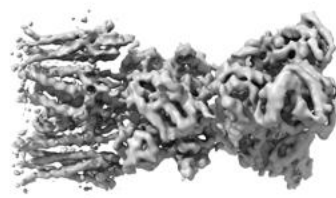
6.4.1 Primary map

| X | Y | Z |
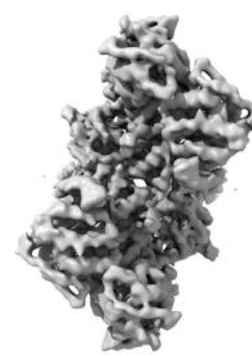
The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ
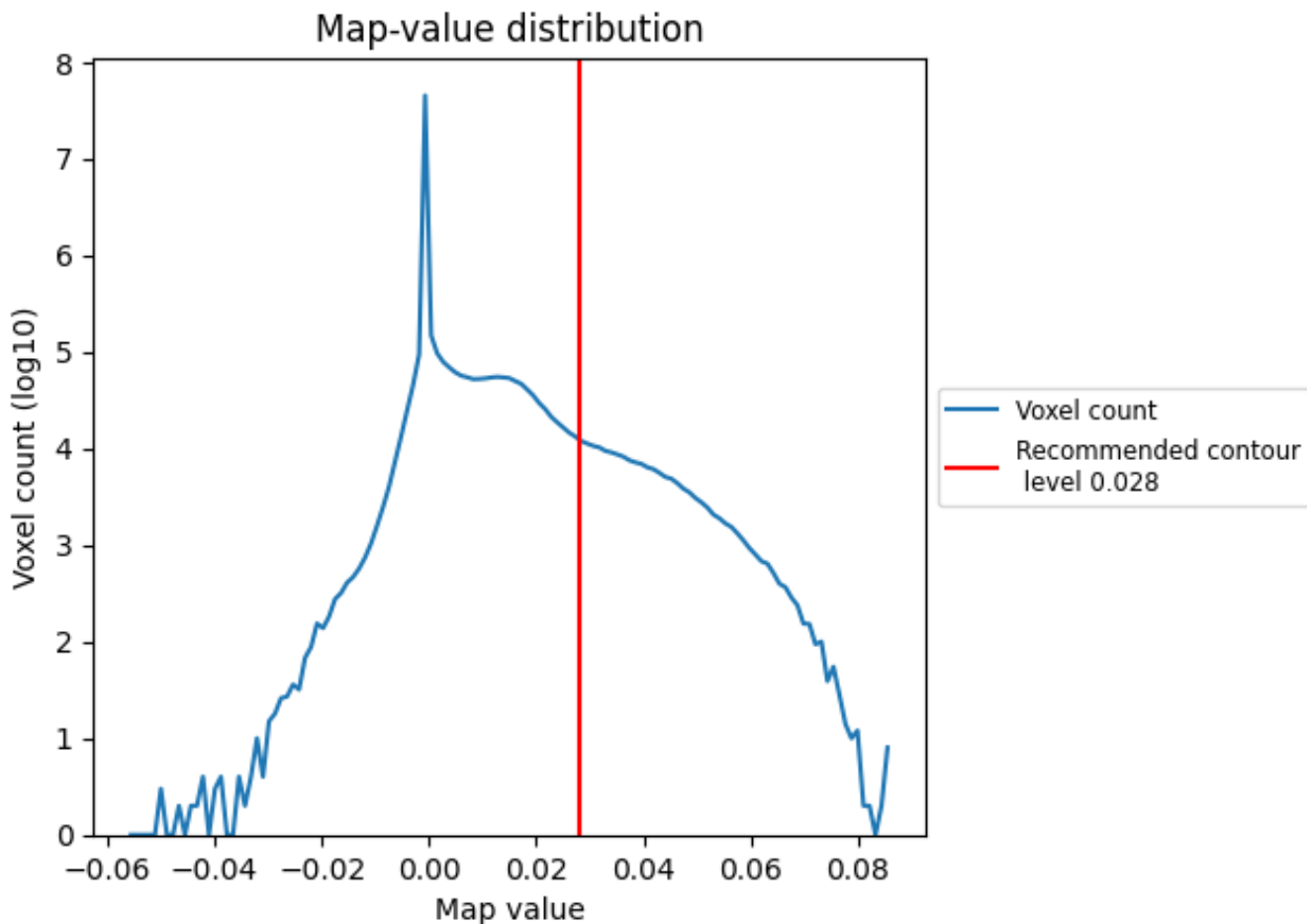
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
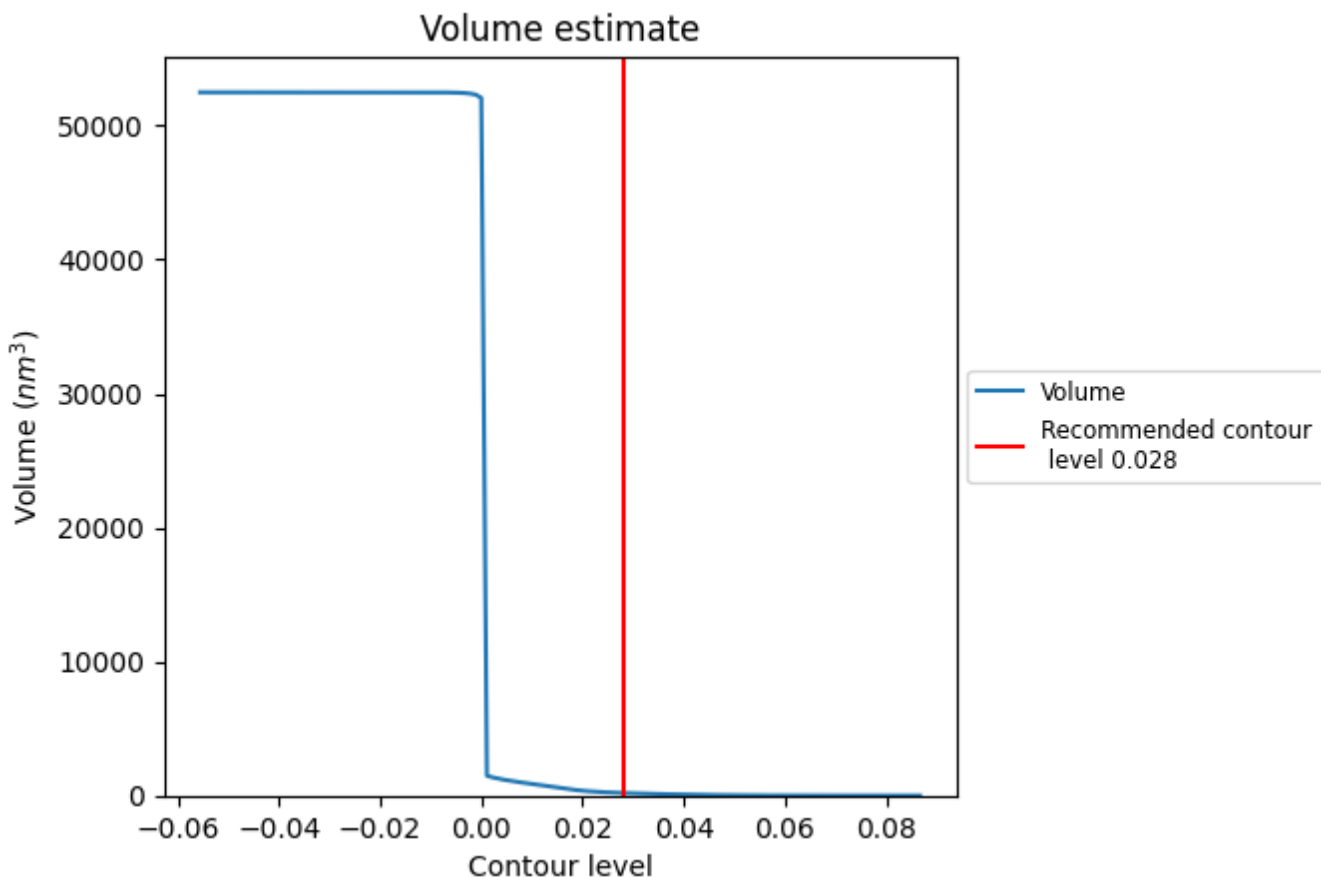
The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 172 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3   Rotationally averaged power spectrum ⓘ

Rotationally averaged power spectrum
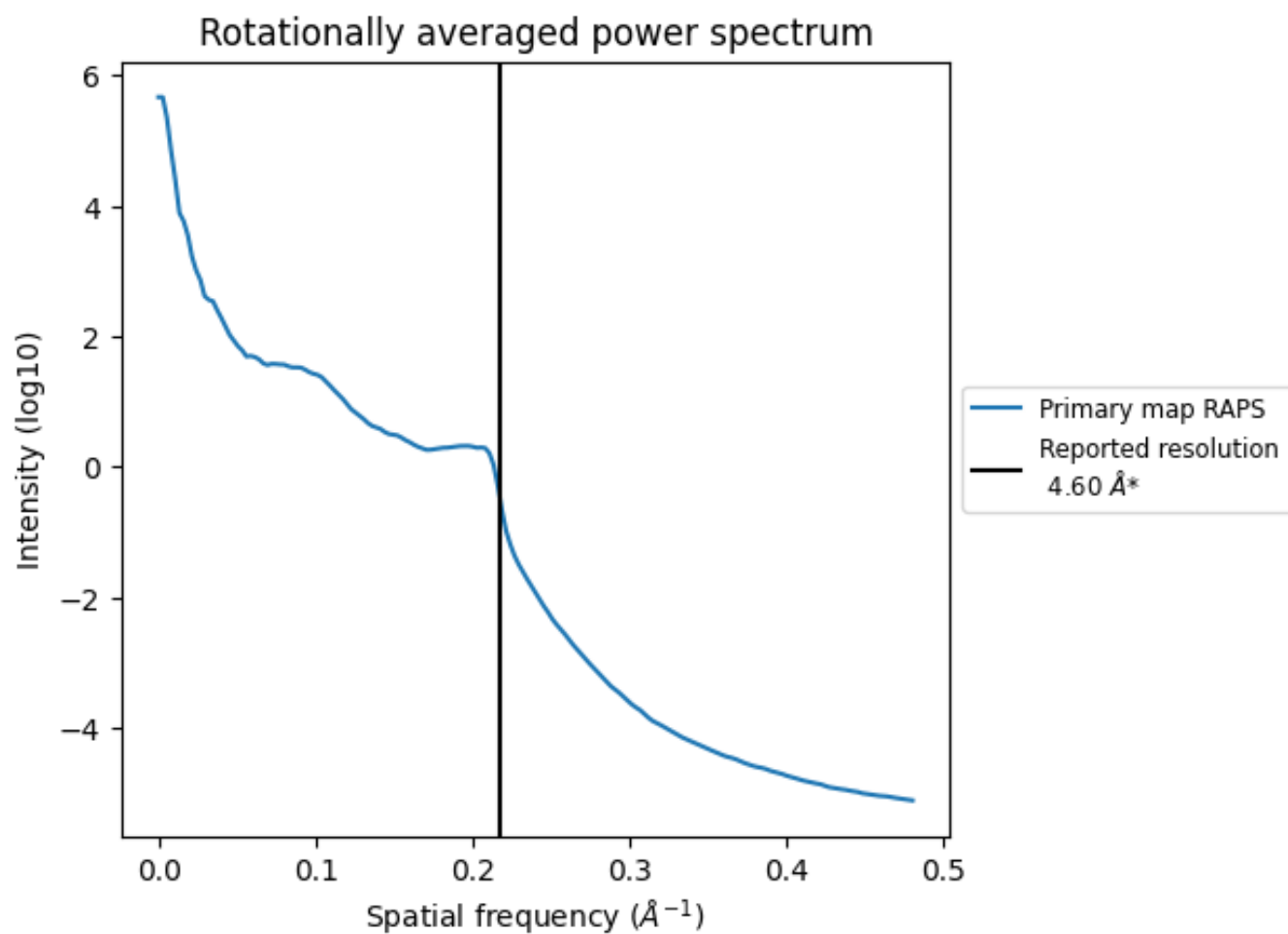
*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8687 and PDB model 5VHY. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

| X | Y | Z |
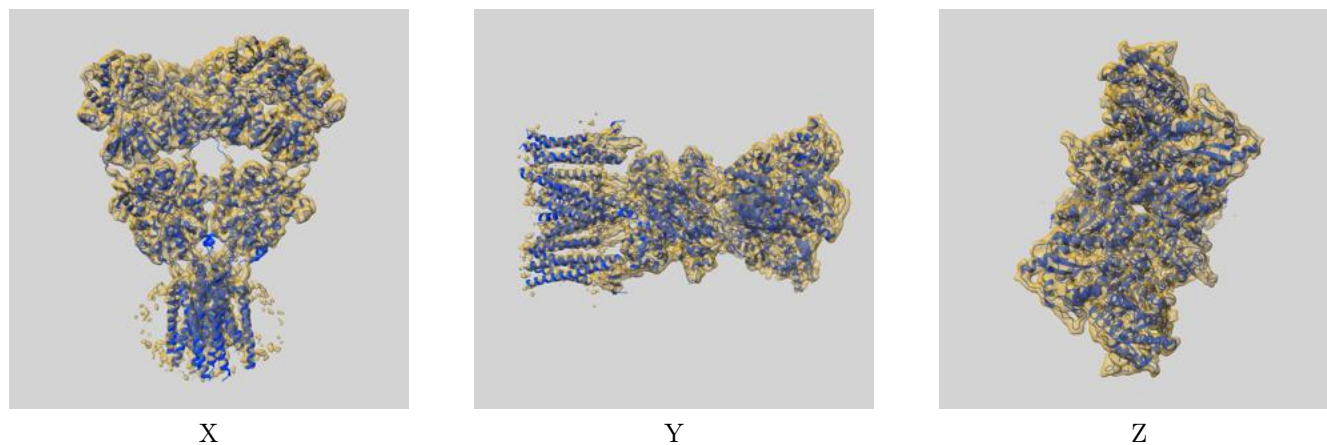
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
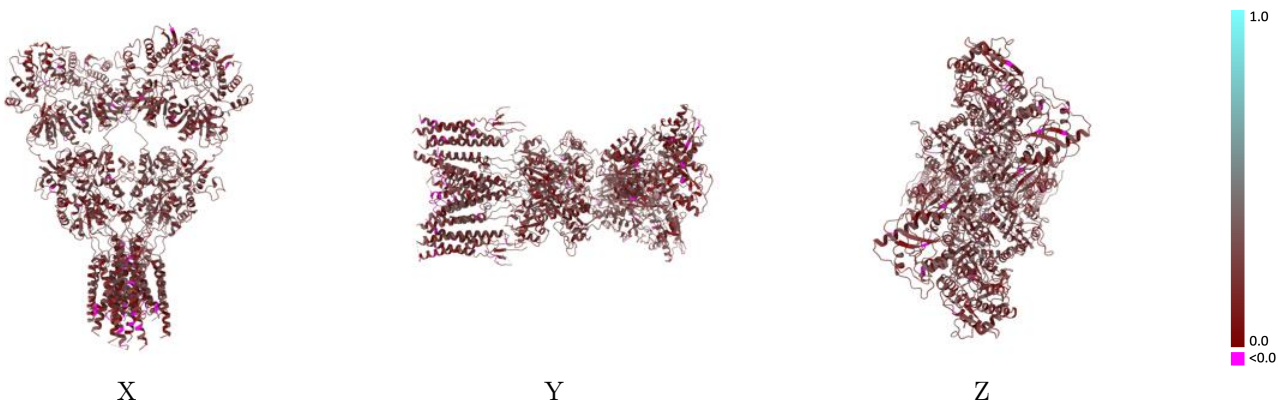
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
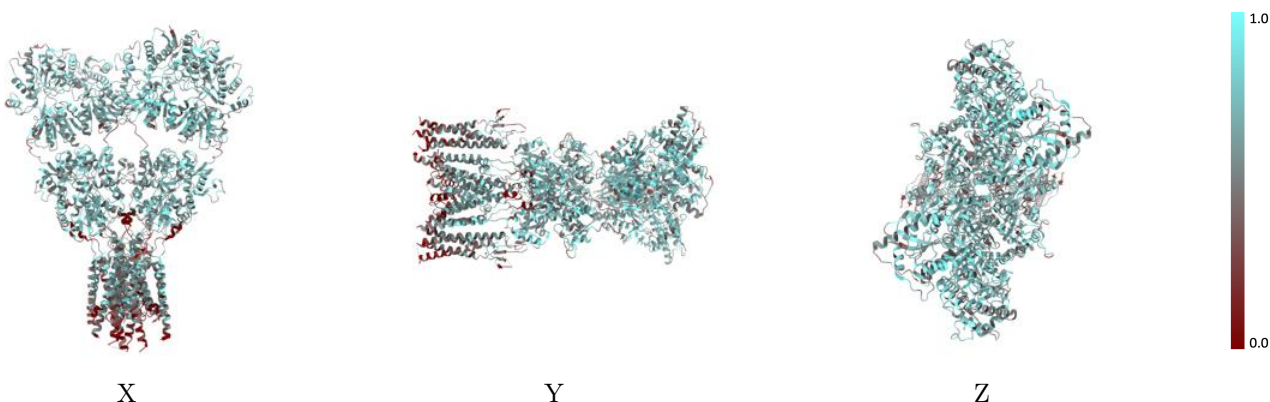
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4   Atom inclusion ⓘ
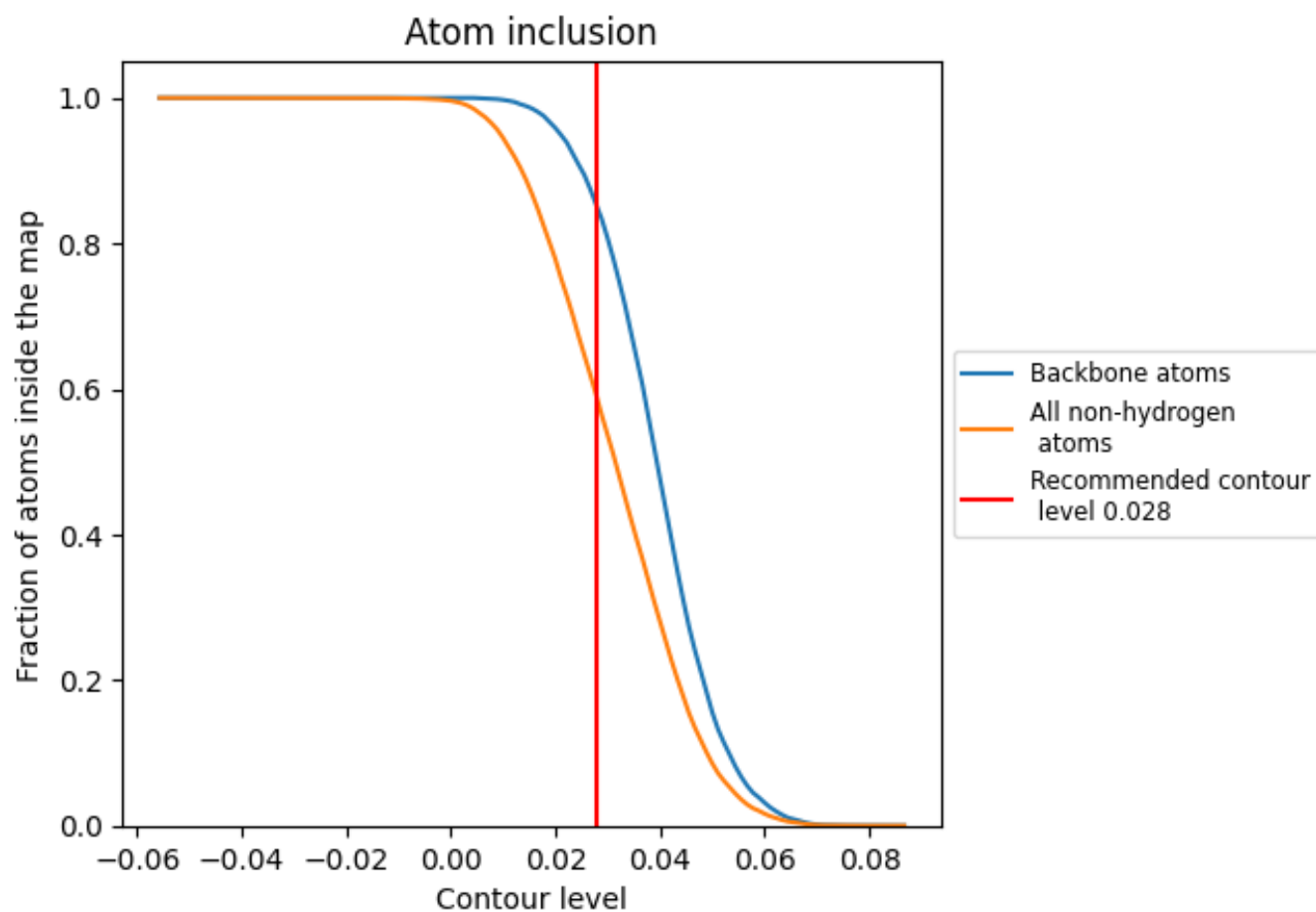
At the recommended contour level, 85% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5870	0.2350
A	0.6091	0.2390
B	0.6044	0.2390
C	0.6101	0.2400
D	0.6040	0.2370
E	0.4162	0.2080
F	0.4068	0.2020

1.0

0.0
<0.0