Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:52 AM EDT

PDB ID	:	5C8J
Title	:	A YidC-like protein in the archaeal plasma membrane
Authors	:	Borowska, M.T.; Dominik, P.K.; Anghel, S.A.; Kossiakoff, A.A.; Keenan, R.J.
Deposited on	:	2015-06-25
Resolution	:	3.50 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 ⓘ 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 ⓘ) were used in the production of this report:

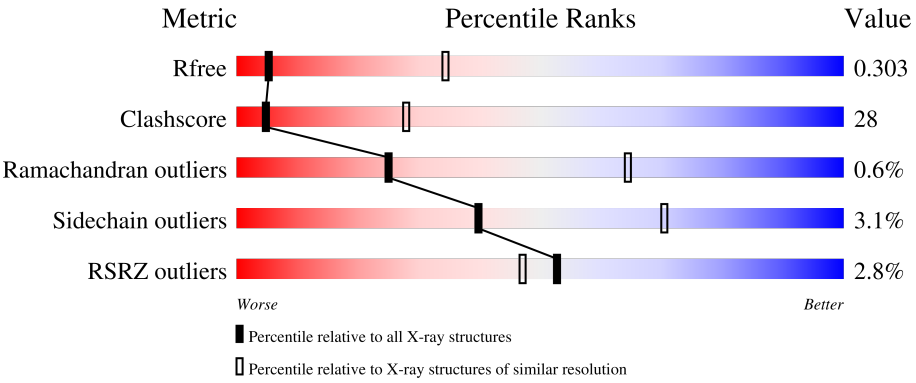
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	239	55% 39%
1	C	239	58% 37%
1	E	239	58% 37%
1	G	239	5% 55% 38%
2	B	215	56% 43%

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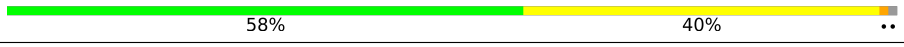
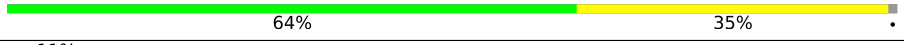
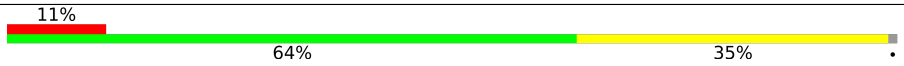
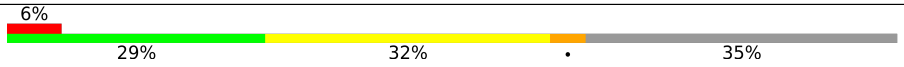
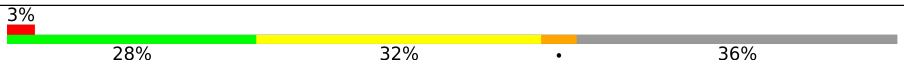
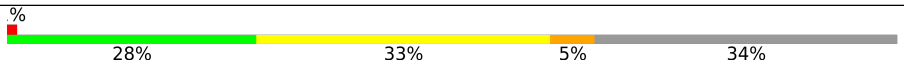
Mol	Chain	Length	Quality of chain
2	D	215	
2	F	215	
2	H	215	
3	I	207	
3	J	207	
3	K	207	
3	L	207	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17889 atoms, of which 46 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 Antibody fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1725	1096	284	338	7			
1	C	230	Total	C	N	O	S	0	0	0
			1733	1100	285	340	8			
1	E	230	Total	C	N	O	S	0	0	0
			1731	1099	285	340	7			
1	G	229	Total	C	N	O	S	0	0	0
			1725	1096	284	338	7			

- Molecule 2 is a protein called Antibody fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1630	1013	277	334	6			
2	D	212	Total	C	N	O	S	0	0	0
			1620	1008	275	331	6			
2	F	213	Total	C	N	O	S	0	0	0
			1623	1010	276	332	5			
2	H	213	Total	C	N	O	S	0	0	0
			1623	1010	276	332	5			

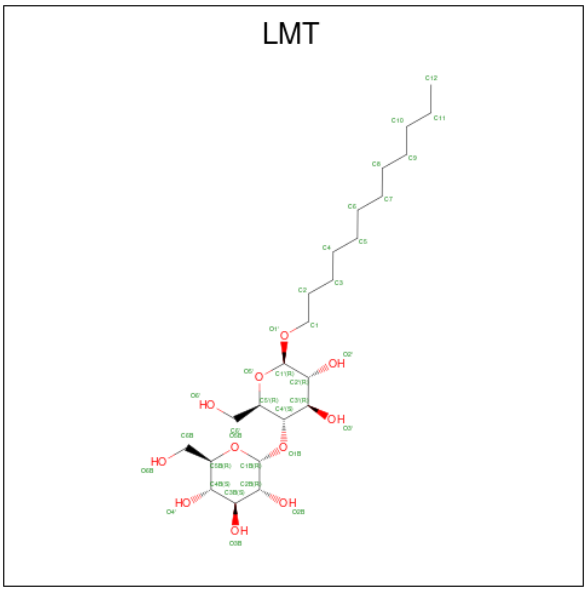
- Molecule 3 is a protein called Protein MJ0480.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	134	Total	C	N	O	S	0	0	0
			1094	760	163	168	3			
3	J	134	Total	C	N	O	S	0	0	0
			1094	760	163	168	3			
3	K	133	Total	C	N	O	S	0	0	0
			1087	756	162	166	3			
3	L	137	Total	C	N	O	S	0	0	0
			1123	779	169	171	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	199	GLY	-	expression tag	UNP Q57904
I	200	SER	-	expression tag	UNP Q57904
I	201	SER	-	expression tag	UNP Q57904
I	202	HIS	-	expression tag	UNP Q57904
I	203	HIS	-	expression tag	UNP Q57904
I	204	HIS	-	expression tag	UNP Q57904
I	205	HIS	-	expression tag	UNP Q57904
I	206	HIS	-	expression tag	UNP Q57904
I	207	HIS	-	expression tag	UNP Q57904
J	199	GLY	-	expression tag	UNP Q57904
J	200	SER	-	expression tag	UNP Q57904
J	201	SER	-	expression tag	UNP Q57904
J	202	HIS	-	expression tag	UNP Q57904
J	203	HIS	-	expression tag	UNP Q57904
J	204	HIS	-	expression tag	UNP Q57904
J	205	HIS	-	expression tag	UNP Q57904
J	206	HIS	-	expression tag	UNP Q57904
J	207	HIS	-	expression tag	UNP Q57904
K	199	GLY	-	expression tag	UNP Q57904
K	200	SER	-	expression tag	UNP Q57904
K	201	SER	-	expression tag	UNP Q57904
K	202	HIS	-	expression tag	UNP Q57904
K	203	HIS	-	expression tag	UNP Q57904
K	204	HIS	-	expression tag	UNP Q57904
K	205	HIS	-	expression tag	UNP Q57904
K	206	HIS	-	expression tag	UNP Q57904
K	207	HIS	-	expression tag	UNP Q57904
L	199	GLY	-	expression tag	UNP Q57904
L	200	SER	-	expression tag	UNP Q57904
L	201	SER	-	expression tag	UNP Q57904
L	202	HIS	-	expression tag	UNP Q57904
L	203	HIS	-	expression tag	UNP Q57904
L	204	HIS	-	expression tag	UNP Q57904
L	205	HIS	-	expression tag	UNP Q57904
L	206	HIS	-	expression tag	UNP Q57904
L	207	HIS	-	expression tag	UNP Q57904

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



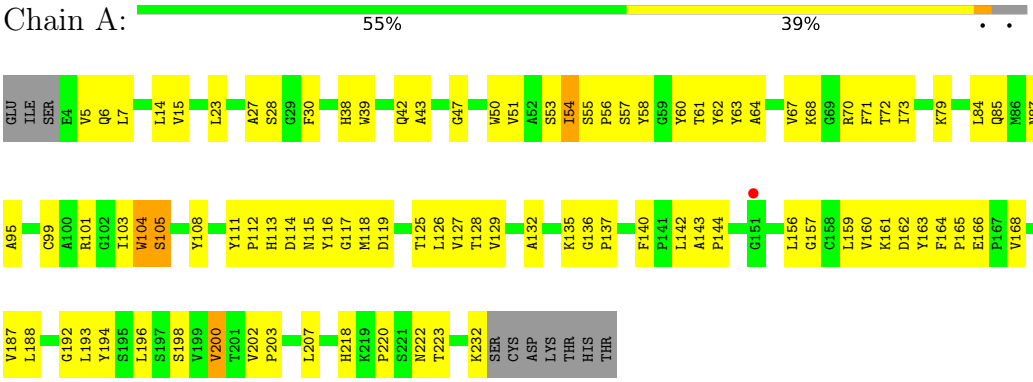
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	L	1	81	24	46	11	0	0

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.

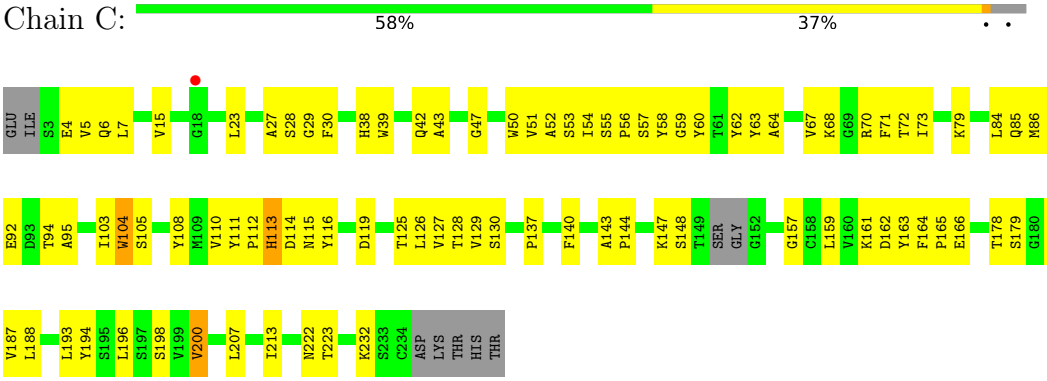
• Molecule 1: Antibody fragment, heavy chain

Chain A:



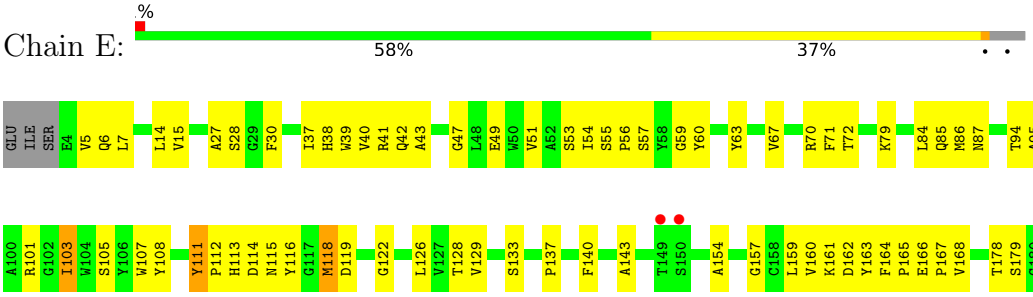
• Molecule 1: Antibody fragment, heavy chain

Chain C:

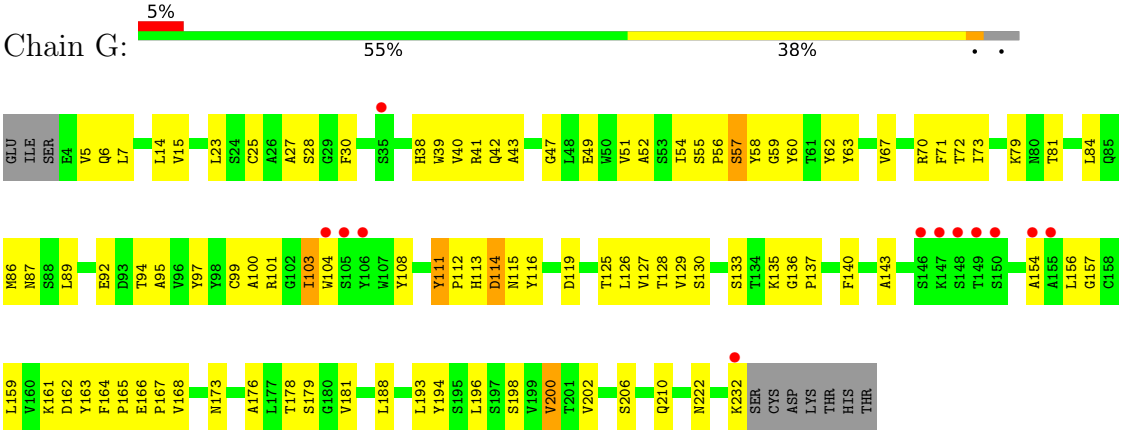


• Molecule 1: Antibody fragment, heavy chain

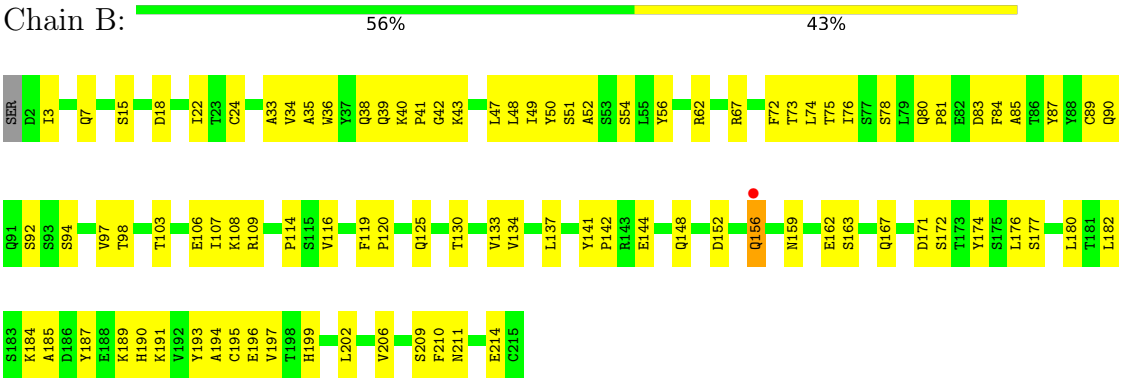
Chain E:



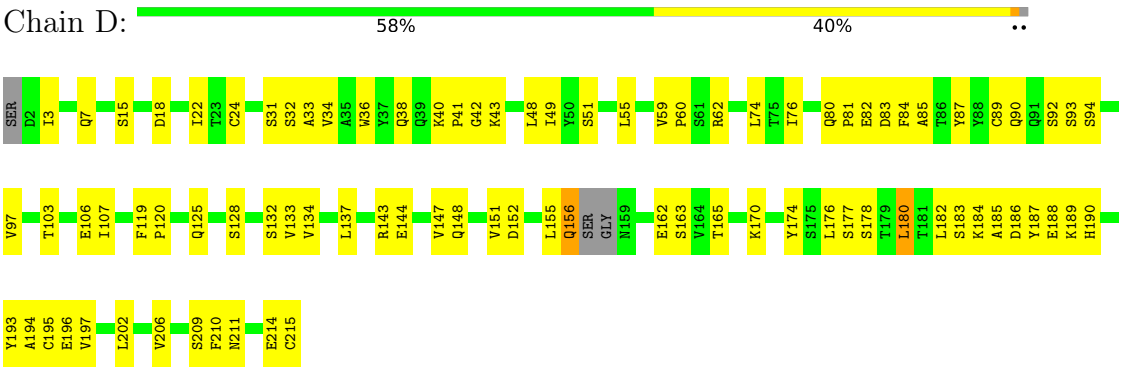
• Molecule 1: Antibody fragment, heavy chain



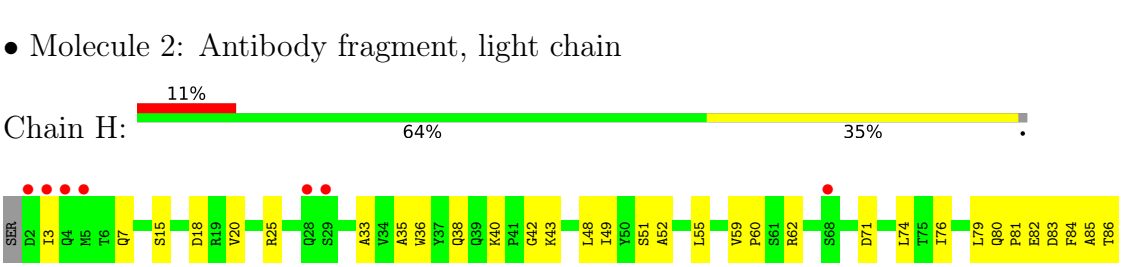
• Molecule 2: Antibody fragment, light chain

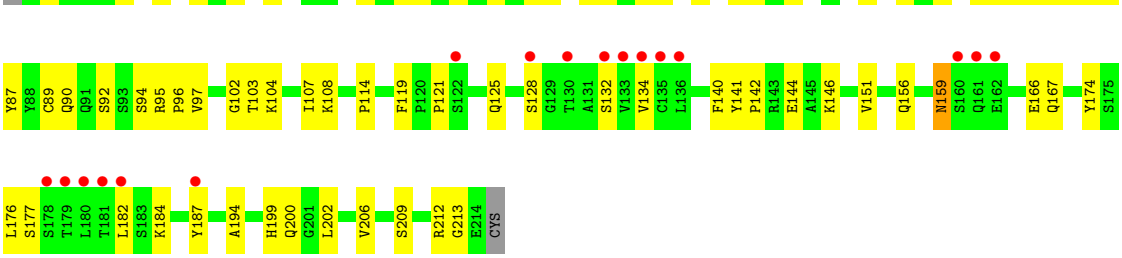


• Molecule 2: Antibody fragment, light chain



• Molecule 2: Antibody fragment, light chain



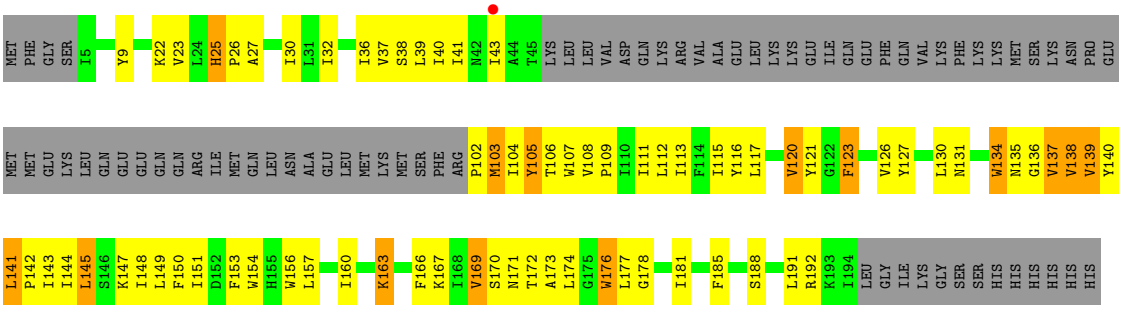


• Molecule 2: Antibody fragment, light chain

Chain H:

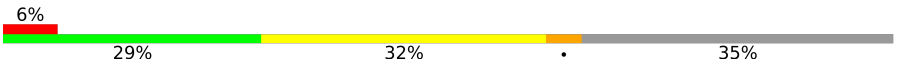
• Molecule 3: Protein MJ0480

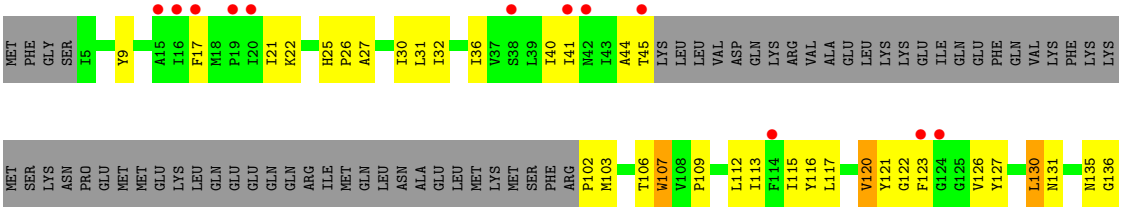
Chain I:

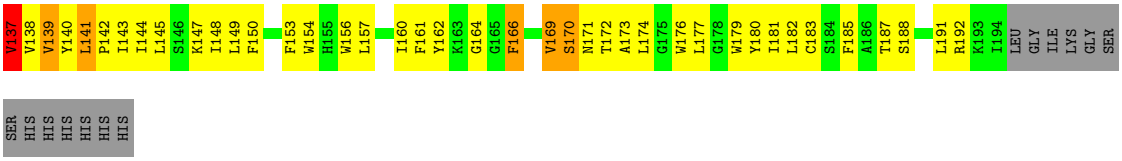


• Molecule 3: Protein MJ0480

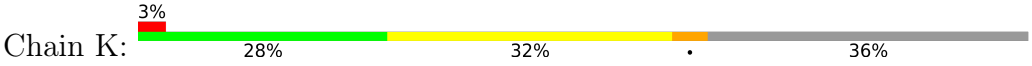
Chain J:

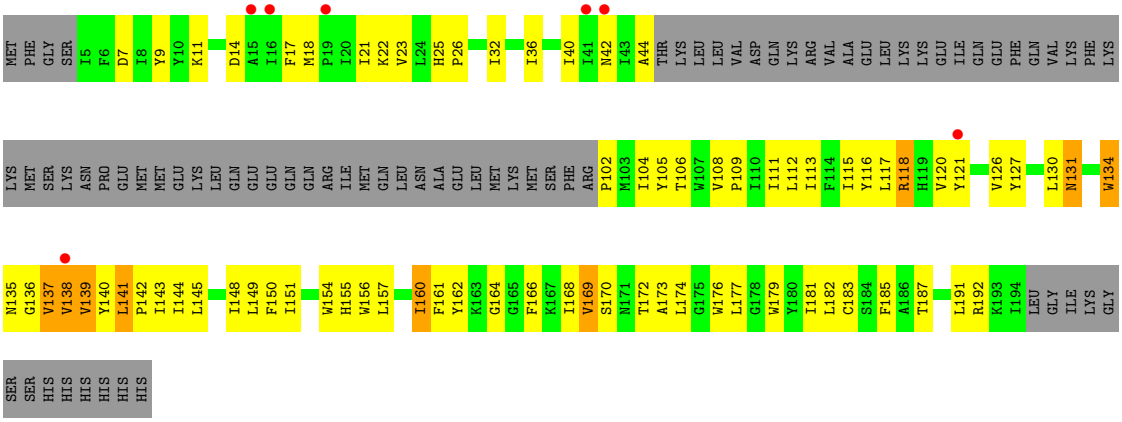




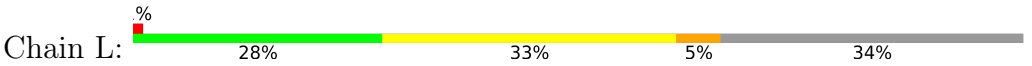


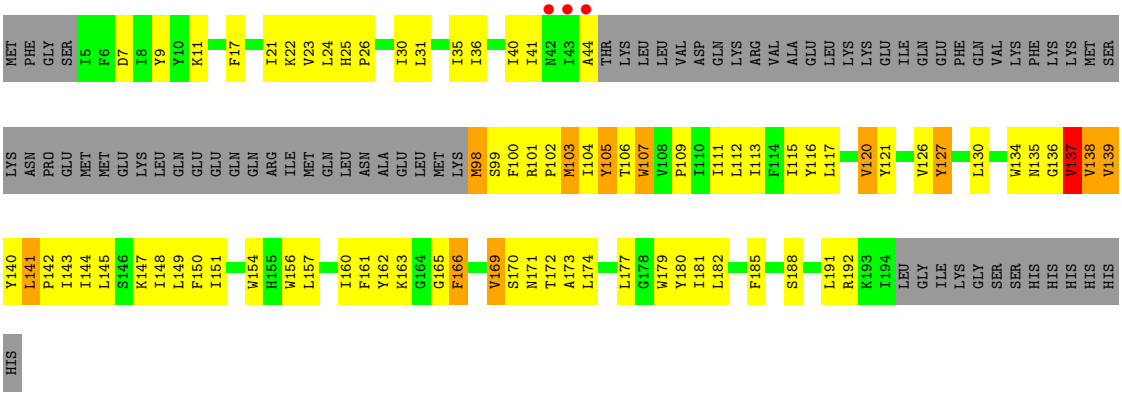
• Molecule 3: Protein MJ0480





• Molecule 3: Protein MJ0480





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.25Å 251.42Å 96.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.77 – 3.50 96.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	86.2 (89.77-3.50) 86.3 (96.11-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.253 , 0.302 0.253 , 0.303	Depositor DCC
R_{free} test set	2448 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	17889	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.31% 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

5.1 Standard geometry

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

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	0.26	0/1774	0.44	0/2422
1	C	0.27	0/1781	0.45	0/2430
1	E	0.26	0/1780	0.43	0/2430
1	G	0.26	0/1774	0.44	0/2422
2	B	0.25	0/1663	0.44	0/2255
2	D	0.24	0/1652	0.43	0/2239
2	F	0.25	0/1656	0.42	0/2247
2	H	0.25	0/1656	0.43	0/2247
3	I	0.25	0/1131	0.39	0/1546
3	J	0.26	0/1131	0.39	0/1546
3	K	0.24	0/1124	0.37	0/1536
3	L	0.25	0/1161	0.39	0/1585
All	All	0.25	0/18283	0.42	0/24905

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	1725	0	1660	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1733	0	1665	88	0
1	E	1731	0	1665	83	0
1	G	1725	0	1660	96	0
2	B	1630	0	1590	82	0
2	D	1620	0	1580	82	0
2	F	1623	0	1585	66	0
2	H	1623	0	1585	69	0
3	I	1094	0	1150	113	0
3	J	1094	0	1150	97	0
3	K	1087	0	1143	99	0
3	L	1123	0	1178	108	0
4	L	35	46	44	1	0
All	All	17843	46	17655	983	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 28.

All (983) 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)
3:L:41:ILE:HD11	3:L:106:THR:HB	1.34	1.06
1:E:103:ILE:HD13	1:E:119:ASP:HB2	1.34	1.05
1:G:137:PRO:HB3	1:G:163:TYR:HB3	1.37	1.03
1:A:135:LYS:HD2	1:A:193:LEU:HD11	1.44	0.99
3:I:148:ILE:HG23	3:L:150:PHE:HB3	1.46	0.97
3:K:109:PRO:HA	3:K:112:LEU:HG	1.48	0.95
2:F:116:VAL:HG21	2:F:197:VAL:HG21	1.50	0.94
3:K:118:ARG:HH11	3:K:118:ARG:HG2	1.29	0.93
3:L:120:VAL:HA	3:L:126:VAL:HG12	1.50	0.93
3:I:173:ALA:HB1	3:L:137:VAL:CG1	2.00	0.92
1:A:137:PRO:HB3	1:A:163:TYR:HB3	1.52	0.91
3:I:22:LYS:HG2	3:I:130:LEU:HD23	1.50	0.91
3:I:103:MET:HG3	3:I:163:LYS:NZ	1.86	0.91
3:L:103:MET:SD	3:L:163:LYS:NZ	2.44	0.90
1:C:137:PRO:HB3	1:C:163:TYR:HB3	1.53	0.88
3:I:169:VAL:HG12	3:I:170:SER:H	1.39	0.87
3:K:141:LEU:HB3	3:K:145:LEU:HD23	1.55	0.86
2:H:7:GLN:NE2	2:H:103:THR:OG1	2.08	0.86
1:A:38:HIS:HD1	1:A:53:SER:HG	1.16	0.85
1:C:143:ALA:HB2	1:C:232:LYS:HE2	1.57	0.84
3:I:141:LEU:HD12	3:I:142:PRO:HD2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:TRP:HA	1:G:108:TYR:HE2	1.43	0.84
3:K:9:TYR:HE2	3:K:116:TYR:HB2	1.43	0.83
3:K:169:VAL:HG12	3:K:170:SER:H	1.40	0.83
2:H:15:SER:N	2:H:18:ASP:OD2	2.12	0.81
2:B:141:TYR:CD2	2:B:142:PRO:HA	2.15	0.81
1:G:188:LEU:HD13	1:G:194:TYR:HE2	1.45	0.81
1:E:166:GLU:HG3	1:E:194:TYR:HD1	1.43	0.81
1:C:166:GLU:HG3	1:C:194:TYR:CD1	2.15	0.81
3:J:41:ILE:HD11	3:J:106:THR:HB	1.62	0.80
4:L:301:LMT:O2B	4:L:301:LMT:O3'	1.99	0.80
1:C:94:THR:HG23	1:C:128:THR:HA	1.62	0.80
1:E:114:ASP:HB3	1:E:116:TYR:CE1	2.17	0.80
3:J:120:VAL:HA	3:J:126:VAL:HG12	1.64	0.80
3:J:169:VAL:HG12	3:J:170:SER:H	1.47	0.79
3:L:169:VAL:HG12	3:L:170:SER:H	1.47	0.79
2:F:133:VAL:HG13	2:F:180:LEU:HB3	1.65	0.79
1:G:115:ASN:HD21	2:H:95:ARG:HH12	1.31	0.79
3:J:137:VAL:CG1	3:K:173:ALA:HB1	2.13	0.79
1:E:105:SER:HB3	1:E:108:TYR:HE2	1.46	0.79
3:L:141:LEU:HB3	3:L:145:LEU:HD23	1.65	0.78
2:D:184:LYS:HE2	2:D:188:GLU:OE2	1.84	0.78
3:L:142:PRO:O	3:L:143:ILE:HG12	1.83	0.78
1:C:56:PRO:O	1:C:57:SER:OG	2.01	0.77
3:I:137:VAL:HG21	3:I:140:TYR:CE1	2.19	0.77
2:B:106:GLU:OE1	2:B:174:TYR:OH	2.03	0.77
1:A:115:ASN:HB2	2:B:92:SER:HB3	1.66	0.76
3:I:173:ALA:HB1	3:L:137:VAL:HG12	1.65	0.76
1:E:166:GLU:HG3	1:E:194:TYR:CD1	2.20	0.76
3:J:120:VAL:HG13	3:J:121:TYR:CD2	2.20	0.76
3:L:109:PRO:HA	3:L:112:LEU:HG	1.66	0.76
1:E:137:PRO:HB3	1:E:163:TYR:HB3	1.66	0.76
1:C:188:LEU:HD13	1:C:194:TYR:HE2	1.51	0.76
3:L:171:ASN:OD1	3:L:172:THR:N	2.18	0.76
2:F:144:GLU:N	2:F:144:GLU:OE1	2.18	0.76
1:C:166:GLU:HG3	1:C:194:TYR:HD1	1.50	0.75
1:A:94:THR:HG23	1:A:128:THR:HA	1.68	0.75
3:L:98:MET:SD	3:L:98:MET:N	2.60	0.75
2:B:84:PHE:CZ	2:B:107:ILE:HG13	2.21	0.75
3:L:141:LEU:HG	3:L:144:ILE:HD11	1.68	0.75
3:I:123:PHE:HE2	3:L:166:PHE:N	1.85	0.75
3:J:148:ILE:HG23	3:K:150:PHE:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TRP:HA	1:C:108:TYR:CE2	2.22	0.74
2:B:148:GLN:HB3	2:B:196:GLU:HB3	1.68	0.74
3:K:120:VAL:HA	3:K:126:VAL:HG12	1.69	0.74
2:F:133:VAL:CG1	2:F:180:LEU:HB3	2.18	0.74
1:E:56:PRO:O	1:E:57:SER:OG	2.04	0.73
1:E:105:SER:HB3	1:E:108:TYR:CE2	2.23	0.73
3:I:112:LEU:HA	3:I:115:ILE:HD11	1.70	0.73
3:L:112:LEU:HA	3:L:115:ILE:HD11	1.70	0.73
2:D:182:LEU:CD1	2:D:187:TYR:HB2	2.18	0.73
2:F:106:GLU:OE1	2:F:174:TYR:OH	2.04	0.73
3:K:109:PRO:HA	3:K:112:LEU:CG	2.18	0.73
2:B:156:GLN:HA	2:B:156:GLN:HE21	1.54	0.73
1:E:143:ALA:HB2	1:E:232:LYS:HE2	1.70	0.73
3:J:138:VAL:CG2	3:J:139:VAL:HG12	2.18	0.73
1:G:166:GLU:HG2	1:G:194:TYR:CD1	2.23	0.73
3:I:120:VAL:HA	3:I:126:VAL:HG12	1.70	0.72
2:D:148:GLN:HB3	2:D:196:GLU:HB3	1.71	0.72
2:H:151:VAL:HB	2:H:156:GLN:HE21	1.54	0.72
3:J:142:PRO:O	3:J:143:ILE:HG12	1.87	0.72
2:F:143:ARG:HB2	2:F:174:TYR:CE2	2.25	0.71
3:K:142:PRO:O	3:K:143:ILE:HG12	1.89	0.71
3:J:135:ASN:OD1	3:J:137:VAL:HG23	1.91	0.71
2:D:3:ILE:HD12	2:D:94:SER:HB2	1.73	0.71
3:J:141:LEU:HG	3:J:144:ILE:HD11	1.73	0.70
1:A:56:PRO:O	1:A:57:SER:OG	2.05	0.70
2:D:214:GLU:HG2	2:D:215:CYS:H	1.56	0.70
1:E:188:LEU:HD12	1:E:194:TYR:HE2	1.55	0.70
1:G:104:TRP:HA	1:G:108:TYR:CE2	2.26	0.70
2:H:84:PHE:CE2	2:H:107:ILE:HD11	2.26	0.70
1:E:211:THR:HG23	1:E:228:LYS:HE3	1.72	0.70
3:J:137:VAL:HG11	3:J:140:TYR:CE1	2.27	0.70
1:G:56:PRO:O	1:G:57:SER:OG	2.04	0.70
3:L:138:VAL:HG22	3:L:139:VAL:HG12	1.74	0.70
1:C:54:ILE:HD12	1:C:60:TYR:O	1.92	0.70
2:F:116:VAL:CG2	2:F:197:VAL:HG21	2.21	0.70
1:G:54:ILE:HD12	1:G:60:TYR:O	1.91	0.70
3:I:171:ASN:OD1	3:I:172:THR:N	2.25	0.70
3:K:118:ARG:HH11	3:K:118:ARG:CG	2.03	0.69
2:D:36:TRP:CZ3	2:D:89:CYS:HB3	2.26	0.69
1:A:166:GLU:HG3	1:A:194:TYR:CD1	2.26	0.69
2:B:202:LEU:HD13	2:B:206:VAL:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:HB3	1:A:116:TYR:CE2	2.27	0.69
1:A:143:ALA:HB2	1:A:232:LYS:HE2	1.73	0.69
2:H:84:PHE:CZ	2:H:107:ILE:HD11	2.28	0.69
3:I:120:VAL:HG13	3:I:121:TYR:CD2	2.27	0.69
2:B:36:TRP:CZ3	2:B:89:CYS:HB3	2.27	0.69
2:D:155:LEU:O	2:D:156:GLN:NE2	2.26	0.69
2:H:25:ARG:HG3	2:H:71:ASP:OD2	1.93	0.69
1:A:135:LYS:CD	1:A:193:LEU:HD11	2.23	0.69
1:C:114:ASP:HB3	1:C:116:TYR:CE2	2.27	0.69
2:H:40:LYS:HD3	2:H:85:ALA:HB2	1.73	0.69
3:I:103:MET:HG3	3:I:163:LYS:HZ3	1.55	0.69
1:E:103:ILE:HD13	1:E:119:ASP:CB	2.17	0.68
1:E:5:VAL:HG21	1:E:101:ARG:HH11	1.58	0.68
2:H:144:GLU:OE1	2:H:144:GLU:N	2.24	0.68
3:I:138:VAL:HG22	3:I:139:VAL:HG12	1.75	0.68
3:I:126:VAL:O	3:I:130:LEU:HD13	1.93	0.68
3:L:137:VAL:HG11	3:L:140:TYR:CE1	2.28	0.68
1:A:38:HIS:ND1	1:A:53:SER:OG	2.16	0.68
3:J:153:PHE:CZ	3:J:157:LEU:HD12	2.28	0.68
3:K:22:LYS:HG2	3:K:130:LEU:CD2	2.24	0.68
1:A:111:TYR:HD1	3:I:23:VAL:HG12	1.59	0.68
2:B:167:GLN:OE1	2:B:172:SER:HB3	1.92	0.68
2:D:143:ARG:HB2	2:D:174:TYR:CE2	2.28	0.68
3:I:141:LEU:HD12	3:I:142:PRO:CD	2.23	0.68
3:I:174:LEU:HD23	3:I:178:GLY:C	2.15	0.68
3:I:123:PHE:HE2	3:L:166:PHE:H	1.41	0.67
3:I:174:LEU:HD11	3:L:145:LEU:HD11	1.76	0.67
1:E:7:LEU:HD23	1:E:99:CYS:SG	2.34	0.67
2:H:33:ALA:HA	2:H:51:SER:HA	1.77	0.67
3:I:9:TYR:HE2	3:I:116:TYR:HB2	1.59	0.67
3:J:150:PHE:HB3	3:K:148:ILE:HG23	1.76	0.67
1:G:59:GLY:O	3:K:134:TRP:N	2.23	0.67
2:F:62:ARG:NE	2:F:83:ASP:OD2	2.28	0.67
1:A:162:ASP:HA	1:A:193:LEU:HB3	1.78	0.66
2:D:156:GLN:HA	2:D:156:GLN:HE21	1.60	0.66
3:J:22:LYS:HD3	3:J:130:LEU:HD21	1.77	0.66
2:B:156:GLN:HB3	2:B:159:ASN:HD21	1.61	0.66
1:C:6:GLN:O	1:C:7:LEU:HD12	1.95	0.66
1:E:54:ILE:HD12	1:E:60:TYR:O	1.95	0.66
1:C:188:LEU:HD13	1:C:194:TYR:CE2	2.29	0.66
1:C:103:ILE:HB	1:C:119:ASP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:CD1	1:C:161:LYS:HB2	2.26	0.66
3:J:22:LYS:HG2	3:J:130:LEU:HD22	1.77	0.66
1:E:94:THR:HG23	1:E:128:THR:HA	1.77	0.66
1:G:114:ASP:HB3	1:G:116:TYR:CE2	2.31	0.66
3:I:141:LEU:HG	3:I:144:ILE:CG1	2.25	0.66
2:B:74:LEU:HD23	2:B:75:THR:N	2.11	0.66
1:G:94:THR:HG23	1:G:128:THR:HA	1.77	0.66
2:D:133:VAL:CG1	2:D:180:LEU:HB3	2.25	0.65
2:D:42:GLY:O	2:D:43:LYS:HD2	1.97	0.65
3:L:120:VAL:HG13	3:L:121:TYR:CD2	2.32	0.65
1:C:38:HIS:HD1	1:C:53:SER:HG	1.43	0.65
3:L:9:TYR:HE2	3:L:116:TYR:HB2	1.60	0.65
2:H:81:PRO:HA	2:H:84:PHE:CE2	2.31	0.65
2:H:104:LYS:NZ	2:H:166:GLU:OE1	2.26	0.65
3:I:137:VAL:HG21	3:I:140:TYR:CD1	2.32	0.65
3:K:173:ALA:O	3:K:174:LEU:HG	1.97	0.65
2:B:83:ASP:O	2:B:87:TYR:OH	2.10	0.65
1:G:166:GLU:HG2	1:G:194:TYR:HD1	1.60	0.65
3:J:141:LEU:HB3	3:J:145:LEU:HD23	1.77	0.65
1:A:188:LEU:HD13	1:A:194:TYR:HE2	1.61	0.64
3:I:142:PRO:O	3:I:143:ILE:HG22	1.97	0.64
3:I:22:LYS:HG2	3:I:130:LEU:CD2	2.27	0.64
3:K:136:GLY:O	3:K:137:VAL:HB	1.98	0.64
2:B:42:GLY:O	2:B:43:LYS:HD2	1.97	0.64
1:C:111:TYR:CE1	3:L:23:VAL:HG12	2.31	0.64
1:G:130:SER:HG	1:G:164:PHE:HZ	1.44	0.64
1:E:159:LEU:CD1	1:E:161:LYS:HB2	2.27	0.64
2:H:182:LEU:CD1	2:H:187:TYR:HB2	2.27	0.64
3:L:141:LEU:HD12	3:L:144:ILE:HG12	1.77	0.64
1:A:111:TYR:CD1	3:I:23:VAL:HG12	2.33	0.64
1:G:43:ALA:HA	1:G:95:ALA:HB2	1.81	0.63
3:L:41:ILE:HD11	3:L:106:THR:CB	2.21	0.63
1:C:162:ASP:HA	1:C:193:LEU:HB3	1.80	0.63
1:G:114:ASP:HB3	1:G:116:TYR:HE2	1.63	0.63
1:A:58:TYR:O	3:I:134:TRP:HA	1.98	0.63
3:J:138:VAL:HG22	3:J:139:VAL:HG12	1.80	0.63
3:I:141:LEU:CD2	3:I:144:ILE:HD11	2.29	0.63
1:A:51:VAL:HG13	1:A:67:VAL:HG21	1.81	0.62
1:G:62:TYR:OH	1:G:113:HIS:ND1	2.26	0.62
3:J:135:ASN:OD1	3:J:136:GLY:N	2.32	0.62
3:L:25:HIS:HD2	3:L:26:PRO:HD2	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:100:PHE:O	3:L:104:ILE:HG12	1.99	0.62
2:H:176:LEU:HD23	2:H:177:SER:N	2.13	0.62
2:F:38:GLN:CB	2:F:48:LEU:HD21	2.29	0.62
2:F:42:GLY:O	2:F:43:LYS:HD2	1.98	0.62
2:H:83:ASP:O	2:H:87:TYR:OH	2.07	0.62
3:K:141:LEU:HD13	3:K:142:PRO:HD2	1.82	0.62
1:G:112:PRO:HG2	1:G:113:HIS:CD2	2.34	0.62
1:C:58:TYR:O	3:L:134:TRP:HA	1.98	0.62
2:D:38:GLN:HB3	2:D:48:LEU:HD21	1.82	0.62
3:I:102:PRO:HG2	3:I:103:MET:SD	2.39	0.62
1:C:43:ALA:HA	1:C:95:ALA:HB2	1.82	0.62
1:C:105:SER:O	1:C:108:TYR:HD2	1.83	0.62
1:G:137:PRO:CB	1:G:163:TYR:HB3	2.22	0.62
3:K:137:VAL:HG11	3:K:140:TYR:CE1	2.35	0.62
2:D:119:PHE:HB2	2:D:134:VAL:HB	1.80	0.61
3:K:138:VAL:HG22	3:K:139:VAL:HG12	1.81	0.61
2:H:167:GLN:HG2	2:H:174:TYR:CE1	2.35	0.61
1:A:57:SER:O	3:I:135:ASN:ND2	2.33	0.61
2:F:74:LEU:HD23	2:F:75:THR:N	2.15	0.61
3:I:30:ILE:HD11	3:I:121:TYR:HE1	1.65	0.61
3:K:118:ARG:HG2	3:K:118:ARG:NH1	2.09	0.61
3:J:138:VAL:HG23	3:J:139:VAL:HG12	1.81	0.61
1:C:70:ARG:HB3	1:C:87:ASN:O	2.01	0.61
1:G:54:ILE:HG13	1:G:55:SER:N	2.15	0.61
3:I:148:ILE:CG2	3:L:150:PHE:HB3	2.25	0.61
3:L:141:LEU:CB	3:L:145:LEU:HD23	2.31	0.61
1:A:188:LEU:HD13	1:A:194:TYR:CE2	2.36	0.61
1:E:162:ASP:HA	1:E:193:LEU:HB3	1.83	0.61
1:E:187:VAL:CG1	2:F:163:SER:HB2	2.31	0.61
1:G:23:LEU:HD22	1:G:125:THR:HG21	1.83	0.61
2:B:144:GLU:N	2:B:144:GLU:OE1	2.32	0.60
3:I:135:ASN:HD22	3:L:169:VAL:HG11	1.66	0.60
2:B:84:PHE:CE1	2:B:107:ILE:HG13	2.36	0.60
3:J:191:LEU:HD12	3:J:192:ARG:N	2.16	0.60
3:I:112:LEU:HA	3:I:115:ILE:CD1	2.30	0.60
3:J:9:TYR:HE2	3:J:116:TYR:HB2	1.65	0.60
3:I:137:VAL:CG2	3:L:173:ALA:HB1	2.31	0.60
3:J:102:PRO:HG2	3:J:103:MET:SD	2.42	0.60
1:C:184:PHE:HA	2:D:165:THR:HG22	1.82	0.60
1:C:27:ALA:HB1	1:C:30:PHE:CE1	2.37	0.60
1:C:54:ILE:HG13	1:C:55:SER:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ASN:OD1	2:H:95:ARG:NH2	2.34	0.60
2:H:38:GLN:HB2	2:H:48:LEU:HD11	1.84	0.60
2:B:125:GLN:HG2	2:B:130:THR:O	2.01	0.60
2:D:194:ALA:HB2	2:D:209:SER:HB2	1.84	0.60
2:F:38:GLN:HB3	2:F:48:LEU:HD21	1.82	0.60
3:J:30:ILE:HD11	3:J:121:TYR:HE1	1.65	0.60
3:K:191:LEU:HD12	3:K:192:ARG:N	2.16	0.60
3:L:112:LEU:HA	3:L:115:ILE:CD1	2.31	0.60
2:F:40:LYS:HD3	2:F:85:ALA:HB2	1.81	0.60
2:F:176:LEU:HD23	2:F:177:SER:N	2.16	0.60
1:G:126:LEU:HD22	1:G:127:VAL:H	1.66	0.60
3:J:141:LEU:CB	3:J:145:LEU:HD23	2.30	0.60
3:K:22:LYS:HG2	3:K:130:LEU:HD22	1.83	0.60
1:C:112:PRO:O	1:C:113:HIS:HB2	2.01	0.60
1:G:5:VAL:HG21	1:G:101:ARG:HH11	1.65	0.60
2:H:48:LEU:HA	2:H:59:VAL:HG21	1.82	0.60
3:I:150:PHE:HB3	3:L:148:ILE:HG23	1.84	0.60
3:K:108:VAL:O	3:K:111:ILE:HG22	2.02	0.60
1:E:6:GLN:C	1:E:7:LEU:HD12	2.21	0.60
3:L:22:LYS:HG2	3:L:130:LEU:HD23	1.82	0.60
1:A:114:ASP:HB3	1:A:116:TYR:HE2	1.65	0.59
2:B:62:ARG:NE	2:B:83:ASP:OD2	2.35	0.59
1:G:126:LEU:HD22	1:G:127:VAL:N	2.17	0.59
3:K:116:TYR:O	3:K:120:VAL:HG23	2.02	0.59
2:D:48:LEU:O	2:D:49:ILE:HD13	2.02	0.59
3:L:100:PHE:O	3:L:104:ILE:N	2.32	0.59
2:B:202:LEU:HD13	2:B:206:VAL:CG2	2.32	0.59
2:D:24:CYS:HB2	2:D:36:TRP:CH2	2.36	0.59
1:A:159:LEU:CD1	1:A:161:LYS:HB2	2.32	0.59
2:F:116:VAL:HG21	2:F:197:VAL:CG2	2.29	0.59
1:C:51:VAL:HG23	1:C:52:ALA:H	1.68	0.59
1:E:137:PRO:HB2	1:E:160:VAL:HG13	1.85	0.59
2:H:36:TRP:CG	2:H:74:LEU:HD13	2.37	0.59
3:J:122:GLY:HA2	3:K:166:PHE:HZ	1.67	0.59
1:C:39:TRP:O	1:C:51:VAL:HG22	2.03	0.59
1:C:143:ALA:CB	1:C:232:LYS:HG2	2.32	0.59
2:F:202:LEU:HD13	2:F:206:VAL:HG23	1.85	0.59
2:H:114:PRO:HD3	2:H:199:HIS:ND1	2.18	0.59
1:A:58:TYR:HB3	1:A:60:TYR:CE2	2.38	0.59
1:C:39:TRP:CG	1:C:84:LEU:HD22	2.38	0.59
1:G:143:ALA:HB2	1:G:232:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:95:ALA:HB2	1.85	0.58
1:A:112:PRO:HG2	1:A:113:HIS:CD2	2.37	0.58
1:G:71:PHE:CE2	1:G:86:MET:HG2	2.38	0.58
3:J:122:GLY:HA2	3:K:166:PHE:CZ	2.38	0.58
1:E:43:ALA:HA	1:E:95:ALA:CB	2.34	0.58
3:L:141:LEU:HD13	3:L:142:PRO:HD2	1.84	0.58
3:I:32:ILE:O	3:I:36:ILE:HD13	2.04	0.58
2:D:40:LYS:HD3	2:D:85:ALA:HB2	1.83	0.58
2:F:194:ALA:CB	2:F:209:SER:HB2	2.34	0.58
1:G:103:ILE:HD13	1:G:119:ASP:HB2	1.84	0.58
1:E:188:LEU:HD12	1:E:194:TYR:CE2	2.38	0.58
1:A:166:GLU:HG3	1:A:194:TYR:HD1	1.68	0.58
1:E:165:PRO:O	1:E:218:HIS:NE2	2.34	0.58
1:E:211:THR:CG2	1:E:228:LYS:HE3	2.33	0.58
3:I:191:LEU:HD12	3:I:192:ARG:N	2.19	0.58
3:J:180:TYR:HA	3:J:183:CYS:HG	1.69	0.58
1:A:157:GLY:HA2	1:A:198:SER:O	2.03	0.58
2:F:194:ALA:HB2	2:F:209:SER:HB2	1.84	0.58
2:H:81:PRO:HA	2:H:84:PHE:HE2	1.67	0.58
3:L:160:ILE:HD12	3:L:161:PHE:CG	2.39	0.58
2:D:38:GLN:CB	2:D:48:LEU:HD21	2.32	0.57
2:D:194:ALA:CB	2:D:209:SER:HB2	2.34	0.57
2:H:60:PRO:HB2	2:H:62:ARG:HG2	1.85	0.57
3:I:103:MET:CG	3:I:163:LYS:HZ3	2.16	0.57
1:C:71:PHE:CE2	1:C:86:MET:HG2	2.39	0.57
1:G:6:GLN:C	1:G:7:LEU:HD12	2.24	0.57
1:G:103:ILE:O	1:G:108:TYR:OH	2.12	0.57
1:A:27:ALA:HB1	1:A:30:PHE:CE1	2.39	0.57
1:A:166:GLU:HG3	1:A:194:TYR:CE1	2.40	0.57
2:B:133:VAL:CG1	2:B:180:LEU:HB3	2.34	0.57
3:I:151:ILE:HD13	3:L:145:LEU:HD12	1.86	0.57
1:G:115:ASN:HD21	2:H:95:ARG:NH1	2.00	0.57
1:A:70:ARG:HB3	1:A:87:ASN:O	2.05	0.57
1:C:43:ALA:HA	1:C:95:ALA:CB	2.35	0.57
1:E:43:ALA:HA	1:E:95:ALA:HB2	1.85	0.57
3:I:188:SER:HB3	3:L:156:TRP:HE1	1.70	0.57
3:J:107:TRP:HE3	3:J:107:TRP:HA	1.70	0.57
3:L:109:PRO:HA	3:L:112:LEU:CG	2.33	0.57
2:D:182:LEU:HD11	2:D:187:TYR:HB2	1.86	0.57
3:L:157:LEU:O	3:L:160:ILE:HG13	2.05	0.56
1:G:114:ASP:N	1:G:114:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:171:ASN:O	3:I:172:THR:OG1	2.17	0.56
3:L:107:TRP:O	3:L:111:ILE:HG22	2.05	0.56
1:G:43:ALA:HA	1:G:95:ALA:CB	2.35	0.56
3:L:107:TRP:HZ2	3:L:161:PHE:HE1	1.54	0.56
1:C:126:LEU:HD22	1:C:127:VAL:H	1.71	0.56
1:E:51:VAL:HG13	1:E:67:VAL:HG11	1.88	0.56
1:E:112:PRO:HG2	1:E:113:HIS:ND1	2.20	0.56
3:L:36:ILE:O	3:L:40:ILE:HG13	2.05	0.56
2:B:48:LEU:O	2:B:49:ILE:HD13	2.06	0.56
2:D:90:GLN:HE21	2:D:97:VAL:HG11	1.70	0.56
2:D:120:PRO:HB3	2:D:210:PHE:CE1	2.40	0.56
1:G:159:LEU:CD1	1:G:161:LYS:HB2	2.36	0.56
2:H:20:VAL:CG2	2:H:79:LEU:HD22	2.36	0.56
3:J:157:LEU:O	3:J:160:ILE:HG13	2.05	0.56
2:B:176:LEU:HD23	2:B:177:SER:N	2.21	0.56
3:K:182:LEU:O	3:K:182:LEU:HD13	2.05	0.56
3:L:138:VAL:CG2	3:L:139:VAL:HG12	2.34	0.56
2:F:15:SER:N	2:F:18:ASP:OD2	2.38	0.56
1:C:23:LEU:HD22	1:C:125:THR:HG21	1.86	0.56
2:F:48:LEU:HA	2:F:59:VAL:HG21	1.86	0.56
1:G:162:ASP:HA	1:G:193:LEU:HB3	1.87	0.56
2:H:86:THR:HA	2:H:103:THR:O	2.06	0.56
3:L:121:TYR:HE2	3:L:127:TYR:HD1	1.54	0.56
2:D:202:LEU:HD13	2:D:206:VAL:HG23	1.87	0.56
3:K:177:LEU:HD23	3:K:181:ILE:HG12	1.88	0.56
3:I:167:LYS:O	3:I:169:VAL:HG23	2.06	0.55
3:K:108:VAL:N	3:K:109:PRO:HD2	2.21	0.55
1:A:222:ASN:HB2	1:G:14:LEU:HD23	1.88	0.55
3:I:173:ALA:O	3:I:174:LEU:HD12	2.06	0.55
3:J:22:LYS:HG2	3:J:130:LEU:CD2	2.36	0.55
3:K:168:ILE:HD12	3:K:168:ILE:H	1.70	0.55
2:D:176:LEU:HD23	2:D:177:SER:N	2.21	0.55
3:J:107:TRP:HA	3:J:107:TRP:CE3	2.40	0.55
2:B:194:ALA:HB2	2:B:209:SER:HB2	1.87	0.55
1:G:7:LEU:HD23	1:G:99:CYS:SG	2.46	0.55
2:H:141:TYR:CG	2:H:142:PRO:HA	2.42	0.55
2:D:84:PHE:CZ	2:D:107:ILE:HG12	2.41	0.55
2:D:133:VAL:HG12	2:D:180:LEU:HB3	1.87	0.55
2:F:156:GLN:HB3	2:F:159:ASN:HD21	1.71	0.55
1:A:137:PRO:HD2	1:A:223:THR:OG1	2.06	0.55
2:B:162:GLU:HA	2:B:177:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HG3	1:C:148:SER:N	2.22	0.55
2:B:194:ALA:CB	2:B:209:SER:HB2	2.36	0.55
3:J:171:ASN:O	3:J:172:THR:OG1	2.09	0.55
3:K:168:ILE:HD12	3:K:168:ILE:N	2.22	0.55
3:L:126:VAL:O	3:L:130:LEU:HD13	2.06	0.55
1:C:51:VAL:HG23	1:C:52:ALA:N	2.22	0.55
1:G:92:GLU:OE1	1:G:92:GLU:N	2.35	0.55
3:K:113:ILE:HG22	3:K:117:LEU:HD12	1.88	0.55
2:F:199:HIS:CD2	2:F:200:GLN:H	2.25	0.55
3:I:137:VAL:HG23	3:L:173:ALA:HB1	1.88	0.55
3:L:135:ASN:OD1	3:L:136:GLY:N	2.40	0.55
3:L:138:VAL:HG22	3:L:139:VAL:CG1	2.37	0.55
2:D:143:ARG:HB2	2:D:174:TYR:HE2	1.68	0.54
3:J:185:PHE:HD1	3:K:156:TRP:CG	2.25	0.54
1:E:71:PHE:CE2	1:E:86:MET:HG2	2.43	0.54
3:J:102:PRO:O	3:J:106:THR:HG23	2.06	0.54
3:K:104:ILE:O	3:K:108:VAL:HG23	2.08	0.54
1:G:137:PRO:HB3	1:G:163:TYR:CB	2.26	0.54
3:I:141:LEU:HG	3:I:144:ILE:HD11	1.90	0.54
3:I:145:LEU:HD11	3:L:151:ILE:HB	1.88	0.54
3:J:160:ILE:HD12	3:J:161:PHE:CD1	2.42	0.54
1:A:54:ILE:HG13	1:A:55:SER:N	2.23	0.54
1:A:67:VAL:HB	1:A:71:PHE:CG	2.43	0.54
2:F:24:CYS:HB2	2:F:36:TRP:CH2	2.42	0.54
1:A:72:THR:OG1	1:A:85:GLN:HB3	2.07	0.54
3:I:177:LEU:HD23	3:I:181:ILE:HG12	1.90	0.54
1:A:6:GLN:C	1:A:7:LEU:HD12	2.28	0.54
2:B:148:GLN:O	2:B:196:GLU:N	2.37	0.54
3:I:103:MET:HG3	3:I:163:LYS:HZ1	1.70	0.54
2:B:182:LEU:CD1	2:B:187:TYR:HB2	2.38	0.54
1:E:51:VAL:HG13	1:E:67:VAL:HG21	1.90	0.54
3:J:139:VAL:CG2	3:J:141:LEU:HD22	2.38	0.54
2:B:162:GLU:HB2	2:B:176:LEU:HD21	1.90	0.54
3:L:174:LEU:CD1	3:L:179:TRP:HB2	2.38	0.54
1:A:137:PRO:HB3	1:A:163:TYR:CB	2.34	0.53
1:E:27:ALA:HB1	1:E:30:PHE:CE1	2.44	0.53
2:F:196:GLU:HG2	2:F:207:THR:OG1	2.07	0.53
3:I:141:LEU:HG	3:I:144:ILE:HG13	1.90	0.53
3:K:109:PRO:CA	3:K:112:LEU:HG	2.31	0.53
3:L:26:PRO:O	3:L:30:ILE:HG12	2.08	0.53
1:A:165:PRO:O	1:A:218:HIS:NE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:102:PRO:O	3:K:106:THR:HG23	2.08	0.53
3:K:120:VAL:HG13	3:K:126:VAL:CG1	2.38	0.53
3:K:169:VAL:HG12	3:K:170:SER:N	2.18	0.53
1:C:15:VAL:HG11	1:C:89:LEU:HD13	1.90	0.53
1:C:92:GLU:OE1	1:C:92:GLU:N	2.32	0.53
1:G:27:ALA:HB1	1:G:30:PHE:CE1	2.44	0.53
1:A:54:ILE:CD1	1:A:61:THR:HG22	2.38	0.53
2:B:180:LEU:HD21	2:B:182:LEU:HD23	1.91	0.53
1:C:108:TYR:HA	1:C:111:TYR:O	2.08	0.53
2:F:36:TRP:CZ3	2:F:89:CYS:HB3	2.44	0.53
2:F:114:PRO:HD3	2:F:199:HIS:ND1	2.24	0.53
1:G:6:GLN:O	1:G:7:LEU:HD12	2.08	0.53
1:G:188:LEU:HD13	1:G:194:TYR:CE2	2.34	0.53
2:H:35:ALA:HA	2:H:49:ILE:O	2.08	0.53
1:A:50:TRP:CE3	1:A:64:ALA:HB2	2.44	0.53
2:H:3:ILE:CD1	2:H:94:SER:HB2	2.37	0.53
1:A:38:HIS:CG	1:A:53:SER:HG	2.22	0.53
1:C:144:PRO:HG3	1:C:207:LEU:HD22	1.91	0.53
2:D:31:SER:HB3	2:D:93:SER:OG	2.09	0.53
2:D:151:VAL:HG23	2:D:156:GLN:HG3	1.90	0.53
2:H:202:LEU:HD13	2:H:206:VAL:HG23	1.91	0.53
3:I:113:ILE:O	3:I:117:LEU:HD23	2.08	0.53
2:F:49:ILE:CD1	2:F:55:LEU:HA	2.38	0.53
1:G:103:ILE:HD13	1:G:119:ASP:CB	2.39	0.53
3:J:138:VAL:HG22	3:J:139:VAL:CG1	2.38	0.53
1:A:126:LEU:HD22	1:A:127:VAL:H	1.74	0.53
2:H:3:ILE:HD12	2:H:94:SER:HB2	1.91	0.53
3:J:32:ILE:O	3:J:36:ILE:HD13	2.09	0.53
1:A:42:GLN:HG3	1:A:47:GLY:O	2.09	0.52
2:H:212:ARG:HH11	2:H:213:GLY:H	1.56	0.52
1:A:63:TYR:CZ	1:A:73:ILE:HG22	2.45	0.52
1:C:115:ASN:HB2	2:D:92:SER:HB2	1.91	0.52
1:C:166:GLU:HG3	1:C:194:TYR:CE1	2.43	0.52
3:L:40:ILE:O	3:L:44:ALA:HB3	2.09	0.52
1:A:42:GLN:O	1:A:95:ALA:HB1	2.09	0.52
2:D:162:GLU:HA	2:D:177:SER:O	2.09	0.52
2:D:15:SER:N	2:D:18:ASP:OD2	2.42	0.52
2:F:49:ILE:HD13	2:F:55:LEU:HA	1.91	0.52
3:K:141:LEU:CB	3:K:145:LEU:HD23	2.33	0.52
3:L:191:LEU:HD12	3:L:192:ARG:N	2.24	0.52
1:A:188:LEU:HD11	1:A:192:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:GLU:OE1	2:D:174:TYR:OH	2.27	0.52
1:G:70:ARG:HB3	1:G:87:ASN:O	2.09	0.52
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.92	0.52
1:C:28:SER:HB3	1:E:79:LYS:NZ	2.25	0.52
2:D:144:GLU:OE1	2:D:144:GLU:N	2.40	0.52
1:A:126:LEU:HD22	1:A:127:VAL:N	2.25	0.52
1:C:79:LYS:NZ	1:E:28:SER:HB3	2.25	0.52
3:I:106:THR:C	3:I:109:PRO:HD2	2.30	0.52
3:K:9:TYR:CE2	3:K:116:TYR:HB2	2.33	0.52
3:L:142:PRO:O	3:L:144:ILE:N	2.41	0.52
3:I:103:MET:SD	3:I:103:MET:N	2.83	0.52
2:B:137:LEU:HD21	2:B:197:VAL:HG13	1.92	0.51
1:G:39:TRP:CG	1:G:84:LEU:HD22	2.44	0.51
1:G:135:LYS:HD3	1:G:136:GLY:O	2.10	0.51
2:H:182:LEU:HD13	2:H:187:TYR:HB2	1.92	0.51
3:L:135:ASN:OD1	3:L:137:VAL:HG23	2.10	0.51
3:I:104:ILE:O	3:I:108:VAL:HG23	2.11	0.51
3:K:32:ILE:O	3:K:36:ILE:HD13	2.10	0.51
3:L:7:ASP:HB3	3:L:11:LYS:HE2	1.93	0.51
3:L:120:VAL:HG13	3:L:121:TYR:CE2	2.45	0.51
3:I:135:ASN:OD1	3:I:135:ASN:N	2.43	0.51
3:J:137:VAL:HG12	3:K:173:ALA:HB1	1.89	0.51
2:B:182:LEU:HD11	2:B:187:TYR:HB2	1.93	0.51
1:E:103:ILE:O	1:E:108:TYR:OH	2.17	0.51
2:F:125:GLN:O	2:F:128:SER:OG	2.24	0.51
1:G:42:GLN:HG3	1:G:47:GLY:O	2.10	0.51
1:G:103:ILE:CG1	1:G:119:ASP:HB2	2.39	0.51
2:H:20:VAL:HG21	2:H:79:LEU:HD22	1.91	0.51
1:G:206:SER:HB2	1:G:210:GLN:CD	2.30	0.51
1:A:54:ILE:HD12	1:A:60:TYR:O	2.09	0.51
1:A:156:LEU:HB2	1:A:200:VAL:HG23	1.93	0.51
2:B:15:SER:N	2:B:18:ASP:OD2	2.43	0.51
2:D:55:LEU:HD21	2:D:59:VAL:HB	1.92	0.51
2:D:62:ARG:NE	2:D:83:ASP:OD2	2.44	0.51
1:E:115:ASN:HD21	2:F:95:ARG:HH12	1.57	0.51
2:D:147:VAL:HG11	2:D:178:SER:HB2	1.93	0.51
1:G:56:PRO:O	1:G:57:SER:CB	2.58	0.51
2:H:212:ARG:HH11	2:H:213:GLY:N	2.08	0.51
3:I:145:LEU:CD1	3:L:151:ILE:HB	2.41	0.51
3:J:162:TYR:O	3:J:164:GLY:N	2.44	0.51
3:I:123:PHE:CE2	3:L:165:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:151:ILE:HD11	3:K:155:HIS:NE2	2.26	0.51
1:A:43:ALA:HA	1:A:95:ALA:CB	2.41	0.51
2:B:34:VAL:HG13	2:B:90:GLN:O	2.10	0.51
3:J:109:PRO:HA	3:J:112:LEU:HG	1.93	0.51
3:J:172:THR:O	3:J:173:ALA:HB3	2.10	0.51
3:J:182:LEU:HD13	3:J:182:LEU:O	2.09	0.51
3:K:137:VAL:HG11	3:K:140:TYR:CD1	2.46	0.51
2:B:35:ALA:HA	2:B:49:ILE:O	2.11	0.51
2:B:119:PHE:HB2	2:B:134:VAL:HB	1.92	0.51
1:C:62:TYR:OH	1:C:113:HIS:ND1	2.38	0.51
2:D:151:VAL:HG23	2:D:156:GLN:CG	2.41	0.51
3:J:17:PHE:O	3:J:21:ILE:HG13	2.11	0.51
1:A:23:LEU:HD22	1:A:125:THR:HG21	1.93	0.50
1:E:70:ARG:HB3	1:E:87:ASN:O	2.11	0.50
1:G:51:VAL:HG23	1:G:52:ALA:N	2.25	0.50
3:I:169:VAL:HG12	3:I:170:SER:N	2.17	0.50
1:A:79:LYS:NZ	1:G:28:SER:HB3	2.25	0.50
1:C:187:VAL:CG1	2:D:163:SER:HB3	2.41	0.50
1:E:55:SER:O	1:E:59:GLY:N	2.45	0.50
3:I:103:MET:CG	3:I:163:LYS:NZ	2.67	0.50
3:I:120:VAL:HG13	3:I:121:TYR:CE2	2.45	0.50
3:L:113:ILE:O	3:L:117:LEU:HD23	2.10	0.50
1:E:137:PRO:CB	1:E:163:TYR:HB3	2.39	0.50
1:E:184:PHE:HA	2:F:165:THR:HG22	1.93	0.50
1:G:57:SER:O	3:K:135:ASN:ND2	2.45	0.50
1:C:137:PRO:CB	1:C:163:TYR:HB3	2.34	0.50
1:E:5:VAL:HG21	1:E:101:ARG:NH1	2.25	0.50
3:I:30:ILE:HD11	3:I:121:TYR:CE1	2.45	0.50
3:J:174:LEU:CD1	3:J:179:TRP:HB2	2.41	0.50
1:A:54:ILE:HD12	1:A:61:THR:HG22	1.93	0.50
2:B:40:LYS:HD2	2:B:85:ALA:HB2	1.94	0.50
3:K:131:ASN:N	3:K:131:ASN:HD22	2.09	0.50
1:A:104:TRP:HA	1:A:108:TYR:CE1	2.47	0.50
2:D:83:ASP:O	2:D:87:TYR:OH	2.22	0.50
2:F:40:LYS:HB3	2:F:41:PRO:HD2	1.94	0.50
1:G:166:GLU:OE2	1:G:167:PRO:HA	2.12	0.50
2:H:199:HIS:CD2	2:H:200:GLN:H	2.29	0.50
3:I:138:VAL:CG2	3:I:139:VAL:HG12	2.40	0.50
3:K:118:ARG:CG	3:K:118:ARG:NH1	2.66	0.50
1:A:126:LEU:HD11	1:A:128:THR:OG1	2.12	0.50
2:B:33:ALA:HA	2:B:51:SER:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASP:OD1	2:B:190:HIS:HB3	2.11	0.50
2:F:67:ARG:HH11	2:F:72:PHE:HE2	1.58	0.50
3:L:25:HIS:HD2	3:L:26:PRO:CD	2.24	0.50
2:B:194:ALA:HB2	2:B:209:SER:CB	2.41	0.50
2:D:211:ASN:HB2	2:D:214:GLU:OE1	2.12	0.50
1:A:28:SER:HB3	1:G:79:LYS:NZ	2.27	0.49
2:F:114:PRO:HB3	2:F:140:PHE:HB3	1.94	0.49
3:K:17:PHE:O	3:K:21:ILE:HG13	2.10	0.49
3:L:17:PHE:O	3:L:21:ILE:HG13	2.12	0.49
1:C:223:THR:HG22	1:E:133:SER:OG	2.12	0.49
2:D:36:TRP:CE3	2:D:89:CYS:HB3	2.47	0.49
3:K:36:ILE:O	3:K:40:ILE:HG13	2.12	0.49
3:K:106:THR:C	3:K:109:PRO:HD2	2.32	0.49
1:C:147:LYS:HG3	1:C:148:SER:H	1.78	0.49
3:I:109:PRO:HA	3:I:112:LEU:HG	1.93	0.49
3:J:174:LEU:HD13	3:J:179:TRP:N	2.27	0.49
1:G:51:VAL:HG23	1:G:52:ALA:H	1.77	0.49
2:H:90:GLN:HE21	2:H:97:VAL:HG11	1.78	0.49
3:I:139:VAL:O	3:L:173:ALA:HA	2.13	0.49
3:J:22:LYS:CD	3:J:130:LEU:HD21	2.41	0.49
3:J:177:LEU:HD23	3:J:181:ILE:HG12	1.94	0.49
2:B:211:ASN:HB2	2:B:214:GLU:OE1	2.12	0.49
2:D:194:ALA:HB2	2:D:209:SER:CB	2.41	0.49
3:I:185:PHE:CE2	3:L:148:ILE:HD11	2.47	0.49
1:A:103:ILE:HB	1:A:119:ASP:HB2	1.94	0.49
1:E:6:GLN:O	1:E:7:LEU:HD12	2.13	0.49
1:E:143:ALA:CB	1:E:232:LYS:HG2	2.43	0.49
3:J:143:ILE:O	3:J:147:LYS:N	2.45	0.49
3:L:174:LEU:HD13	3:L:179:TRP:N	2.28	0.49
1:C:15:VAL:CG1	1:C:129:VAL:HG22	2.43	0.49
2:D:187:TYR:HA	2:D:193:TYR:OH	2.13	0.49
2:F:194:ALA:HB2	2:F:209:SER:CB	2.42	0.49
3:L:121:TYR:CE2	3:L:127:TYR:HD1	2.31	0.49
2:D:7:GLN:HB2	2:D:89:CYS:SG	2.52	0.49
1:E:211:THR:HG22	1:E:213:ILE:HD11	1.95	0.49
3:J:113:ILE:O	3:J:117:LEU:HD23	2.13	0.49
3:J:176:TRP:CZ2	3:K:118:ARG:HD2	2.48	0.49
2:B:185:ALA:O	2:B:189:LYS:HG3	2.13	0.48
1:C:157:GLY:HA2	1:C:198:SER:O	2.13	0.48
3:J:120:VAL:HG13	3:J:121:TYR:CG	2.48	0.48
3:L:109:PRO:O	3:L:113:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:LEU:HD23	2:B:56:TYR:CD2	2.48	0.48
2:B:133:VAL:HG13	2:B:180:LEU:HB3	1.94	0.48
1:G:41:ARG:HB3	1:G:97:TYR:CE2	2.47	0.48
3:I:172:THR:O	3:I:173:ALA:HB3	2.13	0.48
3:I:177:LEU:HD23	3:I:177:LEU:O	2.13	0.48
3:K:40:ILE:O	3:K:44:ALA:HB3	2.13	0.48
3:K:109:PRO:O	3:K:113:ILE:HG13	2.13	0.48
1:A:143:ALA:CB	1:A:232:LYS:HE2	2.42	0.48
1:C:63:TYR:CZ	1:C:73:ILE:HG22	2.48	0.48
1:C:79:LYS:HZ1	1:E:28:SER:HB3	1.78	0.48
1:C:115:ASN:O	1:C:116:TYR:HB2	2.13	0.48
1:C:126:LEU:HD22	1:C:127:VAL:N	2.27	0.48
1:G:39:TRP:O	1:G:51:VAL:HG22	2.12	0.48
2:B:7:GLN:NE2	2:B:103:THR:OG1	2.47	0.48
1:A:5:VAL:HG11	1:A:101:ARG:HH11	1.78	0.48
1:C:181:VAL:HG12	1:C:200:VAL:HG13	1.96	0.48
1:G:103:ILE:CD1	1:G:119:ASP:HB2	2.43	0.48
3:I:141:LEU:HG	3:I:144:ILE:CD1	2.44	0.48
3:I:185:PHE:HD1	3:L:156:TRP:CG	2.31	0.48
2:H:114:PRO:HB3	2:H:140:PHE:HB3	1.95	0.48
3:I:120:VAL:HG13	3:I:121:TYR:CG	2.48	0.48
3:J:25:HIS:CD2	3:J:27:ALA:HB3	2.48	0.48
3:J:120:VAL:HG13	3:J:121:TYR:CE2	2.48	0.48
1:A:132:ALA:HB3	1:A:164:PHE:CZ	2.48	0.48
1:E:112:PRO:HG2	1:E:113:HIS:CE1	2.49	0.48
1:E:210:GLN:O	1:E:211:THR:HB	2.13	0.48
2:F:83:ASP:O	2:F:87:TYR:OH	2.18	0.48
1:G:63:TYR:OH	1:G:73:ILE:N	2.40	0.48
3:J:36:ILE:O	3:J:40:ILE:HG13	2.13	0.48
3:J:169:VAL:HG12	3:J:170:SER:N	2.24	0.48
1:A:135:LYS:NZ	1:A:193:LEU:HD21	2.29	0.48
1:C:164:PHE:CE2	1:C:165:PRO:HB3	2.48	0.48
3:L:174:LEU:HD11	3:L:179:TRP:HB2	1.94	0.48
1:A:140:PHE:CD2	2:B:125:GLN:HB2	2.49	0.48
2:B:187:TYR:HA	2:B:193:TYR:OH	2.14	0.48
1:E:228:LYS:HE2	1:E:230:GLU:OE2	2.14	0.48
1:G:166:GLU:HG2	1:G:194:TYR:CE1	2.49	0.48
3:I:142:PRO:O	3:I:144:ILE:N	2.41	0.48
2:D:214:GLU:HG2	2:D:215:CYS:N	2.24	0.47
1:G:206:SER:HB2	1:G:210:GLN:OE1	2.14	0.47
1:A:62:TYR:OH	1:A:113:HIS:ND1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:VAL:HB	1:C:71:PHE:CG	2.48	0.47
2:D:125:GLN:O	2:D:128:SER:OG	2.26	0.47
1:E:103:ILE:HD12	1:E:103:ILE:HA	1.72	0.47
1:G:163:TYR:CE2	1:G:168:VAL:HG23	2.48	0.47
3:J:30:ILE:HD11	3:J:121:TYR:CE1	2.48	0.47
3:J:131:ASN:N	3:J:131:ASN:HD22	2.12	0.47
3:K:25:HIS:ND1	3:K:26:PRO:HD2	2.29	0.47
3:L:177:LEU:HD23	3:L:181:ILE:HG12	1.96	0.47
2:B:80:GLN:HB3	2:B:81:PRO:HD2	1.96	0.47
1:E:164:PHE:HB2	1:E:193:LEU:HD13	1.96	0.47
3:I:109:PRO:O	3:I:112:LEU:HG	2.12	0.47
1:A:112:PRO:O	1:A:113:HIS:HB2	2.14	0.47
1:C:6:GLN:C	1:C:7:LEU:HD12	2.33	0.47
2:D:152:ASP:OD1	2:D:190:HIS:HB3	2.14	0.47
2:D:156:GLN:NE2	2:D:156:GLN:HA	2.27	0.47
3:I:109:PRO:O	3:I:113:ILE:HG13	2.14	0.47
3:I:173:ALA:C	3:I:174:LEU:HD12	2.35	0.47
3:L:160:ILE:HD12	3:L:161:PHE:CD1	2.49	0.47
2:B:3:ILE:HD12	2:B:94:SER:HB2	1.96	0.47
1:E:140:PHE:CD2	2:F:125:GLN:HB2	2.49	0.47
2:H:107:ILE:HG22	2:H:108:LYS:N	2.29	0.47
3:K:157:LEU:HD23	3:K:157:LEU:O	2.12	0.47
1:A:27:ALA:HB1	1:A:30:PHE:CZ	2.50	0.47
1:A:38:HIS:CB	1:A:118:MET:HE2	2.44	0.47
1:C:137:PRO:HB3	1:C:163:TYR:CB	2.36	0.47
1:C:213:ILE:HD12	1:C:213:ILE:N	2.30	0.47
1:E:111:TYR:HD2	1:E:111:TYR:O	1.97	0.47
1:G:157:GLY:HA2	1:G:198:SER:O	2.14	0.47
2:H:42:GLY:O	2:H:43:LYS:HD2	2.15	0.47
3:J:154:TRP:CH2	3:J:177:LEU:HD22	2.50	0.47
1:A:163:TYR:CE1	1:A:168:VAL:HG23	2.50	0.47
2:B:191:LYS:NZ	2:B:191:LYS:HB3	2.30	0.47
2:F:74:LEU:HD23	2:F:75:THR:H	1.79	0.47
1:G:126:LEU:HD11	1:G:128:THR:OG1	2.13	0.47
2:H:125:GLN:O	2:H:128:SER:OG	2.30	0.47
3:K:113:ILE:CG2	3:K:117:LEU:HD12	2.45	0.47
1:A:79:LYS:HZ1	1:G:28:SER:HB3	1.78	0.47
1:C:108:TYR:CE1	1:C:114:ASP:O	2.68	0.47
2:D:82:GLU:OE1	2:D:82:GLU:N	2.39	0.47
1:E:211:THR:HG23	1:E:228:LYS:CE	2.44	0.47
2:H:84:PHE:CZ	2:H:107:ILE:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:25:HIS:ND1	3:I:26:PRO:HD2	2.30	0.47
3:L:144:ILE:HG13	3:L:145:LEU:N	2.28	0.47
3:L:177:LEU:HD23	3:L:177:LEU:O	2.14	0.47
2:B:50:TYR:O	2:B:54:SER:HB3	2.15	0.46
2:B:156:GLN:HE21	2:B:156:GLN:CA	2.26	0.46
2:H:121:PRO:HB3	2:H:132:SER:O	2.16	0.46
3:I:106:THR:O	3:I:109:PRO:HD2	2.14	0.46
3:K:141:LEU:CD1	3:K:144:ILE:HG12	2.45	0.46
1:C:178:THR:O	1:C:181:VAL:HG22	2.15	0.46
1:E:38:HIS:ND1	1:E:53:SER:OG	2.44	0.46
3:J:173:ALA:HA	3:K:139:VAL:O	2.15	0.46
3:K:177:LEU:HD23	3:K:177:LEU:O	2.15	0.46
3:L:169:VAL:HG12	3:L:170:SER:N	2.24	0.46
2:B:120:PRO:HB3	2:B:210:PHE:CE1	2.51	0.46
1:C:222:ASN:HB2	1:E:14:LEU:HD23	1.97	0.46
2:D:36:TRP:CD2	2:D:74:LEU:HG	2.51	0.46
1:E:163:TYR:CE2	1:E:168:VAL:HG23	2.50	0.46
3:J:40:ILE:O	3:J:44:ALA:HB3	2.15	0.46
2:B:159:ASN:OD1	2:B:180:LEU:HG	2.15	0.46
2:F:40:LYS:HD3	2:F:85:ALA:CB	2.44	0.46
1:G:15:VAL:CG1	1:G:129:VAL:HG22	2.45	0.46
3:I:22:LYS:CG	3:I:130:LEU:HD23	2.35	0.46
2:D:22:ILE:HG12	2:D:103:THR:HG21	1.97	0.46
1:E:37:ILE:HB	1:E:54:ILE:CG2	2.45	0.46
3:K:105:TYR:O	3:K:109:PRO:HD3	2.16	0.46
3:K:141:LEU:HD12	3:K:144:ILE:HG12	1.98	0.46
1:A:136:GLY:HA3	1:A:223:THR:HG21	1.98	0.46
1:C:15:VAL:HG11	1:C:89:LEU:CD1	2.44	0.46
1:A:108:TYR:HA	1:A:111:TYR:O	2.16	0.46
2:D:137:LEU:HD21	2:D:197:VAL:HG13	1.98	0.46
1:E:63:TYR:OH	1:E:72:THR:HA	2.16	0.46
3:J:142:PRO:O	3:J:144:ILE:N	2.38	0.46
3:K:26:PRO:HB3	3:K:121:TYR:HE2	1.81	0.46
3:L:141:LEU:HD13	3:L:141:LEU:HA	1.76	0.46
2:F:116:VAL:HA	2:F:136:LEU:O	2.16	0.46
2:H:49:ILE:CD1	2:H:55:LEU:HA	2.46	0.46
3:I:169:VAL:CG1	3:I:170:SER:H	2.21	0.46
3:K:154:TRP:CH2	3:K:177:LEU:HD22	2.50	0.46
3:L:149:LEU:N	3:L:149:LEU:HD22	2.31	0.46
1:E:154:ALA:N	1:E:202:VAL:O	2.43	0.46
1:G:154:ALA:N	1:G:202:VAL:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:172:THR:O	3:K:173:ALA:HB3	2.15	0.46
1:A:92:GLU:OE1	1:A:92:GLU:N	2.43	0.46
1:A:144:PRO:HG3	1:A:207:LEU:HD22	1.97	0.46
2:H:82:GLU:OE1	2:H:82:GLU:N	2.41	0.46
2:B:67:ARG:HH11	2:B:72:PHE:HE2	1.64	0.45
2:D:34:VAL:HG13	2:D:90:GLN:O	2.15	0.45
2:F:149:TRP:CE3	2:F:180:LEU:HD22	2.51	0.45
2:H:76:ILE:N	2:H:76:ILE:HD12	2.31	0.45
3:J:26:PRO:O	3:J:30:ILE:HG12	2.16	0.45
3:J:122:GLY:CA	3:K:166:PHE:HZ	2.28	0.45
3:K:109:PRO:HA	3:K:112:LEU:CD2	2.46	0.45
1:A:165:PRO:HD2	1:A:220:PRO:CB	2.47	0.45
1:E:164:PHE:HA	1:E:165:PRO:HA	1.71	0.45
2:H:48:LEU:O	2:H:49:ILE:HD13	2.16	0.45
3:I:176:TRP:HA	3:L:138:VAL:HG11	1.98	0.45
3:J:166:PHE:CE1	3:K:136:GLY:HA3	2.51	0.45
2:F:146:LYS:HA	2:F:146:LYS:HD3	1.68	0.45
2:H:7:GLN:HE22	2:H:102:GLY:C	2.19	0.45
2:H:49:ILE:HD13	2:H:55:LEU:HA	1.98	0.45
2:B:24:CYS:HB2	2:B:36:TRP:CH2	2.51	0.45
2:B:90:GLN:HE21	2:B:97:VAL:HG11	1.81	0.45
1:C:111:TYR:HE1	3:L:23:VAL:HG12	1.76	0.45
2:D:202:LEU:HD13	2:D:206:VAL:CG2	2.45	0.45
1:E:41:ARG:HB3	1:E:97:TYR:CD2	2.52	0.45
1:E:157:GLY:HA2	1:E:198:SER:O	2.16	0.45
3:K:7:ASP:HB3	3:K:11:LYS:HE2	1.98	0.45
3:K:149:LEU:N	3:K:149:LEU:HD22	2.31	0.45
1:C:126:LEU:HD11	1:C:128:THR:OG1	2.16	0.45
2:D:76:ILE:HD12	2:D:76:ILE:N	2.32	0.45
3:L:105:TYR:HD1	3:L:105:TYR:O	2.00	0.45
1:A:223:THR:HG22	1:G:133:SER:OG	2.17	0.45
1:C:72:THR:OG1	1:C:85:GLN:HB3	2.16	0.45
2:D:48:LEU:HA	2:D:59:VAL:HG21	1.99	0.45
1:G:140:PHE:CE2	2:H:125:GLN:HG3	2.52	0.45
1:C:130:SER:HG	1:C:164:PHE:HZ	1.64	0.45
2:D:148:GLN:O	2:D:195:CYS:HA	2.17	0.45
2:F:35:ALA:HA	2:F:49:ILE:O	2.17	0.45
3:I:136:GLY:O	3:I:137:VAL:O	2.34	0.45
1:C:112:PRO:O	1:C:113:HIS:CB	2.64	0.45
3:I:102:PRO:HA	3:I:105:TYR:HB3	1.98	0.45
3:I:138:VAL:C	3:I:139:VAL:HG12	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:112:LEU:HA	3:J:115:ILE:HD11	1.98	0.45
3:J:148:ILE:CG2	3:K:150:PHE:HB3	2.41	0.45
3:K:112:LEU:HA	3:K:115:ILE:HD11	1.97	0.45
3:L:109:PRO:CA	3:L:112:LEU:HG	2.43	0.45
2:B:76:ILE:HD12	2:B:76:ILE:N	2.32	0.45
1:C:15:VAL:HG13	1:C:129:VAL:HG22	1.99	0.45
2:D:33:ALA:HA	2:D:51:SER:HA	1.98	0.45
2:H:167:GLN:HG2	2:H:174:TYR:CZ	2.51	0.45
3:I:143:ILE:CG2	3:I:144:ILE:N	2.80	0.45
3:J:139:VAL:O	3:K:173:ALA:HA	2.17	0.45
1:A:105:SER:O	1:A:108:TYR:HD1	1.99	0.45
2:F:109:ARG:HD2	2:F:171:ASP:O	2.16	0.45
3:J:117:LEU:O	3:J:120:VAL:HG12	2.16	0.45
2:D:84:PHE:CE2	2:D:107:ILE:HG12	2.51	0.44
2:F:48:LEU:O	2:F:49:ILE:HD13	2.17	0.44
1:G:42:GLN:O	1:G:95:ALA:HB1	2.17	0.44
3:I:38:SER:O	3:I:41:ILE:HG22	2.16	0.44
1:A:6:GLN:O	1:A:7:LEU:HD12	2.17	0.44
2:B:109:ARG:HG3	2:B:141:TYR:CD1	2.52	0.44
3:I:108:VAL:O	3:I:111:ILE:HG22	2.17	0.44
3:J:185:PHE:HA	3:K:156:TRP:CE2	2.52	0.44
2:B:36:TRP:HB3	2:B:74:LEU:HD12	1.99	0.44
3:I:141:LEU:CD2	3:L:179:TRP:HZ3	2.31	0.44
3:I:166:PHE:HD2	3:L:135:ASN:O	2.00	0.44
3:L:154:TRP:HH2	3:L:177:LEU:HD22	1.82	0.44
1:A:7:LEU:HD23	1:A:99:CYS:SG	2.56	0.44
2:D:40:LYS:HB3	2:D:41:PRO:HD2	1.98	0.44
1:E:38:HIS:CB	1:E:118:MET:HE2	2.47	0.44
3:I:141:LEU:CG	3:I:144:ILE:HD11	2.47	0.44
3:K:22:LYS:HG2	3:K:130:LEU:HD21	1.98	0.44
1:A:14:LEU:HD21	1:G:222:ASN:ND2	2.33	0.44
2:D:31:SER:OG	2:D:32:SER:N	2.50	0.44
2:F:81:PRO:HA	2:F:84:PHE:CE2	2.52	0.44
3:K:137:VAL:HG11	3:K:140:TYR:HE1	1.80	0.44
2:D:133:VAL:HG13	2:D:180:LEU:HB3	1.97	0.44
1:E:42:GLN:HG3	1:E:47:GLY:O	2.17	0.44
1:G:41:ARG:HB3	1:G:97:TYR:CD2	2.53	0.44
3:I:160:ILE:HD11	3:L:192:ARG:HH22	1.83	0.44
3:J:185:PHE:CE2	3:K:148:ILE:HD11	2.52	0.44
2:B:116:VAL:HG22	2:B:197:VAL:HG21	2.00	0.44
1:C:39:TRP:NE1	1:C:84:LEU:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:C	1:C:196:LEU:HD12	2.38	0.44
2:F:80:GLN:HB3	2:F:81:PRO:HD2	1.99	0.44
2:H:146:LYS:HD3	2:H:146:LYS:HA	1.79	0.44
3:I:156:TRP:HE1	3:L:188:SER:HB3	1.83	0.44
3:J:109:PRO:O	3:J:113:ILE:HG13	2.18	0.44
3:K:112:LEU:HA	3:K:115:ILE:CD1	2.47	0.44
3:K:138:VAL:C	3:K:139:VAL:HG12	2.38	0.44
1:A:51:VAL:HG13	1:A:67:VAL:HG11	1.98	0.44
1:C:71:PHE:HE2	1:C:86:MET:HE2	1.83	0.44
2:F:76:ILE:N	2:F:76:ILE:HD12	2.32	0.44
3:I:149:LEU:HD22	3:I:149:LEU:N	2.33	0.44
3:I:166:PHE:CE2	3:L:136:GLY:HA2	2.53	0.44
1:A:137:PRO:CB	1:A:163:TYR:HB3	2.35	0.43
1:E:39:TRP:CG	1:E:84:LEU:HD22	2.53	0.43
2:F:132:SER:HA	2:F:180:LEU:O	2.18	0.43
1:G:67:VAL:HB	1:G:71:PHE:CG	2.52	0.43
2:H:156:GLN:HB3	2:H:159:ASN:OD1	2.18	0.43
1:G:164:PHE:HA	1:G:165:PRO:HA	1.80	0.43
2:H:141:TYR:CD2	2:H:142:PRO:HA	2.53	0.43
3:K:143:ILE:CG1	3:K:144:ILE:N	2.81	0.43
2:F:51:SER:O	2:F:52:ALA:HB3	2.17	0.43
2:F:211:ASN:HB2	2:F:214:GLU:OE1	2.18	0.43
3:K:14:ASP:O	3:K:18:MET:HG2	2.17	0.43
2:B:15:SER:HB3	2:B:18:ASP:OD2	2.18	0.43
3:I:141:LEU:HD23	3:I:144:ILE:HD11	2.00	0.43
3:J:103:MET:SD	3:J:103:MET:N	2.91	0.43
3:K:143:ILE:HG13	3:K:144:ILE:N	2.33	0.43
3:L:172:THR:O	3:L:173:ALA:HB3	2.18	0.43
1:C:140:PHE:CD2	2:D:125:GLN:HB2	2.54	0.43
1:E:41:ARG:HB3	1:E:97:TYR:CE2	2.53	0.43
3:J:106:THR:O	3:J:109:PRO:HD2	2.19	0.43
3:L:31:LEU:O	3:L:35:ILE:HG13	2.17	0.43
3:L:182:LEU:HD13	3:L:182:LEU:O	2.18	0.43
1:A:178:THR:O	1:A:181:VAL:HG22	2.19	0.43
1:A:202:VAL:HG13	1:A:203:PRO:HD2	2.01	0.43
2:D:80:GLN:OE1	2:D:81:PRO:HD2	2.18	0.43
1:E:55:SER:HB3	1:E:60:TYR:HB2	2.00	0.43
2:F:162:GLU:HA	2:F:177:SER:O	2.18	0.43
3:I:36:ILE:O	3:I:40:ILE:HG13	2.18	0.43
3:I:105:TYR:O	3:I:109:PRO:HD3	2.18	0.43
3:L:98:MET:HE1	3:L:99:SER:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:143:ILE:O	3:L:147:LYS:N	2.51	0.43
1:A:51:VAL:CG1	1:A:67:VAL:HG21	2.48	0.43
1:A:115:ASN:C	1:A:117:GLY:H	2.22	0.43
2:D:147:VAL:HG11	2:D:178:SER:CB	2.49	0.43
2:D:148:GLN:O	2:D:196:GLU:N	2.47	0.43
1:E:112:PRO:O	1:E:113:HIS:HB2	2.18	0.43
3:K:120:VAL:HB	3:K:121:TYR:CD1	2.53	0.43
1:A:68:LYS:HE3	1:A:68:LYS:HB2	1.89	0.43
1:A:115:ASN:O	1:A:116:TYR:HB2	2.18	0.43
1:A:196:LEU:HD12	1:A:196:LEU:C	2.38	0.43
1:E:137:PRO:HB3	1:E:163:TYR:CB	2.44	0.43
2:F:15:SER:HB2	2:F:108:LYS:HE2	2.00	0.43
2:H:182:LEU:HD12	2:H:182:LEU:O	2.18	0.43
3:J:141:LEU:HD13	3:J:141:LEU:HA	1.72	0.43
1:A:165:PRO:HD2	1:A:220:PRO:HB2	2.01	0.43
3:I:37:VAL:HG21	3:L:180:TYR:OH	2.19	0.43
3:J:136:GLY:O	3:J:137:VAL:O	2.36	0.43
1:E:54:ILE:HG13	1:E:55:SER:N	2.34	0.43
2:F:62:ARG:HD2	2:F:78:SER:O	2.19	0.43
2:F:141:TYR:CG	2:F:142:PRO:HA	2.54	0.43
2:H:79:LEU:CD2	2:H:84:PHE:HE1	2.31	0.43
3:J:180:TYR:HA	3:J:183:CYS:SG	2.58	0.43
1:A:28:SER:HB3	1:G:79:LYS:HZ1	1.84	0.42
1:E:72:THR:OG1	1:E:85:GLN:HB3	2.19	0.42
3:I:148:ILE:HD11	3:L:185:PHE:HE2	1.84	0.42
3:L:25:HIS:CD2	3:L:26:PRO:HD2	2.49	0.42
2:B:62:ARG:HD2	2:B:78:SER:O	2.19	0.42
2:B:80:GLN:OE1	2:B:81:PRO:HD2	2.19	0.42
2:B:148:GLN:O	2:B:195:CYS:HA	2.19	0.42
2:F:82:GLU:OE1	2:F:82:GLU:N	2.41	0.42
3:J:120:VAL:HG23	3:J:126:VAL:HG11	2.00	0.42
3:K:160:ILE:H	3:K:160:ILE:HG12	1.54	0.42
1:A:187:VAL:CG1	2:B:163:SER:HB3	2.50	0.42
2:D:137:LEU:HD12	2:D:137:LEU:N	2.34	0.42
2:D:155:LEU:HD23	2:D:155:LEU:HA	1.81	0.42
2:H:60:PRO:HG2	2:H:62:ARG:NH2	2.35	0.42
3:J:141:LEU:HD21	3:K:179:TRP:CZ3	2.54	0.42
3:J:191:LEU:HD12	3:J:191:LEU:C	2.40	0.42
2:B:156:GLN:HA	2:B:156:GLN:NE2	2.28	0.42
1:C:178:THR:HG23	1:C:179:SER:N	2.35	0.42
2:D:170:LYS:N	2:D:170:LYS:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:39:LEU:O	3:I:43:ILE:HG13	2.20	0.42
2:B:74:LEU:HD23	2:B:75:THR:H	1.84	0.42
3:I:166:PHE:CD2	3:L:135:ASN:O	2.72	0.42
3:L:24:LEU:HD12	3:L:25:HIS:H	1.85	0.42
1:A:79:LYS:NZ	1:G:27:ALA:O	2.53	0.42
2:B:51:SER:O	2:B:52:ALA:HB3	2.20	0.42
1:C:55:SER:O	1:C:59:GLY:N	2.50	0.42
1:E:15:VAL:CG1	1:E:129:VAL:HG22	2.49	0.42
2:F:33:ALA:HA	2:F:51:SER:HA	2.01	0.42
1:G:173:ASN:HB3	1:G:176:ALA:HB3	2.02	0.42
3:I:147:LYS:HZ3	3:J:147:LYS:HG2	1.84	0.42
3:J:149:LEU:N	3:J:149:LEU:HD22	2.35	0.42
2:B:40:LYS:HB3	2:B:41:PRO:HD2	2.02	0.42
2:B:194:ALA:HB2	2:B:209:SER:OG	2.19	0.42
1:C:108:TYR:OH	1:C:115:ASN:O	2.37	0.42
1:E:40:VAL:HG13	1:E:49:GLU:O	2.20	0.42
1:E:126:LEU:HD11	1:E:128:THR:OG1	2.20	0.42
1:E:178:THR:HG23	1:E:179:SER:H	1.85	0.42
2:F:74:LEU:HD22	2:F:76:ILE:CD1	2.50	0.42
2:F:119:PHE:HB2	2:F:134:VAL:HB	2.01	0.42
2:F:152:ASP:OD1	2:F:190:HIS:HB3	2.20	0.42
1:G:181:VAL:HG12	1:G:200:VAL:HG13	2.01	0.42
3:I:153:PHE:O	3:I:157:LEU:HB2	2.20	0.42
3:J:41:ILE:O	3:J:45:THR:OG1	2.37	0.42
1:C:137:PRO:HD2	1:C:223:THR:OG1	2.19	0.42
2:D:60:PRO:HB2	2:D:62:ARG:HG2	2.02	0.42
1:G:113:HIS:O	2:H:95:ARG:NH2	2.53	0.42
1:G:156:LEU:HB2	1:G:200:VAL:HG23	2.01	0.42
1:G:178:THR:HG23	1:G:179:SER:N	2.34	0.42
3:I:102:PRO:O	3:I:106:THR:HG23	2.20	0.42
3:I:147:LYS:HZ1	3:J:147:LYS:HB3	1.84	0.42
3:J:120:VAL:HG23	3:J:126:VAL:CG1	2.49	0.42
2:B:114:PRO:HD3	2:B:199:HIS:ND1	2.35	0.42
1:C:27:ALA:HB1	1:C:30:PHE:CZ	2.55	0.42
1:C:42:GLN:HG3	1:C:47:GLY:O	2.20	0.42
1:C:143:ALA:HB1	1:C:232:LYS:HG2	2.01	0.42
1:G:40:VAL:HG13	1:G:49:GLU:O	2.20	0.42
3:I:145:LEU:HD12	3:I:145:LEU:O	2.20	0.42
3:L:112:LEU:HA	3:L:115:ILE:CG1	2.50	0.42
1:A:137:PRO:HB2	1:A:160:VAL:HG13	2.02	0.41
1:E:51:VAL:CG1	1:E:67:VAL:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:TYR:HD2	1:E:122:GLY:O	2.02	0.41
1:G:89:LEU:HD23	1:G:89:LEU:HA	1.92	0.41
1:A:15:VAL:CG1	1:A:129:VAL:HG22	2.50	0.41
2:B:108:LYS:HE2	2:B:108:LYS:HB3	1.86	0.41
1:C:68:LYS:HE3	1:C:68:LYS:HB2	1.93	0.41
1:C:111:TYR:CD1	3:L:23:VAL:HG12	2.55	0.41
1:G:113:HIS:HE1	3:K:131:ASN:OD1	2.02	0.41
3:I:154:TRP:CH2	3:I:177:LEU:HD22	2.55	0.41
3:J:141:LEU:CG	3:J:144:ILE:HD11	2.47	0.41
2:F:42:GLY:C	2:F:43:LYS:HD2	2.41	0.41
2:F:81:PRO:HA	2:F:84:PHE:HE2	1.85	0.41
3:J:144:ILE:HG13	3:J:145:LEU:N	2.34	0.41
1:A:142:LEU:HD13	2:B:119:PHE:CD2	2.55	0.41
2:D:132:SER:HA	2:D:180:LEU:O	2.20	0.41
2:D:183:SER:OG	2:D:186:ASP:OD2	2.37	0.41
1:G:38:HIS:N	1:G:100:ALA:O	2.47	0.41
3:J:191:LEU:HD11	3:K:42:ASN:ND2	2.36	0.41
3:L:101:ARG:N	3:L:102:PRO:HD2	2.35	0.41
1:C:50:TRP:CE3	1:C:64:ALA:HB2	2.56	0.41
2:D:156:GLN:HE21	2:D:156:GLN:CA	2.30	0.41
1:G:58:TYR:O	3:K:134:TRP:HD1	2.03	0.41
1:G:126:LEU:HD13	1:G:126:LEU:C	2.40	0.41
2:H:79:LEU:HG	2:H:84:PHE:CE1	2.56	0.41
2:H:80:GLN:OE1	2:H:81:PRO:HD2	2.20	0.41
3:L:115:ILE:H	3:L:115:ILE:HG12	1.65	0.41
1:A:164:PHE:HA	1:A:165:PRO:HA	1.77	0.41
2:B:22:ILE:O	2:B:73:THR:HG23	2.20	0.41
2:B:141:TYR:CG	2:B:142:PRO:HA	2.56	0.41
1:G:116:TYR:H	2:H:92:SER:HB3	1.85	0.41
1:G:143:ALA:CB	1:G:232:LYS:HG2	2.51	0.41
2:H:184:LYS:HE2	2:H:184:LYS:HB3	1.92	0.41
2:H:194:ALA:HB2	2:H:209:SER:HB2	2.02	0.41
3:J:160:ILE:HD12	3:J:161:PHE:CG	2.56	0.41
3:J:183:CYS:O	3:J:187:THR:N	2.49	0.41
3:K:141:LEU:HD12	3:K:144:ILE:CG1	2.50	0.41
1:A:39:TRP:CG	1:A:84:LEU:HD22	2.56	0.41
2:B:116:VAL:CG2	2:B:197:VAL:HG21	2.50	0.41
2:H:51:SER:O	2:H:52:ALA:HB3	2.21	0.41
3:J:141:LEU:CD1	3:J:142:PRO:HD2	2.51	0.41
3:J:188:SER:HB3	3:K:156:TRP:HE1	1.85	0.41
1:C:140:PHE:CE2	2:D:125:GLN:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:PHE:CE1	2:D:107:ILE:HG12	2.55	0.41
1:E:166:GLU:CB	1:E:167:PRO:HA	2.51	0.41
1:G:25:CYS:O	1:G:81:THR:HG23	2.21	0.41
1:G:111:TYR:CD2	1:G:111:TYR:N	2.88	0.41
2:H:80:GLN:HB3	2:H:81:PRO:HD2	2.02	0.41
3:I:153:PHE:CZ	3:I:157:LEU:HD12	2.56	0.41
3:J:166:PHE:CE1	3:K:136:GLY:CA	3.03	0.41
3:K:106:THR:O	3:K:109:PRO:HD2	2.20	0.41
3:K:142:PRO:O	3:K:144:ILE:N	2.43	0.41
3:L:113:ILE:HG23	3:L:117:LEU:HD23	2.03	0.41
1:C:4:GLU:O	1:C:29:GLY:HA3	2.21	0.41
1:C:116:TYR:H	2:D:92:SER:HB2	1.86	0.41
2:D:55:LEU:HD13	2:D:55:LEU:C	2.40	0.41
2:D:185:ALA:O	2:D:189:LYS:HG3	2.21	0.41
1:E:67:VAL:HB	1:E:71:PHE:CG	2.55	0.41
1:E:178:THR:HG23	1:E:179:SER:N	2.35	0.41
2:F:137:LEU:HD12	2:F:137:LEU:N	2.35	0.41
1:G:178:THR:HG23	1:G:179:SER:H	1.85	0.41
3:I:27:ALA:HB2	3:I:138:VAL:O	2.21	0.41
3:J:31:LEU:C	3:J:31:LEU:HD23	2.41	0.41
3:J:157:LEU:O	3:J:157:LEU:HD23	2.21	0.41
3:K:183:CYS:O	3:K:187:THR:N	2.51	0.41
3:L:141:LEU:CD1	3:L:144:ILE:HG12	2.47	0.41
2:B:36:TRP:CE3	2:B:89:CYS:HB3	2.55	0.41
1:E:166:GLU:OE2	1:E:186:ALA:HB3	2.21	0.41
1:G:111:TYR:HB3	3:K:23:VAL:O	2.20	0.41
2:H:36:TRP:CZ3	2:H:89:CYS:HB3	2.55	0.41
3:I:135:ASN:ND2	3:L:169:VAL:HG11	2.35	0.41
3:L:162:TYR:O	3:L:163:LYS:HB2	2.21	0.41
1:A:113:HIS:CE1	3:I:131:ASN:ND2	2.89	0.40
1:A:113:HIS:HE1	3:I:131:ASN:ND2	2.19	0.40
2:B:3:ILE:O	2:B:98:THR:HG21	2.21	0.40
1:E:213:ILE:N	1:E:213:ILE:HD12	2.36	0.40
2:H:119:PHE:HB2	2:H:134:VAL:HB	2.03	0.40
3:I:141:LEU:HD12	3:I:141:LEU:HA	1.70	0.40
3:K:120:VAL:HG13	3:K:126:VAL:HG11	2.02	0.40
2:B:107:ILE:HG22	2:B:108:LYS:N	2.36	0.40
2:B:171:ASP:OD1	2:B:171:ASP:N	2.53	0.40
1:G:63:TYR:OH	1:G:72:THR:HA	2.21	0.40
3:J:173:ALA:HB2	3:K:140:TYR:CD1	2.55	0.40
2:B:39:GLN:O	2:B:85:ALA:HB1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:VAL:HG13	2:D:193:TYR:CE2	2.56	0.40
1:G:178:THR:O	1:G:181:VAL:HG22	2.22	0.40
2:H:76:ILE:HG21	2:H:79:LEU:HD12	2.03	0.40
2:H:95:ARG:HA	2:H:96:PRO:C	2.41	0.40
3:K:162:TYR:O	3:K:164:GLY:N	2.53	0.40
1:C:5:VAL:O	1:C:6:GLN:HB3	2.21	0.40
1:E:178:THR:O	1:E:181:VAL:HG22	2.21	0.40
2:F:67:ARG:NH1	2:F:72:PHE:CE2	2.89	0.40
1:G:196:LEU:C	1:G:196:LEU:HD12	2.41	0.40
3:I:135:ASN:HD22	3:L:169:VAL:CG1	2.33	0.40
3:K:160:ILE:HB	3:K:161:PHE:HD1	1.86	0.40
1:A:50:TRP:CZ3	1:A:64:ALA:HB2	2.56	0.40
1:A:112:PRO:HG2	1:A:113:HIS:HD2	1.85	0.40
1:A:112:PRO:O	1:A:113:HIS:CB	2.69	0.40
2:B:184:LYS:HE2	2:B:184:LYS:HB3	1.90	0.40
2:D:193:TYR:O	2:D:209:SER:OG	2.25	0.40
2:F:81:PRO:O	2:F:84:PHE:HD2	2.04	0.40
3:J:156:TRP:CG	3:K:185:PHE:HD1	2.38	0.40
3:L:143:ILE:CG1	3:L:144:ILE:N	2.85	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	227/239 (95%)	214 (94%)	13 (6%)	0	100	100
1	C	226/239 (95%)	216 (96%)	9 (4%)	1 (0%)	34	72
1	E	228/239 (95%)	214 (94%)	14 (6%)	0	100	100
1	G	227/239 (95%)	215 (95%)	11 (5%)	1 (0%)	34	72
2	B	212/215 (99%)	206 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	208/215 (97%)	201 (97%)	7 (3%)	0	100 100
2	F	211/215 (98%)	204 (97%)	7 (3%)	0	100 100
2	H	211/215 (98%)	203 (96%)	8 (4%)	0	100 100
3	I	130/207 (63%)	119 (92%)	7 (5%)	4 (3%)	4 30
3	J	130/207 (63%)	118 (91%)	10 (8%)	2 (2%)	10 45
3	K	129/207 (62%)	117 (91%)	9 (7%)	3 (2%)	6 36
3	L	133/207 (64%)	119 (90%)	12 (9%)	2 (2%)	10 45
All	All	2272/2644 (86%)	2146 (94%)	113 (5%)	13 (1%)	25 64

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	57	SER
3	I	137	VAL
3	I	169	VAL
3	J	137	VAL
3	J	169	VAL
3	K	169	VAL
3	L	169	VAL
3	L	137	VAL
3	I	134	TRP
3	I	163	LYS
3	K	134	TRP
3	K	137	VAL
1	C	113	HIS

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	191/201 (95%)	187 (98%)	4 (2%)	53 79
1	C	193/201 (96%)	190 (98%)	3 (2%)	62 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	192/201 (96%)	187 (97%)	5 (3%)	46 74
1	G	191/201 (95%)	187 (98%)	4 (2%)	53 79
2	B	189/190 (100%)	188 (100%)	1 (0%)	88 94
2	D	188/190 (99%)	186 (99%)	2 (1%)	73 88
2	F	188/190 (99%)	188 (100%)	0	100 100
2	H	188/190 (99%)	187 (100%)	1 (0%)	88 94
3	I	117/185 (63%)	105 (90%)	12 (10%)	7 32
3	J	117/185 (63%)	107 (92%)	10 (8%)	10 39
3	K	116/185 (63%)	108 (93%)	8 (7%)	15 47
3	L	120/185 (65%)	109 (91%)	11 (9%)	9 36
All	All	1990/2304 (86%)	1929 (97%)	61 (3%)	40 70

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	104	TRP
1	A	105	SER
1	A	200	VAL
2	B	156	GLN
1	C	104	TRP
1	C	110	VAL
1	C	200	VAL
2	D	156	GLN
2	D	180	LEU
1	E	103	ILE
1	E	107	TRP
1	E	111	TYR
1	E	118	MET
1	E	200	VAL
1	G	103	ILE
1	G	111	TYR
1	G	114	ASP
1	G	200	VAL
2	H	159	ASN
3	I	25	HIS
3	I	103	MET
3	I	105	TYR

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Mol	Chain	Res	Type
3	I	107	TRP
3	I	120	VAL
3	I	123	PHE
3	I	127	TYR
3	I	138	VAL
3	I	139	VAL
3	I	141	LEU
3	I	145	LEU
3	I	176	TRP
3	J	107	TRP
3	J	120	VAL
3	J	123	PHE
3	J	127	TYR
3	J	130	LEU
3	J	137	VAL
3	J	139	VAL
3	J	141	LEU
3	J	166	PHE
3	J	170	SER
3	K	118	ARG
3	K	127	TYR
3	K	131	ASN
3	K	138	VAL
3	K	139	VAL
3	K	141	LEU
3	K	160	ILE
3	K	176	TRP
3	L	98	MET
3	L	103	MET
3	L	105	TYR
3	L	107	TRP
3	L	120	VAL
3	L	127	TYR
3	L	137	VAL
3	L	138	VAL
3	L	139	VAL
3	L	141	LEU
3	L	166	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
2	F	156	GLN
2	H	7	GLN
2	H	138	ASN
2	H	156	GLN
3	J	131	ASN
3	L	25	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

1 ligand is 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	$\#\|Z\| > 2$
4	LMT	L	301	-	36,36,36	1.13	5 (13%)	47,47,47	1.02	2 (4%)

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
4	LMT	L	301	-	-	13/21/61/61	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	LMT	O3'-C3'	-2.72	1.36	1.43
4	L	301	LMT	O3B-C3B	-2.47	1.37	1.43
4	L	301	LMT	O2B-C2B	-2.26	1.37	1.43
4	L	301	LMT	O2'-C2'	-2.20	1.37	1.43
4	L	301	LMT	O4'-C4B	-2.16	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	301	LMT	C1-O1'-C1'	3.78	120.12	113.84
4	L	301	LMT	O1'-C1'-C2'	2.68	112.49	108.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

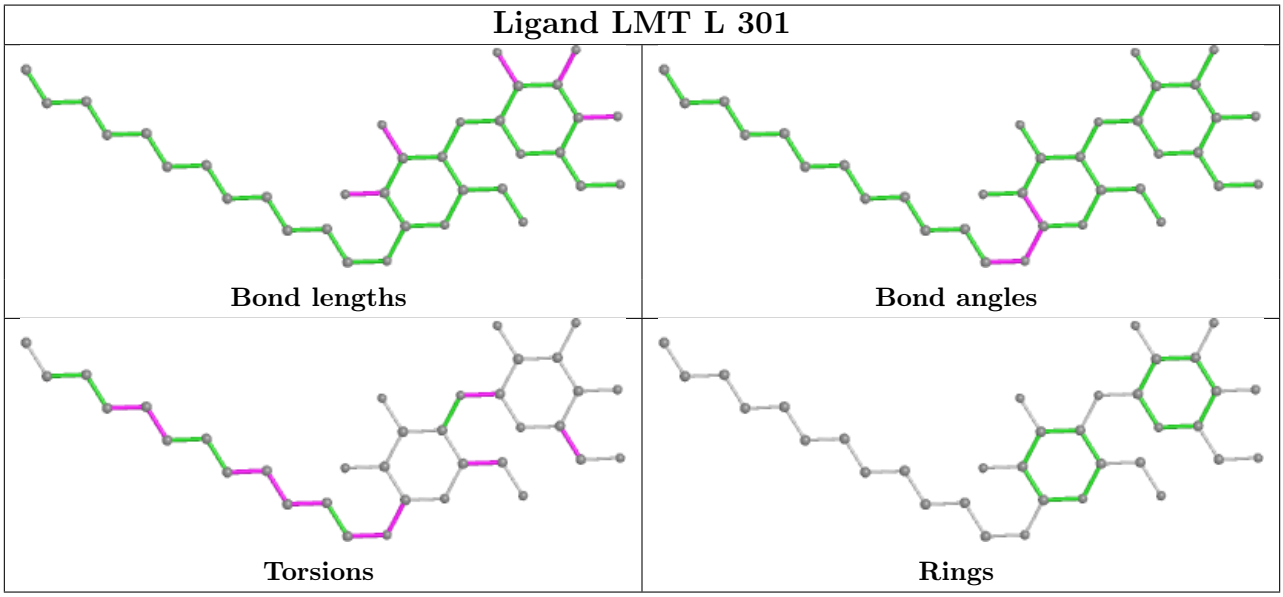
Mol	Chain	Res	Type	Atoms
4	L	301	LMT	C2-C1-O1'-C1'
4	L	301	LMT	O5B-C5B-C6B-O6B
4	L	301	LMT	O5'-C5'-C6'-O6'
4	L	301	LMT	C2B-C1B-O1B-C4'
4	L	301	LMT	C2'-C1'-O1'-C1
4	L	301	LMT	O5B-C1B-O1B-C4'
4	L	301	LMT	C4B-C5B-C6B-O6B
4	L	301	LMT	C1-C2-C3-C4
4	L	301	LMT	C6-C7-C8-C9
4	L	301	LMT	C2-C3-C4-C5
4	L	301	LMT	C4'-C5'-C6'-O6'
4	L	301	LMT	C7-C8-C9-C10
4	L	301	LMT	C3-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	LMT	1	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	229/239 (95%)	-0.10	1 (0%) 92 90	65, 90, 131, 238	0
1	C	230/239 (96%)	-0.18	1 (0%) 92 90	51, 84, 131, 227	0
1	E	230/239 (96%)	-0.11	2 (0%) 84 79	64, 95, 178, 234	0
1	G	229/239 (95%)	0.18	12 (5%) 27 24	71, 114, 208, 242	0
2	B	214/215 (99%)	-0.23	1 (0%) 91 88	58, 95, 141, 184	0
2	D	212/215 (98%)	-0.27	0 100 100	68, 101, 139, 202	0
2	F	213/215 (99%)	-0.19	1 (0%) 91 88	69, 107, 148, 174	0
2	H	213/215 (99%)	0.28	24 (11%) 5 6	82, 135, 204, 239	0
3	I	134/207 (64%)	-0.15	1 (0%) 87 83	60, 112, 182, 229	0
3	J	134/207 (64%)	0.22	12 (8%) 9 10	81, 133, 220, 263	0
3	K	133/207 (64%)	0.40	7 (5%) 26 24	90, 145, 255, 279	0
3	L	137/207 (66%)	-0.09	3 (2%) 62 56	58, 107, 190, 256	0
All	All	2308/2644 (87%)	-0.04	65 (2%) 53 47	51, 105, 195, 279	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	42	ASN	6.6
2	H	178	SER	4.9
2	H	3	ILE	4.7
2	H	182	LEU	4.7
3	J	42	ASN	4.3
3	K	19	PRO	4.1
1	G	150	SER	4.0
1	G	35	SER	3.9
1	G	232	LYS	3.8
3	J	123	PHE	3.5
3	J	41	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
3	K	15	ALA	3.4
3	J	124	GLY	3.4
3	K	16	ILE	3.3
1	G	147	LYS	3.3
2	H	160	SER	3.3
2	H	134	VAL	3.3
2	H	181	THR	3.3
1	G	148	SER	3.2
2	H	132	SER	3.2
1	G	104	TRP	3.1
3	L	43	ILE	3.1
3	J	19	PRO	3.0
1	G	106	TYR	3.0
3	L	42	ASN	3.0
3	J	15	ALA	3.0
2	H	68	SER	2.9
1	G	155	ALA	2.9
2	H	4	GLN	2.7
2	H	187	TYR	2.7
2	H	135	CYS	2.7
2	H	2	ASP	2.7
3	L	44	ALA	2.6
1	E	149	THR	2.6
2	H	130	THR	2.6
2	H	161	GLN	2.5
3	K	41	ILE	2.5
1	A	151	GLY	2.5
1	G	105	SER	2.5
1	G	154	ALA	2.5
3	J	114	PHE	2.5
2	B	156	GLN	2.4
2	H	122	SER	2.4
2	H	162	GLU	2.4
3	J	17	PHE	2.4
3	J	45	THR	2.4
1	G	149	THR	2.3
2	H	5	MET	2.3
2	H	180	LEU	2.3
1	E	150	SER	2.3
2	H	128	SER	2.2
1	C	18	GLY	2.2
1	G	146	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	136	LEU	2.2
3	I	43	ILE	2.2
2	H	28	GLN	2.1
2	H	29	SER	2.1
3	J	20	ILE	2.1
3	J	38	SER	2.1
2	H	179	THR	2.1
2	H	133	VAL	2.1
3	K	121	TYR	2.1
3	K	138	VAL	2.0
2	H	136	LEU	2.0
3	J	16	ILE	2.0

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)

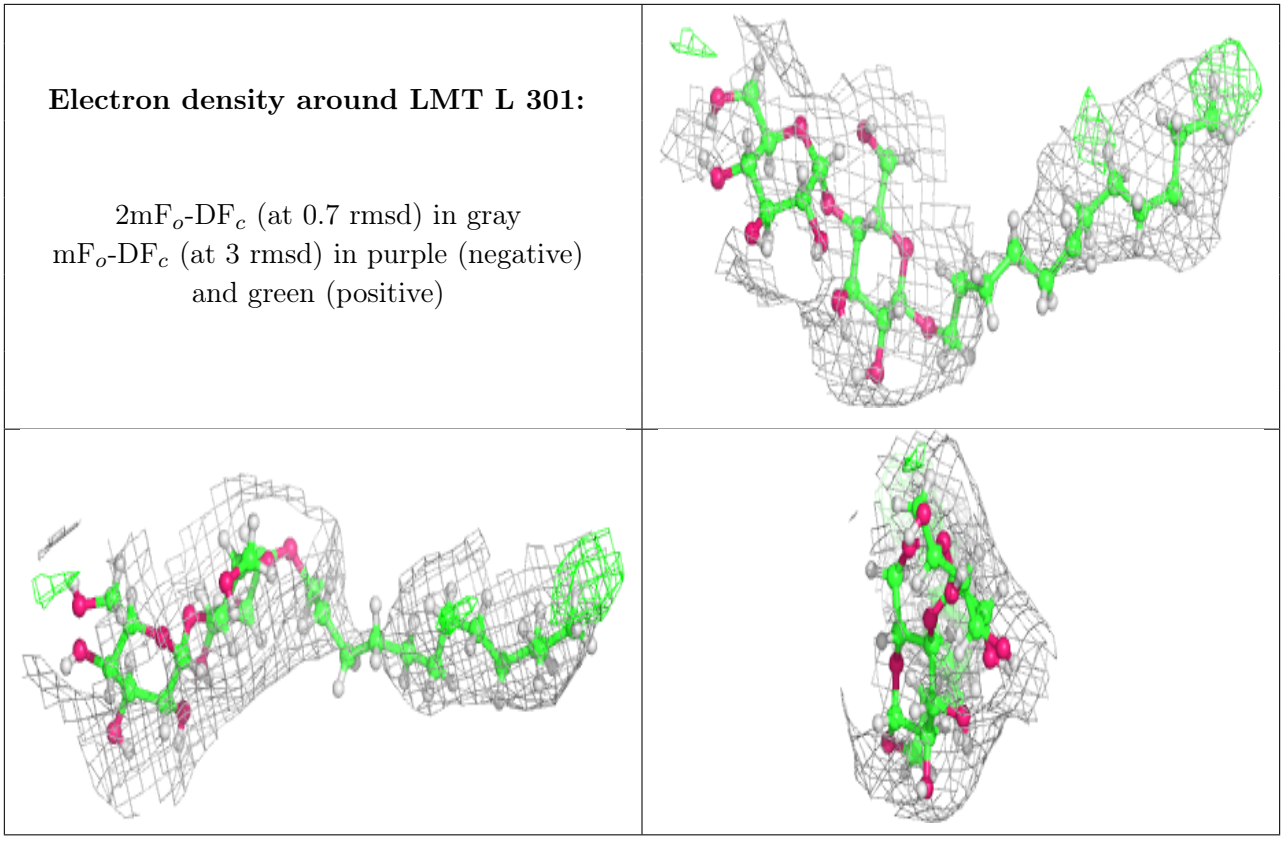
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	LMT	L	301	35/35	0.65	0.21	139,193,233,236	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT L 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.