Full wwPDB EM Validation Report (i)

Nov 17, 2022 – 01:41 AM EST

PDB ID	:	7LF2
EMDB ID	:	EMD-23298
Title	:	Trimeric human Arginase 1 in complex with mAb4
Authors	:	Gomez-Llorente, Y.; Scapin, G.; Palte, R.L.
Deposited on	:	2021-01-15
Resolution	:	3.72 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

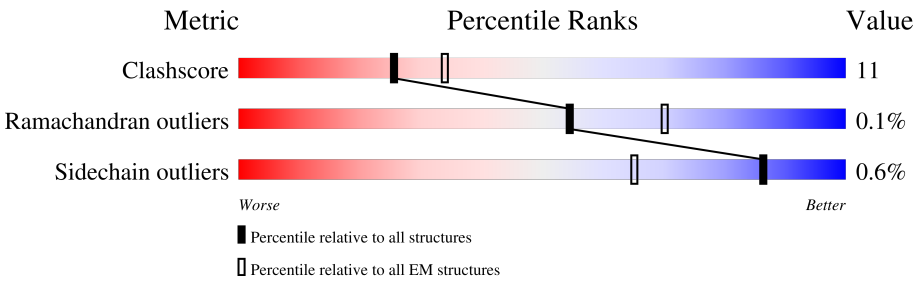
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.72 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)	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%

Mol	Chain	Length	Quality of chain
1	A	322	78% 20% •
1	B	322	80% 18% •
1	C	322	80% 19% •
1	J	322	82% 17% •
1	Q	322	83% 16% •
1	R	322	83% 16% •
2	D	443	31% 16% • 52%
2	F	443	30% 17% • 52%
2	G	443	30% 16% • 52%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	443	31% 16% 52%
2	O	443	31% 16% 52%
2	P	443	30% 16% 52%
3	E	214	63% 36%
3	H	214	61% 38%
3	I	214	63% 36%
3	L	214	62% 37%
3	M	214	63% 36%
3	N	214	61% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33798 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 Arginase-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	317	2409	1535	411	457	6	0	0
1	B	317	2409	1535	411	457	6	0	0
1	C	317	2409	1535	411	457	6	0	0
1	J	317	2409	1535	411	457	6	0	0
1	Q	317	2409	1535	411	457	6	0	0
1	R	317	2409	1535	411	457	6	0	0

- Molecule 2 is a protein called mAb4 monoclonal antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	211	1581	1008	249	317	7	0	0
2	G	211	1581	1008	249	317	7	0	0
2	F	211	1581	1008	249	317	7	0	0
2	K	211	1581	1008	249	317	7	0	0
2	O	211	1581	1008	249	317	7	0	0
2	P	211	1581	1008	249	317	7	0	0

- Molecule 3 is a protein called mAb4 monoclonal antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	214	1641	1025	280	331	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	214	1641	1025	280	331	5	0	0
3	H	214	1641	1025	280	331	5	0	0
3	L	214	1641	1025	280	331	5	0	0
3	M	214	1641	1025	280	331	5	0	0
3	N	214	1641	1025	280	331	5	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

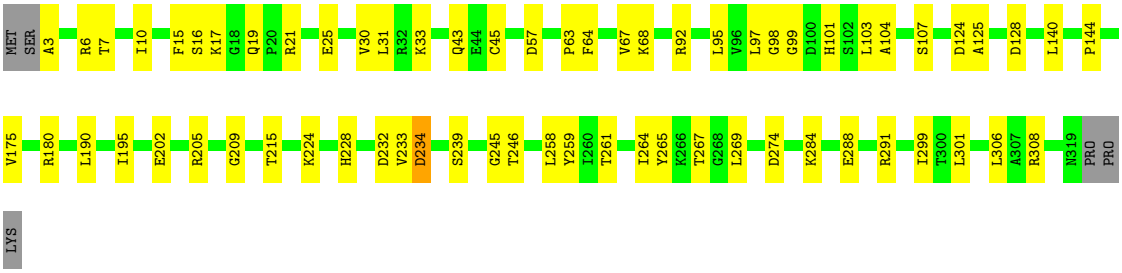
Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
4	A	2	2	2	0
4	B	2	2	2	0
4	C	2	2	2	0
4	J	2	2	2	0
4	Q	2	2	2	0
4	R	2	2	2	0

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. 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. 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.

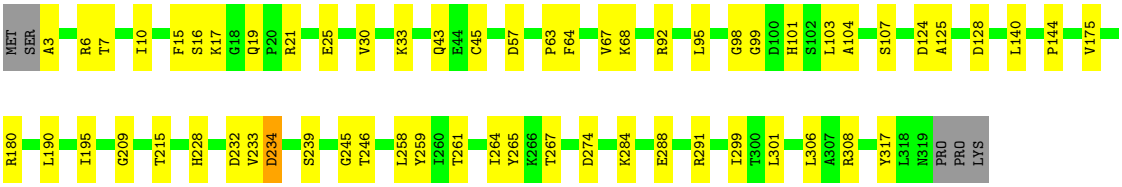
• Molecule 1: Arginase-1

Chain A:



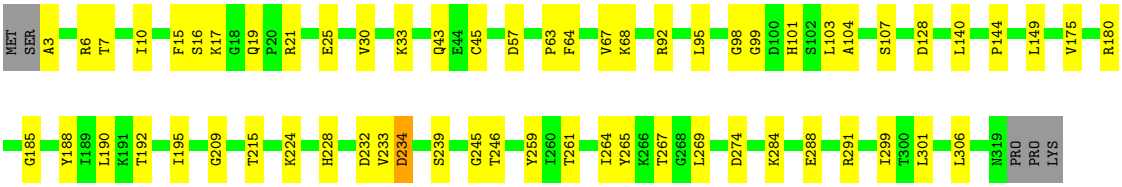
• Molecule 1: Arginase-1

Chain B:



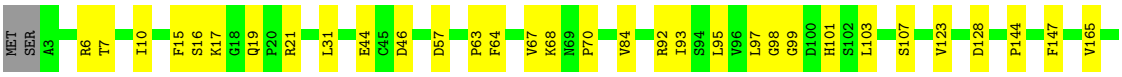
• Molecule 1: Arginase-1

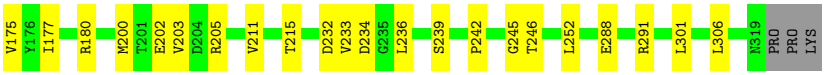
Chain C:



• Molecule 1: Arginase-1

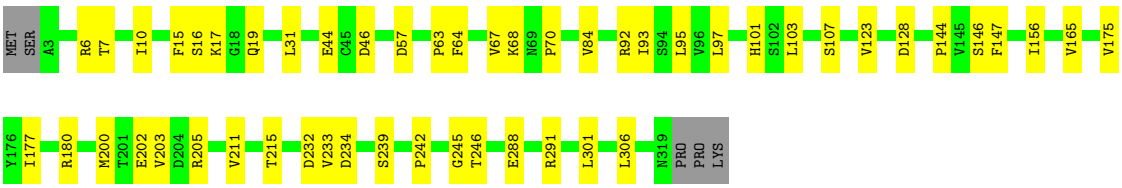
Chain J:





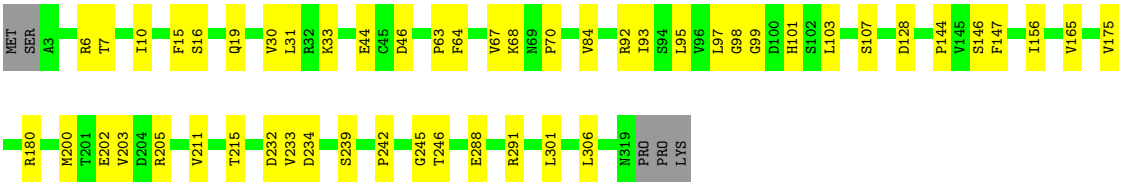
• Molecule 1: Arginase-1

Chain Q:



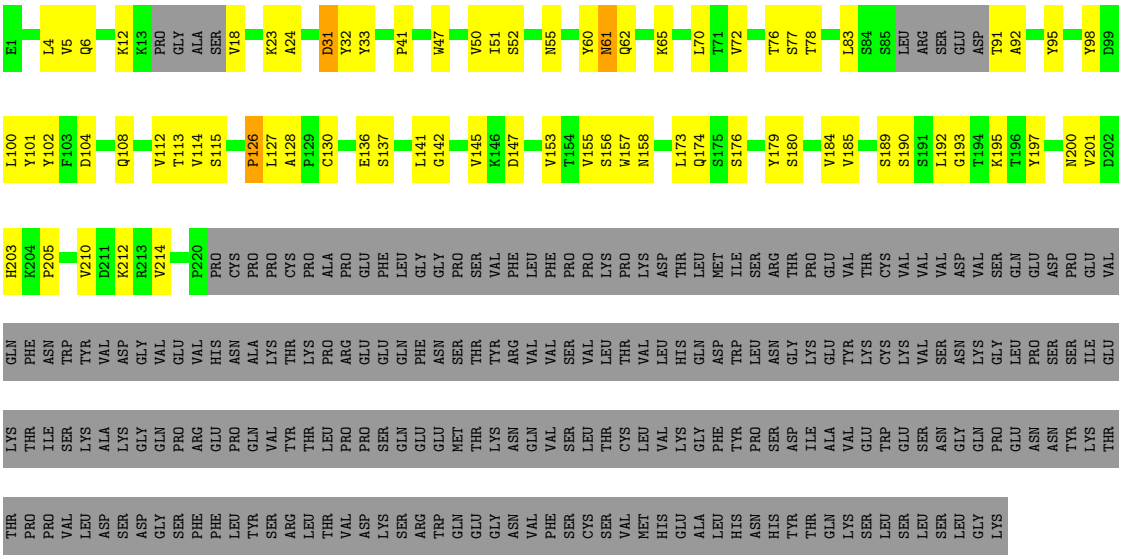
• Molecule 1: Arginase-1

Chain R:



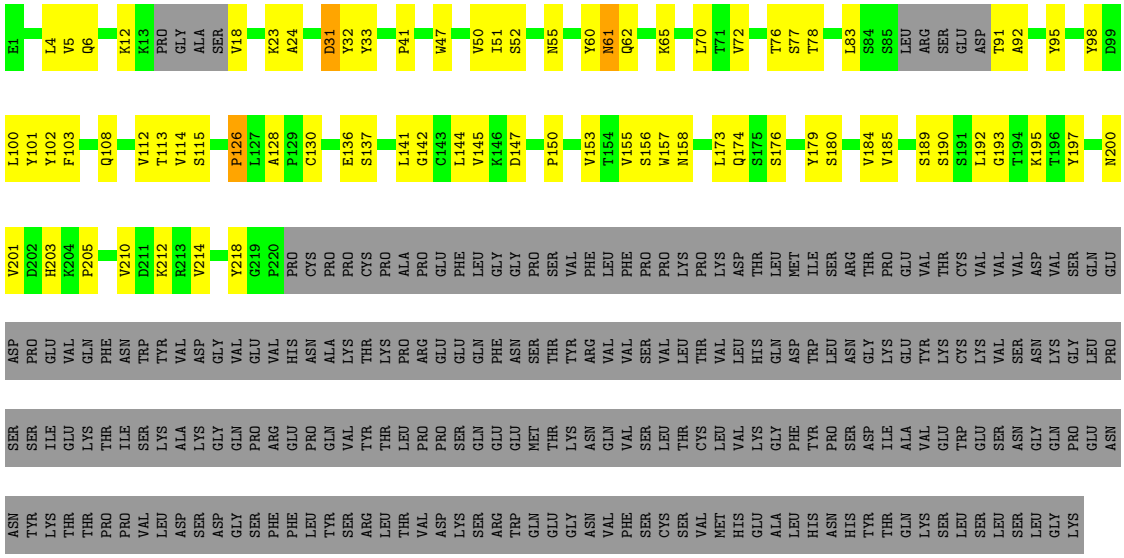
• Molecule 2: mAb4 monoclonal antibody heavy chain

Chain D:



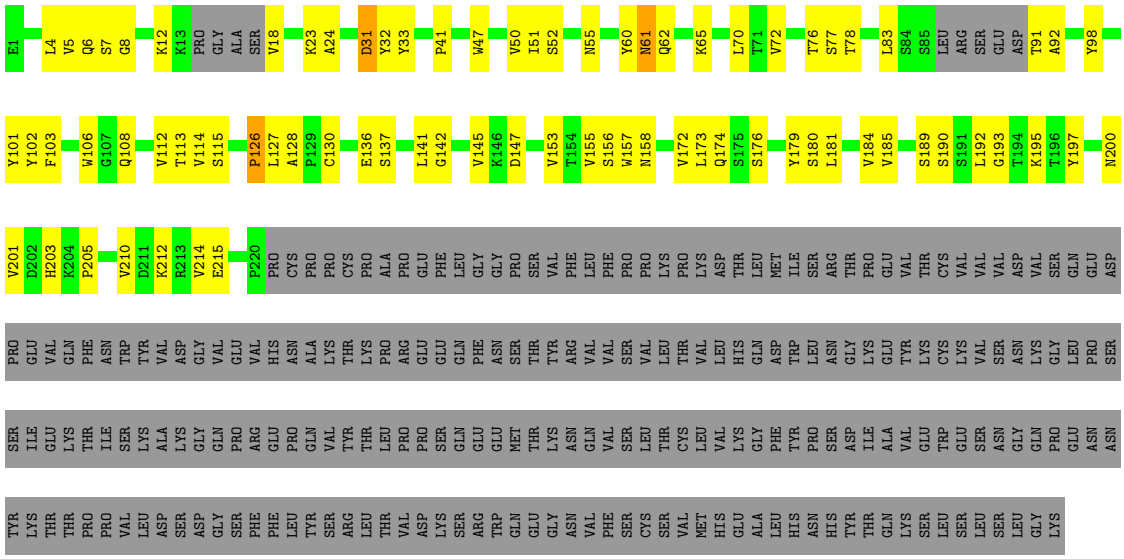
• Molecule 2: mAb4 monoclonal antibody heavy chain

Chain G:



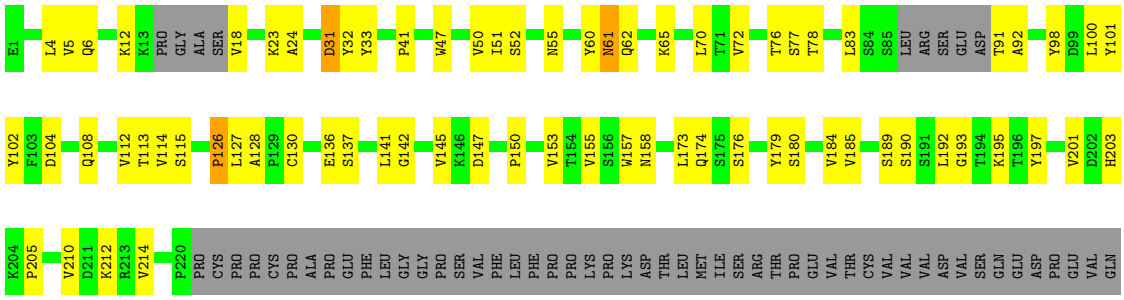
• Molecule 2: mAb4 monoclonal antibody heavy chain

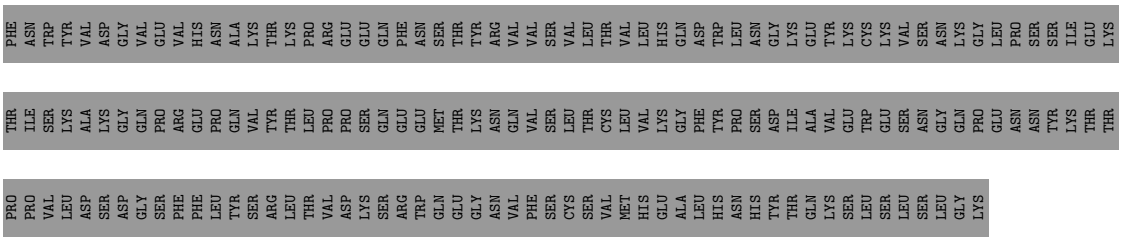
Chain F: 30% 17% • 52%



• Molecule 2: mAb4 monoclonal antibody heavy chain

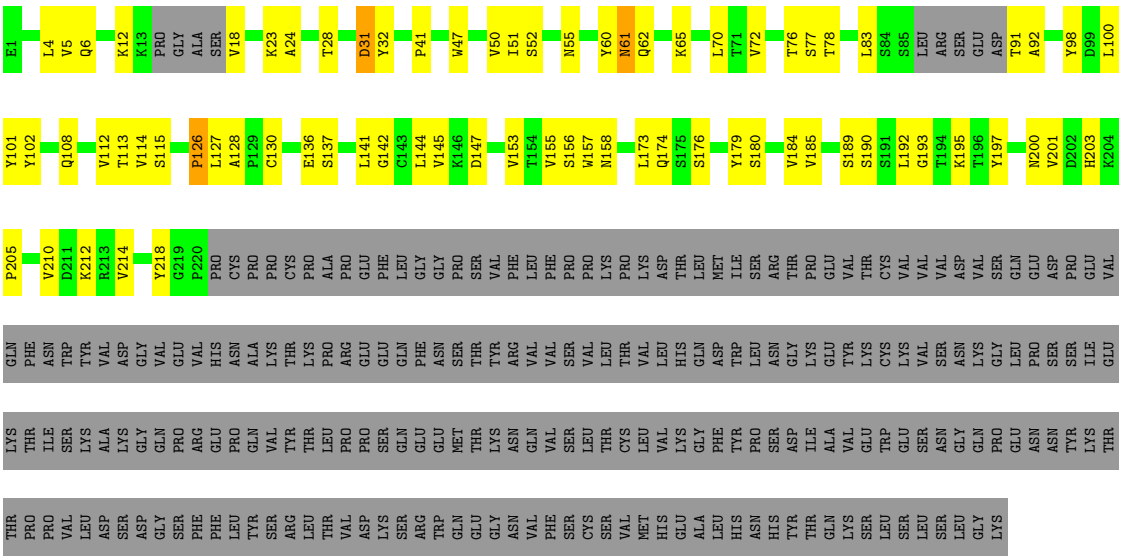
Chain K: 31% 16% • 52%





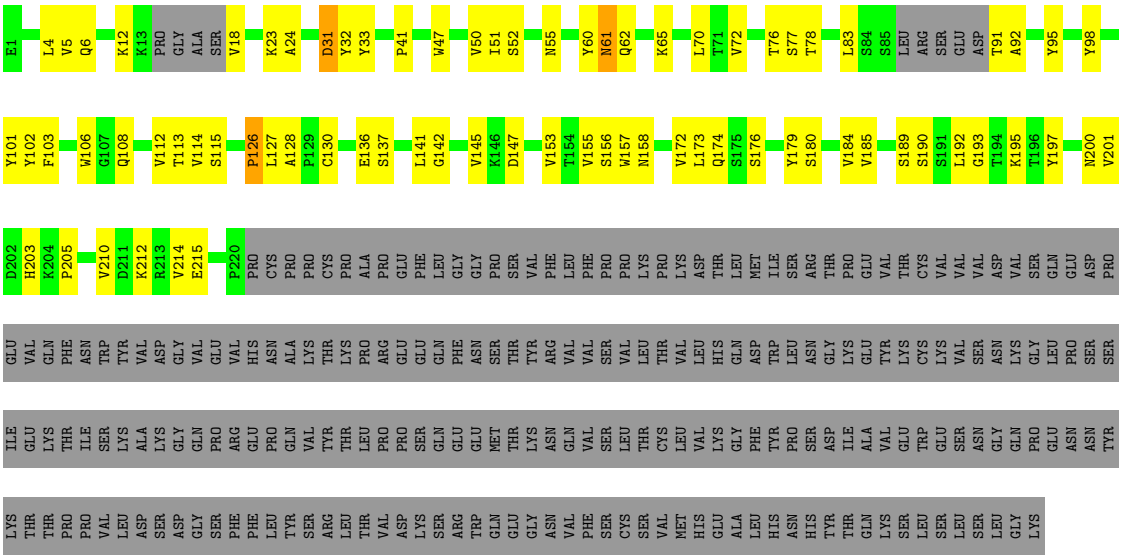
• Molecule 2: mAb4 monoclonal antibody heavy chain

Chain O: 31% 16% • 52%



• Molecule 2: mAb4 monoclonal antibody heavy chain

Chain P: 30% 16% • 52%



• Molecule 3: mAb4 monoclonal antibody light chain

Chain E: 63% 36%

E1 I2 Q6 L11 P15 A19 T20 S26 Q27 R28 I29 D32 L33 H34 Q37 L46 L47 I48 K49 Y50 Q53 I58 P59 S60 R61 T74 I75 S76 S77 L78 E79 P80 E81 D82 V85 Y86 Y87 Q90 S91 P95 R96 T97 G101 T102 K103

L104 E105 R108 T109 P113 I117 F118 S131 V132 V133 C134 L135 L136 N137 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 N158 V163 T164 S174 L175 L179 T180 Y186 E187 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201 N210 R211 G212

E213 C214

- Molecule 3: mAb4 monoclonal antibody light chain

Chain I: 63% 36%

E1 I2 Q6 L11 P15 A19 T20 S26 Q27 R28 I29 D32 L33 H34 Q37 L47 I48 K49 Y50 Q53 I58 P59 S60 R61 D70 T74 I75 S76 S77 L78 E79 P80 E81 D82 V85 Y86 Y87 Q90 S91 P95 R96 T97 G101 T102

K103 L104 E105 R108 T109 P113 I117 F118 S131 V132 V133 C134 L135 L136 N137 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 N158 V163 T164 S174 L175 L179 T180 Y186 E187 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201 N210 R211

G212 E213 C214

- Molecule 3: mAb4 monoclonal antibody light chain

Chain H: 61% 38%

E1 I2 Q6 L11 P15 A19 T20 S26 Q27 R28 I29 D32 L33 H34 Q37 P44 R45 L46 L47 I48 K49 Y50 Q53 I58 P59 S60 R61 D70 T74 I75 S76 S77 L78 E79 P80 E81 D82 V85 Y86 Y87 Q90 S91 P95 R96 T97

G101 T102 K103 L104 E105 R108 T109 P113 I117 F118 S131 V132 V133 C134 L135 L136 N137 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 N158 S159 Q160 V163 T164 S174 L175 L179 T180 Y186 E187 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199

G200 L201 N210 R211 G212 E213 C214

- Molecule 3: mAb4 monoclonal antibody light chain

Chain L: 62% 37%

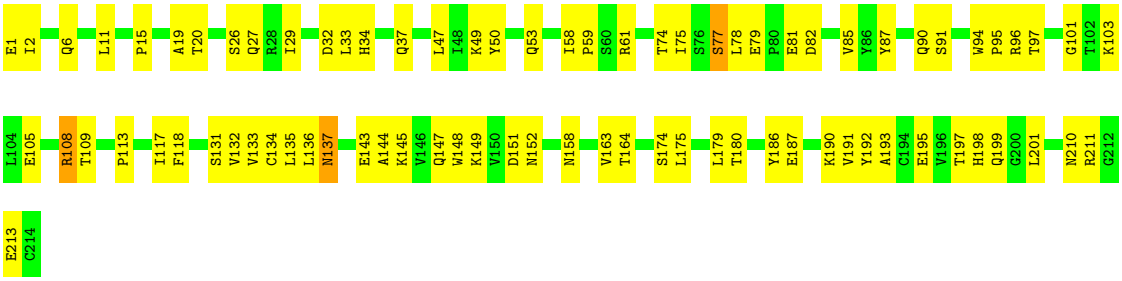
E1 I2 Q6 L11 P15 A19 T20 S26 Q27 R28 I29 D32 L33 H34 Q37 L46 L47 I48 K49 Y50 Q53 I58 P59 S60 R61 D70 T74 I75 S76 S77 L78 E79 P80 E81 D82 V85 Y86 Y87 Q90 S91 W94 P95 R96 T97

G101 T102 K103 L104 E105 R108 T109 P113 I117 F118 S131 V132 V133 C134 L135 L136 N137 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 N158 V163 T164 S174 L175 L179 T180 Y186 E187 K190 V191 Y192 A193 C194 E195 V196 T197 H198 Q199 G200 L201

N210 R211 G212 E213 C214

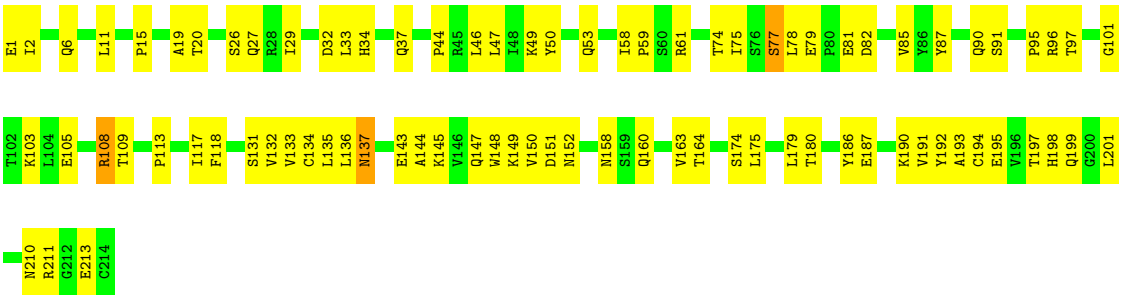
• Molecule 3: mAb4 monoclonal antibody light chain

Chain M: 63% 36%



• Molecule 3: mAb4 monoclonal antibody light chain

Chain N: 61% 38%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31797	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 ($e^-/Å^2$)	44.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	0/2459	0.62	1/3336 (0.0%)
1	B	0.49	0/2459	0.61	1/3336 (0.0%)
1	C	0.49	0/2459	0.61	1/3336 (0.0%)
1	J	0.30	0/2459	0.53	0/3336
1	Q	0.30	0/2459	0.53	0/3336
1	R	0.30	0/2459	0.53	0/3336
2	D	0.38	0/1620	0.65	1/2213 (0.0%)
2	F	0.38	0/1620	0.65	1/2213 (0.0%)
2	G	0.38	0/1620	0.65	1/2213 (0.0%)
2	K	0.38	0/1620	0.65	1/2213 (0.0%)
2	O	0.38	0/1620	0.65	1/2213 (0.0%)
2	P	0.38	0/1620	0.65	1/2213 (0.0%)
3	E	0.38	0/1676	0.62	1/2273 (0.0%)
3	H	0.38	0/1676	0.62	1/2273 (0.0%)
3	I	0.38	0/1676	0.62	1/2273 (0.0%)
3	L	0.38	0/1676	0.62	1/2273 (0.0%)
3	M	0.38	0/1676	0.62	1/2273 (0.0%)
3	N	0.38	0/1676	0.62	1/2273 (0.0%)
All	All	0.39	0/34530	0.61	15/46932 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2
2	F	0	2
2	G	0	2
2	K	0	2
2	O	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
3	E	0	3
3	H	0	3
3	I	0	3
3	L	0	3
3	M	0	3
3	N	0	3
All	All	0	30

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	234	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	234	ASP	CB-CG-OD1	5.83	123.55	118.30
3	L	33	LEU	CA-CB-CG	5.72	128.47	115.30
3	I	33	LEU	CA-CB-CG	5.72	128.45	115.30
3	E	33	LEU	CA-CB-CG	5.72	128.45	115.30
3	N	33	LEU	CA-CB-CG	5.71	128.44	115.30
3	H	33	LEU	CA-CB-CG	5.71	128.44	115.30
3	M	33	LEU	CA-CB-CG	5.71	128.42	115.30
1	C	234	ASP	CB-CG-OD1	5.59	123.33	118.30
2	P	31	ASP	CB-CG-OD2	5.27	123.04	118.30
2	K	31	ASP	CB-CG-OD2	5.20	122.98	118.30
2	F	31	ASP	CB-CG-OD2	5.19	122.97	118.30
2	G	31	ASP	CB-CG-OD2	5.17	122.95	118.30
2	O	31	ASP	CB-CG-OD2	5.16	122.94	118.30
2	D	31	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	102	TYR	Peptide
2	D	126	PRO	Peptide
3	E	53	GLN	Peptide
3	E	58	ILE	Peptide
3	E	77	SER	Peptide
2	F	102	TYR	Peptide
2	F	126	PRO	Peptide
2	G	102	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	G	126	PRO	Peptide
3	H	53	GLN	Peptide
3	H	58	ILE	Peptide
3	H	77	SER	Peptide
3	I	53	GLN	Peptide
3	I	58	ILE	Peptide
3	I	77	SER	Peptide
2	K	102	TYR	Peptide
2	K	126	PRO	Peptide
3	L	53	GLN	Peptide
3	L	58	ILE	Peptide
3	L	77	SER	Peptide
3	M	53	GLN	Peptide
3	M	58	ILE	Peptide
3	M	77	SER	Peptide
3	N	53	GLN	Peptide
3	N	58	ILE	Peptide
3	N	77	SER	Peptide
2	O	102	TYR	Peptide
2	O	126	PRO	Peptide
2	P	102	TYR	Peptide
2	P	126	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2409	0	2456	37	0
1	B	2409	0	2456	36	0
1	C	2409	0	2456	35	0
1	J	2409	0	2456	34	0
1	Q	2409	0	2456	31	0
1	R	2409	0	2456	32	0
2	D	1581	0	1506	47	0
2	F	1581	0	1506	55	0
2	G	1581	0	1506	52	0
2	K	1581	0	1506	47	0
2	O	1581	0	1506	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1581	0	1506	53	0
3	E	1641	0	1592	47	0
3	H	1641	0	1592	52	0
3	I	1641	0	1592	49	0
3	L	1641	0	1592	49	0
3	M	1641	0	1592	51	0
3	N	1641	0	1592	52	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	J	2	0	0	0	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	33798	0	33324	767	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 11.

All (767) 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)
2:O:28:THR:HG23	2:O:31:ASP:OD2	1.65	0.94
2:O:28:THR:CG2	2:O:31:ASP:OD2	2.30	0.79
3:L:90:GLN:HE21	3:L:97:THR:H	1.36	0.74
3:I:90:GLN:HE21	3:I:97:THR:H	1.36	0.74
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.71	0.72
2:G:60:TYR:HE1	2:G:70:LEU:HG	1.55	0.72
3:N:90:GLN:HE21	3:N:97:THR:H	1.36	0.72
2:K:60:TYR:HE1	2:K:70:LEU:HG	1.55	0.71
2:P:60:TYR:HE1	2:P:70:LEU:HG	1.55	0.71
3:H:90:GLN:HE21	3:H:97:THR:H	1.36	0.71
3:M:90:GLN:HE21	3:M:97:THR:H	1.36	0.71
3:E:90:GLN:HE21	3:E:97:THR:H	1.36	0.71
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.73	0.71
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.72	0.71
2:F:60:TYR:HE1	2:F:70:LEU:HG	1.55	0.70
2:O:60:TYR:HE1	2:O:70:LEU:HG	1.55	0.69
2:D:60:TYR:HE1	2:D:70:LEU:HG	1.55	0.69
2:K:60:TYR:CE1	2:K:70:LEU:HG	2.28	0.69
2:P:60:TYR:CE1	2:P:70:LEU:HG	2.28	0.69
2:G:60:TYR:CE1	2:G:70:LEU:HG	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:TYR:CE1	2:D:70:LEU:HG	2.28	0.69
2:F:60:TYR:CE1	2:F:70:LEU:HG	2.28	0.68
2:O:60:TYR:CE1	2:O:70:LEU:HG	2.28	0.68
2:P:51:ILE:HD13	2:P:72:VAL:HG22	1.77	0.67
2:D:51:ILE:HD13	2:D:72:VAL:HG22	1.77	0.67
2:K:51:ILE:HD13	2:K:72:VAL:HG22	1.77	0.66
3:E:147:GLN:HB2	3:E:195:GLU:HB3	1.78	0.66
2:F:51:ILE:HD13	2:F:72:VAL:HG22	1.77	0.66
1:R:128:ASP:HB3	1:R:144:PRO:HD2	1.78	0.66
2:F:174:GLN:HA	3:H:160:GLN:HE22	1.60	0.66
1:Q:128:ASP:HB3	1:Q:144:PRO:HD2	1.78	0.65
2:F:101:TYR:O	3:H:34:HIS:NE2	2.30	0.65
2:P:101:TYR:O	3:N:34:HIS:NE2	2.29	0.65
2:O:51:ILE:HD13	2:O:72:VAL:HG22	1.77	0.65
3:N:147:GLN:HB2	3:N:195:GLU:HB3	1.78	0.65
2:P:174:GLN:HA	3:N:160:GLN:HE22	1.60	0.65
1:A:101:HIS:ND1	1:A:128:ASP:OD2	2.29	0.65
3:L:145:LYS:HB2	3:L:197:THR:HB	1.79	0.65
2:G:51:ILE:HD13	2:G:72:VAL:HG22	1.77	0.65
3:M:145:LYS:HB2	3:M:197:THR:HB	1.79	0.65
3:I:145:LYS:HB2	3:I:197:THR:HB	1.79	0.65
3:H:145:LYS:HB2	3:H:197:THR:HB	1.79	0.65
3:H:147:GLN:HB2	3:H:195:GLU:HB3	1.78	0.65
1:J:128:ASP:HB3	1:J:144:PRO:HD2	1.78	0.64
3:M:147:GLN:HB2	3:M:195:GLU:HB3	1.78	0.64
1:C:101:HIS:ND1	1:C:128:ASP:OD2	2.30	0.64
3:E:145:LYS:HB2	3:E:197:THR:HB	1.79	0.64
1:C:64:PHE:HB3	1:C:67:VAL:HB	1.78	0.64
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.78	0.64
3:N:145:LYS:HB2	3:N:197:THR:HB	1.79	0.64
1:B:101:HIS:ND1	1:B:128:ASP:OD2	2.30	0.64
1:A:64:PHE:HB3	1:A:67:VAL:HB	1.78	0.64
3:E:149:LYS:HB2	3:E:193:ALA:HB3	1.80	0.64
1:B:64:PHE:HB3	1:B:67:VAL:HB	1.79	0.64
3:I:147:GLN:HB2	3:I:195:GLU:HB3	1.78	0.64
2:D:128:ALA:HA	2:D:141:LEU:HB2	1.80	0.64
3:H:149:LYS:HB2	3:H:193:ALA:HB3	1.80	0.64
3:N:149:LYS:HB2	3:N:193:ALA:HB3	1.80	0.64
2:P:128:ALA:HA	2:P:141:LEU:HB2	1.81	0.63
3:M:149:LYS:HB2	3:M:193:ALA:HB3	1.80	0.63
2:F:128:ALA:HA	2:F:141:LEU:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:142:GLY:HA3	2:G:185:VAL:HG12	1.81	0.63
2:O:128:ALA:HA	2:O:141:LEU:HB2	1.80	0.63
2:K:142:GLY:HA3	2:K:185:VAL:HG12	1.81	0.62
2:G:128:ALA:HA	2:G:141:LEU:HB2	1.80	0.62
2:F:142:GLY:HA3	2:F:185:VAL:HG12	1.81	0.62
3:E:29:ILE:HG22	3:E:32:ASP:HB2	1.82	0.62
3:I:29:ILE:HG22	3:I:32:ASP:HB2	1.82	0.62
3:L:149:LYS:HB3	3:L:152:ASN:HA	1.82	0.62
3:N:29:ILE:HG22	3:N:32:ASP:HB2	1.82	0.62
3:E:149:LYS:HB3	3:E:152:ASN:HA	1.82	0.62
1:Q:10:ILE:HG12	1:Q:95:LEU:HD23	1.82	0.62
3:L:29:ILE:HG22	3:L:32:ASP:HB2	1.82	0.62
3:L:149:LYS:HB2	3:L:193:ALA:HB3	1.80	0.62
3:H:29:ILE:HG22	3:H:32:ASP:HB2	1.82	0.62
2:K:128:ALA:HA	2:K:141:LEU:HB2	1.81	0.62
3:M:29:ILE:HG22	3:M:32:ASP:HB2	1.82	0.62
1:R:10:ILE:HG12	1:R:95:LEU:HD23	1.82	0.62
2:P:142:GLY:HA3	2:P:185:VAL:HG12	1.81	0.61
1:B:180:ARG:NH1	1:B:234:ASP:O	2.30	0.61
1:R:63:PRO:HB3	1:R:68:LYS:HA	1.82	0.61
3:N:149:LYS:HB3	3:N:152:ASN:HA	1.82	0.61
2:D:185:VAL:HG11	3:E:135:LEU:HD21	1.82	0.61
3:I:149:LYS:HB3	3:I:152:ASN:HA	1.82	0.61
2:D:142:GLY:HA3	2:D:185:VAL:HG12	1.81	0.61
1:J:180:ARG:NH1	1:J:234:ASP:O	2.31	0.61
1:J:10:ILE:HG12	1:J:95:LEU:HD23	1.83	0.61
1:Q:63:PRO:HB3	1:Q:68:LYS:HA	1.83	0.61
3:I:149:LYS:HB2	3:I:193:ALA:HB3	1.80	0.61
2:O:142:GLY:HA3	2:O:185:VAL:HG12	1.81	0.61
3:H:149:LYS:HB3	3:H:152:ASN:HA	1.82	0.61
2:K:185:VAL:HG11	3:L:135:LEU:HD21	1.81	0.60
1:R:180:ARG:NH1	1:R:234:ASP:O	2.31	0.60
3:M:85:VAL:HG22	3:M:103:LYS:HG2	1.83	0.60
2:K:100:LEU:O	3:L:96:ARG:NH1	2.34	0.60
3:L:85:VAL:HG22	3:L:103:LYS:HG2	1.83	0.60
3:N:85:VAL:HG22	3:N:103:LYS:HG2	1.83	0.60
1:B:10:ILE:HG12	1:B:95:LEU:HD23	1.83	0.60
1:C:180:ARG:NH1	1:C:234:ASP:O	2.30	0.60
3:M:149:LYS:HB3	3:M:152:ASN:HA	1.82	0.60
1:A:180:ARG:NH1	1:A:234:ASP:O	2.30	0.60
3:E:85:VAL:HG22	3:E:103:LYS:HG2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:ILE:HA	3:L:134:CYS:HA	1.84	0.59
3:I:117:ILE:HA	3:I:134:CYS:HA	1.83	0.59
2:D:100:LEU:O	3:E:96:ARG:NH1	2.34	0.59
3:H:85:VAL:HG22	3:H:103:LYS:HG2	1.83	0.59
3:E:15:PRO:HA	3:E:78:LEU:HD12	1.84	0.59
3:I:85:VAL:HG22	3:I:103:LYS:HG2	1.83	0.59
3:H:117:ILE:HA	3:H:134:CYS:HA	1.83	0.59
2:G:130:CYS:HB3	2:G:193:GLY:HA2	1.85	0.59
3:M:15:PRO:HA	3:M:78:LEU:HD12	1.84	0.59
2:K:130:CYS:HB3	2:K:193:GLY:HA2	1.85	0.59
3:I:15:PRO:HA	3:I:78:LEU:HD12	1.84	0.59
2:O:130:CYS:HB3	2:O:193:GLY:HA2	1.85	0.59
3:M:117:ILE:HA	3:M:134:CYS:HA	1.84	0.58
2:D:128:ALA:H	2:D:214:VAL:HB	1.68	0.58
3:E:117:ILE:HA	3:E:134:CYS:HA	1.83	0.58
3:N:15:PRO:HA	3:N:78:LEU:HD12	1.84	0.58
3:N:117:ILE:HA	3:N:134:CYS:HA	1.84	0.58
3:L:15:PRO:HA	3:L:78:LEU:HD12	1.84	0.58
2:D:130:CYS:HB3	2:D:193:GLY:HA2	1.85	0.58
2:F:128:ALA:H	2:F:214:VAL:HB	1.68	0.58
2:O:128:ALA:H	2:O:214:VAL:HB	1.68	0.58
3:I:151:ASP:HA	3:I:191:VAL:HB	1.86	0.58
3:L:151:ASP:HA	3:L:191:VAL:HB	1.86	0.58
2:F:130:CYS:HB3	2:F:193:GLY:HA2	1.85	0.58
2:P:130:CYS:HB3	2:P:193:GLY:HA2	1.85	0.58
2:K:128:ALA:H	2:K:214:VAL:HB	1.68	0.58
3:H:15:PRO:HA	3:H:78:LEU:HD12	1.84	0.57
3:L:143:GLU:OE1	3:L:199:GLN:NE2	2.37	0.57
1:C:239:SER:O	1:C:291:ARG:NH1	2.38	0.57
3:I:143:GLU:OE1	3:I:199:GLN:NE2	2.37	0.57
1:Q:180:ARG:NH1	1:Q:234:ASP:O	2.31	0.57
3:H:190:LYS:HG2	3:H:211:ARG:HB3	1.86	0.57
3:M:143:GLU:OE1	3:M:199:GLN:NE2	2.37	0.57
3:N:190:LYS:HG2	3:N:211:ARG:HB3	1.86	0.57
1:J:63:PRO:HB3	1:J:68:LYS:HA	1.85	0.57
3:H:143:GLU:OE1	3:H:199:GLN:NE2	2.37	0.57
3:M:190:LYS:HG2	3:M:211:ARG:HB3	1.86	0.57
3:E:190:LYS:HG2	3:E:211:ARG:HB3	1.86	0.57
2:G:128:ALA:H	2:G:214:VAL:HB	1.68	0.57
2:D:101:TYR:O	3:E:34:HIS:NE2	2.38	0.56
3:E:143:GLU:OE1	3:E:199:GLN:NE2	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:ARG:HE	1:J:44:GLU:HB2	1.70	0.56
3:I:190:LYS:HG2	3:I:211:ARG:HB3	1.86	0.56
3:L:190:LYS:HG2	3:L:211:ARG:HB3	1.86	0.56
2:G:5:VAL:HB	2:G:23:LYS:HB3	1.87	0.56
2:K:5:VAL:HB	2:K:23:LYS:HB3	1.87	0.56
2:P:128:ALA:H	2:P:214:VAL:HB	1.68	0.56
3:N:143:GLU:OE1	3:N:199:GLN:NE2	2.37	0.56
2:F:5:VAL:HB	2:F:23:LYS:HB3	1.87	0.56
1:B:239:SER:O	1:B:291:ARG:NH1	2.38	0.56
1:Q:101:HIS:ND1	1:Q:128:ASP:OD2	2.38	0.56
1:A:21:ARG:NH1	3:I:1:GLU:O	2.32	0.56
3:E:151:ASP:HA	3:E:191:VAL:HB	1.86	0.56
3:L:136:LEU:HB2	3:L:175:LEU:HB2	1.88	0.56
3:M:151:ASP:HA	3:M:191:VAL:HB	1.86	0.56
2:G:24:ALA:HB3	2:G:77:SER:HB3	1.88	0.56
2:K:101:TYR:O	3:L:34:HIS:NE2	2.38	0.56
3:H:136:LEU:HB2	3:H:175:LEU:HB2	1.88	0.56
3:N:151:ASP:HA	3:N:191:VAL:HB	1.86	0.56
3:E:186:TYR:O	3:E:192:TYR:OH	2.24	0.56
2:K:24:ALA:HB3	2:K:77:SER:HB3	1.88	0.56
2:O:24:ALA:HB3	2:O:77:SER:HB3	1.88	0.56
3:H:151:ASP:HA	3:H:191:VAL:HB	1.86	0.56
3:M:136:LEU:HB2	3:M:175:LEU:HB2	1.88	0.56
2:F:24:ALA:HB3	2:F:77:SER:HB3	1.88	0.56
3:M:186:TYR:O	3:M:192:TYR:OH	2.24	0.56
3:I:136:LEU:HB2	3:I:175:LEU:HB2	1.88	0.55
3:E:61:ARG:NE	3:E:82:ASP:OD2	2.36	0.55
2:P:5:VAL:HB	2:P:23:LYS:HB3	1.87	0.55
2:D:24:ALA:HB3	2:D:77:SER:HB3	1.88	0.55
1:C:63:PRO:HB3	1:C:68:LYS:HA	1.89	0.55
3:E:136:LEU:HB2	3:E:175:LEU:HB2	1.88	0.55
1:C:17:LYS:NZ	1:C:57:ASP:OD1	2.40	0.55
2:O:5:VAL:HB	2:O:23:LYS:HB3	1.87	0.55
1:R:239:SER:O	1:R:291:ARG:NH1	2.39	0.55
2:G:91:THR:HB	2:G:114:VAL:HB	1.89	0.55
1:B:17:LYS:NZ	1:B:57:ASP:OD1	2.39	0.55
2:K:91:THR:HB	2:K:114:VAL:HB	1.89	0.55
2:P:24:ALA:HB3	2:P:77:SER:HB3	1.88	0.55
3:H:186:TYR:O	3:H:192:TYR:OH	2.24	0.55
3:N:136:LEU:HB2	3:N:175:LEU:HB2	1.88	0.55
1:J:15:PHE:HB3	1:J:103:LEU:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:126:PRO:HG3	2:O:212:LYS:HB3	1.89	0.55
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.36	0.55
2:F:91:THR:HB	2:F:114:VAL:HB	1.89	0.55
2:P:189:SER:H	2:P:192:LEU:HD12	1.73	0.55
1:R:101:HIS:ND1	1:R:128:ASP:OD2	2.39	0.55
3:I:186:TYR:O	3:I:192:TYR:OH	2.24	0.55
1:A:17:LYS:NZ	1:A:57:ASP:OD1	2.40	0.54
1:A:234:ASP:OD2	1:A:246:THR:OG1	2.25	0.54
2:F:47:TRP:HZ2	2:F:50:VAL:HG23	1.72	0.54
1:Q:6:ARG:HE	1:Q:44:GLU:HB2	1.71	0.54
3:N:186:TYR:O	3:N:192:TYR:OH	2.24	0.54
2:D:5:VAL:HB	2:D:23:LYS:HB3	1.87	0.54
2:F:126:PRO:HG3	2:F:212:LYS:HB3	1.90	0.54
1:A:6:ARG:NH1	1:A:265:TYR:OH	2.41	0.54
1:C:10:ILE:HG12	1:C:95:LEU:HD23	1.89	0.54
3:M:1:GLU:HG3	3:M:95:PRO:HD2	1.90	0.54
1:J:239:SER:O	1:J:291:ARG:NH1	2.40	0.54
2:K:189:SER:H	2:K:192:LEU:HD12	1.72	0.54
3:H:1:GLU:HG3	3:H:95:PRO:HD2	1.90	0.54
3:L:1:GLU:HG3	3:L:95:PRO:HD2	1.90	0.54
2:F:31:ASP:OD1	2:F:31:ASP:O	2.26	0.54
2:O:18:VAL:N	2:O:83:LEU:O	2.41	0.54
2:O:189:SER:H	2:O:192:LEU:HD12	1.73	0.54
1:Q:245:GLY:O	3:L:27:GLN:NE2	2.41	0.54
2:O:91:THR:HB	2:O:114:VAL:HB	1.89	0.54
3:L:186:TYR:O	3:L:192:TYR:OH	2.24	0.54
3:E:1:GLU:HG3	3:E:95:PRO:HD2	1.90	0.54
1:J:245:GLY:O	3:M:27:GLN:NE2	2.40	0.54
2:K:47:TRP:HZ2	2:K:50:VAL:HG23	1.72	0.54
2:D:91:THR:HB	2:D:114:VAL:HB	1.89	0.54
2:F:113:THR:O	2:F:115:SER:N	2.41	0.54
2:D:18:VAL:N	2:D:83:LEU:O	2.41	0.54
2:D:31:ASP:OD1	2:D:31:ASP:O	2.26	0.54
2:G:113:THR:O	2:G:115:SER:N	2.41	0.54
2:F:18:VAL:N	2:F:83:LEU:O	2.41	0.54
2:F:189:SER:H	2:F:192:LEU:HD12	1.73	0.54
2:K:31:ASP:O	2:K:31:ASP:OD1	2.25	0.54
1:R:6:ARG:HE	1:R:44:GLU:HB2	1.71	0.54
1:R:245:GLY:O	3:N:27:GLN:NE2	2.41	0.54
3:I:1:GLU:HG3	3:I:95:PRO:HD2	1.90	0.54
1:C:234:ASP:OD2	1:C:246:THR:OG1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:HIS:ND1	1:J:128:ASP:OD2	2.38	0.53
2:K:126:PRO:HG3	2:K:212:LYS:HB3	1.89	0.53
2:O:113:THR:O	2:O:115:SER:N	2.41	0.53
2:P:113:THR:O	2:P:115:SER:N	2.41	0.53
2:G:31:ASP:OD1	2:G:31:ASP:O	2.25	0.53
2:G:126:PRO:HG3	2:G:212:LYS:HB3	1.90	0.53
2:K:18:VAL:N	2:K:83:LEU:O	2.41	0.53
2:P:18:VAL:N	2:P:83:LEU:O	2.41	0.53
3:N:1:GLU:HG3	3:N:95:PRO:HD2	1.90	0.53
3:N:61:ARG:NE	3:N:82:ASP:OD2	2.36	0.53
2:D:189:SER:H	2:D:192:LEU:HD12	1.72	0.53
2:P:31:ASP:O	2:P:31:ASP:OD1	2.25	0.53
2:K:91:THR:N	2:K:112:VAL:O	2.42	0.53
2:O:47:TRP:HZ2	2:O:50:VAL:HG23	1.73	0.53
2:O:91:THR:N	2:O:112:VAL:O	2.42	0.53
2:G:18:VAL:N	2:G:83:LEU:O	2.41	0.53
2:P:91:THR:HB	2:P:114:VAL:HB	1.89	0.53
2:P:91:THR:N	2:P:112:VAL:O	2.42	0.53
1:Q:64:PHE:HB3	1:Q:67:VAL:HB	1.91	0.53
2:D:47:TRP:HZ2	2:D:50:VAL:HG23	1.72	0.53
2:P:126:PRO:HG3	2:P:212:LYS:HB3	1.90	0.53
2:G:47:TRP:HZ2	2:G:50:VAL:HG23	1.73	0.53
2:P:47:TRP:HZ2	2:P:50:VAL:HG23	1.72	0.53
1:R:64:PHE:HB3	1:R:67:VAL:HB	1.90	0.53
3:I:79:GLU:HG3	3:I:81:GLU:HG2	1.91	0.53
2:D:126:PRO:HG3	2:D:212:LYS:HB3	1.90	0.53
2:G:189:SER:H	2:G:192:LEU:HD12	1.72	0.53
1:B:234:ASP:OD2	1:B:246:THR:OG1	2.26	0.53
3:E:79:GLU:HG3	3:E:81:GLU:HG2	1.91	0.53
2:F:91:THR:N	2:F:112:VAL:O	2.42	0.53
3:N:79:GLU:HG3	3:N:81:GLU:HG2	1.91	0.53
1:A:239:SER:O	1:A:291:ARG:NH1	2.41	0.53
1:C:15:PHE:HB3	1:C:103:LEU:HD11	1.90	0.53
2:K:113:THR:O	2:K:115:SER:N	2.41	0.53
3:H:79:GLU:HG3	3:H:81:GLU:HG2	1.91	0.53
1:J:64:PHE:HB3	1:J:67:VAL:HB	1.91	0.52
1:R:15:PHE:HB3	1:R:103:LEU:HD11	1.90	0.52
3:H:61:ARG:NE	3:H:82:ASP:OD2	2.36	0.52
3:N:144:ALA:HB2	3:N:198:HIS:HD2	1.75	0.52
3:M:144:ALA:HB2	3:M:198:HIS:HD2	1.75	0.52
2:D:113:THR:O	2:D:115:SER:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:144:ALA:HB2	3:E:198:HIS:HD2	1.74	0.52
1:B:7:THR:HG22	1:B:92:ARG:HG2	1.90	0.52
2:D:155:VAL:HG22	2:D:201:VAL:HG22	1.92	0.52
2:G:91:THR:N	2:G:112:VAL:O	2.42	0.52
2:D:91:THR:N	2:D:112:VAL:O	2.42	0.52
1:Q:15:PHE:HB3	1:Q:103:LEU:HD11	1.91	0.52
3:I:61:ARG:NE	3:I:82:ASP:OD2	2.36	0.52
3:H:144:ALA:HB2	3:H:198:HIS:HD2	1.75	0.52
2:G:155:VAL:HG22	2:G:201:VAL:HG22	1.92	0.52
2:F:155:VAL:HG22	2:F:201:VAL:HG22	1.92	0.52
1:A:7:THR:HG22	1:A:92:ARG:HG2	1.91	0.52
1:C:245:GLY:O	3:H:27:GLN:NE2	2.43	0.52
2:P:155:VAL:HG22	2:P:201:VAL:HG22	1.92	0.52
2:P:185:VAL:HG11	3:N:135:LEU:HD21	1.92	0.52
1:Q:63:PRO:HA	1:Q:70:PRO:HD3	1.92	0.52
3:L:79:GLU:HG3	3:L:81:GLU:HG2	1.91	0.52
3:M:79:GLU:HG3	3:M:81:GLU:HG2	1.91	0.52
1:A:10:ILE:HG12	1:A:95:LEU:HD23	1.92	0.51
1:C:7:THR:HG22	1:C:92:ARG:HG2	1.92	0.51
2:O:155:VAL:HG22	2:O:201:VAL:HG22	1.92	0.51
3:I:108:ARG:NE	3:I:109:THR:O	2.42	0.51
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.75	0.51
1:A:63:PRO:HB3	1:A:68:LYS:HA	1.92	0.51
3:I:144:ALA:HB2	3:I:198:HIS:HD2	1.75	0.51
2:F:185:VAL:HG11	3:H:135:LEU:HD21	1.92	0.51
2:K:155:VAL:HG22	2:K:201:VAL:HG22	1.92	0.51
1:A:245:GLY:O	3:I:27:GLN:NE2	2.44	0.51
1:B:15:PHE:HB3	1:B:103:LEU:HD11	1.91	0.51
1:J:147:PHE:HB3	1:J:165:VAL:HG11	1.93	0.51
3:I:19:ALA:HB3	3:I:75:ILE:HB	1.93	0.51
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.93	0.51
1:Q:147:PHE:HB3	1:Q:165:VAL:HG11	1.92	0.51
2:D:52:SER:OG	2:D:55:ASN:O	2.30	0.51
1:B:264:ILE:O	1:B:267:THR:OG1	2.24	0.51
2:O:52:SER:OG	2:O:55:ASN:O	2.29	0.51
3:M:19:ALA:HB3	3:M:75:ILE:HB	1.93	0.51
1:A:15:PHE:HB3	1:A:103:LEU:HD11	1.93	0.50
3:E:108:ARG:NE	3:E:109:THR:O	2.42	0.50
1:J:63:PRO:HA	1:J:70:PRO:HD3	1.93	0.50
3:E:19:ALA:HB3	3:E:75:ILE:HB	1.93	0.50
1:B:63:PRO:HB3	1:B:68:LYS:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:147:PHE:HB3	1:R:165:VAL:HG11	1.93	0.50
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.93	0.50
2:F:52:SER:OG	2:F:55:ASN:O	2.29	0.50
1:R:63:PRO:HA	1:R:70:PRO:HD3	1.92	0.50
3:I:137:ASN:ND2	3:I:174:SER:OG	2.45	0.50
3:M:61:ARG:NE	3:M:82:ASP:OD2	2.36	0.50
3:I:6:GLN:OE1	3:I:101:GLY:N	2.44	0.50
1:B:228:HIS:NE2	1:B:274:ASP:OD2	2.41	0.50
3:H:19:ALA:HB3	3:H:75:ILE:HB	1.93	0.50
3:H:2:ILE:HG23	3:H:26:SER:HB3	1.94	0.50
3:L:137:ASN:ND2	3:L:174:SER:OG	2.45	0.50
3:M:137:ASN:ND2	3:M:174:SER:OG	2.45	0.50
3:N:137:ASN:ND2	3:N:174:SER:OG	2.45	0.50
2:G:52:SER:OG	2:G:55:ASN:O	2.29	0.49
2:K:52:SER:OG	2:K:55:ASN:O	2.29	0.49
1:Q:239:SER:O	1:Q:291:ARG:NH1	2.44	0.49
3:I:158:ASN:O	3:I:180:THR:N	2.45	0.49
3:H:108:ARG:NE	3:H:109:THR:O	2.42	0.49
1:B:3:ALA:O	1:B:7:THR:OG1	2.31	0.49
3:H:137:ASN:ND2	3:H:174:SER:OG	2.45	0.49
3:L:2:ILE:HG23	3:L:26:SER:HB3	1.94	0.49
3:N:19:ALA:HB3	3:N:75:ILE:HB	1.93	0.49
3:E:137:ASN:ND2	3:E:174:SER:OG	2.45	0.49
3:M:2:ILE:HG23	3:M:26:SER:HB3	1.94	0.49
2:P:52:SER:OG	2:P:55:ASN:O	2.29	0.49
3:N:6:GLN:OE1	3:N:101:GLY:N	2.45	0.49
1:B:6:ARG:NH1	1:B:265:TYR:OH	2.45	0.49
1:A:264:ILE:O	1:A:267:THR:OG1	2.25	0.49
2:K:6:GLN:HB2	2:K:108:GLN:HB2	1.95	0.49
3:E:2:ILE:HG23	3:E:26:SER:HB3	1.94	0.49
1:J:175:VAL:HG11	1:J:215:THR:HG23	1.94	0.49
1:J:288:GLU:HG2	1:J:291:ARG:HH21	1.78	0.49
1:J:7:THR:HG22	1:J:92:ARG:HG2	1.95	0.48
1:R:175:VAL:HG11	1:R:215:THR:HG23	1.95	0.48
1:R:288:GLU:HG2	1:R:291:ARG:HH21	1.77	0.48
3:E:27:GLN:NE2	1:B:245:GLY:O	2.45	0.48
2:G:6:GLN:HB2	2:G:108:GLN:HB2	1.95	0.48
1:Q:7:THR:HG22	1:Q:92:ARG:HG2	1.95	0.48
2:G:185:VAL:HG11	3:I:135:LEU:HD21	1.96	0.48
2:F:103:PHE:H	3:H:46:LEU:HD22	1.78	0.48
3:I:2:ILE:HG23	3:I:26:SER:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:158:ASN:O	3:H:180:THR:N	2.44	0.48
3:M:158:ASN:O	3:M:180:THR:N	2.44	0.48
3:N:2:ILE:HG23	3:N:26:SER:HB3	1.94	0.48
1:A:30:VAL:HA	1:A:33:LYS:HG2	1.95	0.48
2:K:150:PRO:O	2:K:203:HIS:NE2	2.40	0.48
1:R:180:ARG:HB3	1:R:200:MET:HG3	1.96	0.48
2:D:145:VAL:HG11	2:D:153:VAL:HG21	1.96	0.48
2:G:158:ASN:HD21	2:G:197:TYR:HA	1.78	0.48
2:G:145:VAL:HG11	2:G:153:VAL:HG21	1.96	0.48
2:O:4:LEU:HD21	2:O:98:TYR:HE2	1.79	0.48
2:O:185:VAL:HG11	3:M:135:LEU:HD21	1.96	0.48
2:P:103:PHE:H	3:N:46:LEU:HD22	1.78	0.48
2:F:6:GLN:HB2	2:F:108:GLN:HB2	1.95	0.48
2:K:145:VAL:HG11	2:K:153:VAL:HG21	1.96	0.48
2:G:144:LEU:HD11	3:I:131:SER:HB2	1.96	0.48
2:G:150:PRO:O	2:G:203:HIS:NE2	2.40	0.48
3:L:6:GLN:OE1	3:L:101:GLY:N	2.44	0.48
1:B:284:LYS:N	1:B:288:GLU:OE1	2.40	0.48
2:K:158:ASN:HD21	2:K:197:TYR:HA	1.78	0.48
2:O:145:VAL:HG11	2:O:153:VAL:HG21	1.96	0.48
2:D:158:ASN:HD21	2:D:197:TYR:HA	1.78	0.47
2:O:6:GLN:HB2	2:O:108:GLN:HB2	1.95	0.47
2:P:4:LEU:HD21	2:P:98:TYR:HE2	1.79	0.47
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.97	0.47
2:F:145:VAL:HG11	2:F:153:VAL:HG21	1.96	0.47
1:R:7:THR:HG22	1:R:92:ARG:HG2	1.95	0.47
3:H:6:GLN:OE1	3:H:101:GLY:N	2.44	0.47
2:P:6:GLN:HB2	2:P:108:GLN:HB2	1.95	0.47
2:P:145:VAL:HG11	2:P:153:VAL:HG21	1.96	0.47
1:Q:175:VAL:HG11	1:Q:215:THR:HG23	1.96	0.47
1:J:21:ARG:NH1	3:M:1:GLU:O	2.36	0.47
3:M:108:ARG:NE	3:M:109:THR:O	2.42	0.47
2:D:6:GLN:HB2	2:D:108:GLN:HB2	1.95	0.47
3:E:6:GLN:OE1	3:E:101:GLY:N	2.44	0.47
3:E:158:ASN:O	3:E:180:THR:N	2.44	0.47
2:G:4:LEU:HD21	2:G:98:TYR:HE2	1.79	0.47
2:F:4:LEU:HD21	2:F:98:TYR:HE2	1.79	0.47
2:F:158:ASN:HD21	2:F:197:TYR:HA	1.78	0.47
1:C:6:ARG:NH1	1:C:265:TYR:OH	2.48	0.47
3:N:158:ASN:O	3:N:180:THR:N	2.44	0.47
1:A:232:ASP:OD1	1:A:233:VAL:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:GLU:O	1:B:21:ARG:NH1	2.35	0.47
1:C:3:ALA:O	1:C:7:THR:OG1	2.31	0.47
1:J:234:ASP:OD2	1:J:246:THR:OG1	2.33	0.47
3:L:158:ASN:O	3:L:180:THR:N	2.44	0.47
3:M:163:VAL:HG22	3:M:175:LEU:HD21	1.97	0.47
2:P:158:ASN:HD21	2:P:197:TYR:HA	1.78	0.47
3:H:163:VAL:HG22	3:H:175:LEU:HD21	1.97	0.47
1:A:284:LYS:N	1:A:288:GLU:OE1	2.40	0.47
2:D:4:LEU:HD21	2:D:98:TYR:HE2	1.79	0.47
2:D:136:GLU:O	2:D:190:SER:OG	2.33	0.47
2:O:144:LEU:HD11	3:M:131:SER:HB2	1.96	0.47
2:O:158:ASN:HD21	2:O:197:TYR:HA	1.78	0.47
2:F:136:GLU:O	2:F:190:SER:OG	2.33	0.47
3:N:163:VAL:HG22	3:N:175:LEU:HD21	1.97	0.47
2:K:136:GLU:O	2:K:190:SER:OG	2.33	0.46
1:R:234:ASP:OD2	1:R:246:THR:OG1	2.33	0.46
1:B:258:LEU:HD13	1:B:308:ARG:HD3	1.97	0.46
1:C:16:SER:HB3	1:C:25:GLU:HG3	1.97	0.46
2:O:203:HIS:CE1	2:O:205:PRO:HG2	2.51	0.46
2:P:136:GLU:O	2:P:190:SER:OG	2.33	0.46
2:K:4:LEU:HD21	2:K:98:TYR:HE2	1.79	0.46
2:O:136:GLU:O	2:O:190:SER:OG	2.33	0.46
1:Q:234:ASP:OD2	1:Q:246:THR:OG1	2.33	0.46
1:Q:288:GLU:HG2	1:Q:291:ARG:HH21	1.80	0.46
3:M:6:GLN:OE1	3:M:101:GLY:N	2.44	0.46
1:C:261:THR:HG21	1:C:299:ILE:HG23	1.97	0.46
1:J:7:THR:O	1:J:93:ILE:N	2.47	0.46
2:D:32:TYR:HB3	2:D:98:TYR:HB3	1.98	0.46
1:C:30:VAL:HA	1:C:33:LYS:HG2	1.96	0.46
3:I:132:VAL:HB	3:I:179:LEU:HB3	1.97	0.46
3:I:163:VAL:HG22	3:I:175:LEU:HD21	1.97	0.46
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.97	0.46
3:M:148:TRP:CE2	3:M:179:LEU:HB2	2.51	0.46
2:D:61:ASN:HD22	2:D:62:GLN:H	1.63	0.46
2:O:147:ASP:HA	2:O:179:TYR:HB3	1.98	0.46
3:E:132:VAL:HB	3:E:179:LEU:HB3	1.97	0.46
3:E:163:VAL:HG22	3:E:175:LEU:HD21	1.97	0.46
2:G:136:GLU:O	2:G:190:SER:OG	2.33	0.46
1:J:16:SER:HB2	1:J:19:GLN:HE21	1.80	0.46
1:R:7:THR:O	1:R:93:ILE:N	2.48	0.46
3:H:148:TRP:CE2	3:H:179:LEU:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:ARG:NE	3:L:109:THR:O	2.42	0.46
3:M:132:VAL:HB	3:M:179:LEU:HB3	1.97	0.46
3:E:148:TRP:CE2	3:E:179:LEU:HB2	2.51	0.46
1:C:98:GLY:HA3	1:C:99:GLY:HA3	1.72	0.46
3:L:148:TRP:CE2	3:L:179:LEU:HB2	2.51	0.46
1:A:228:HIS:NE2	1:A:274:ASP:OD2	2.41	0.46
2:G:147:ASP:HA	2:G:179:TYR:HB3	1.98	0.46
1:J:98:GLY:HA3	1:J:99:GLY:HA3	1.70	0.46
2:K:147:ASP:HA	2:K:179:TYR:HB3	1.98	0.46
1:Q:301:LEU:HB3	1:Q:306:LEU:HD13	1.98	0.46
1:R:16:SER:HB2	1:R:19:GLN:HE21	1.81	0.46
3:L:163:VAL:HG22	3:L:175:LEU:HD21	1.97	0.46
3:E:20:THR:HA	3:E:74:THR:HA	1.98	0.46
2:O:61:ASN:HD22	2:O:62:GLN:H	1.64	0.46
2:O:192:LEU:HD22	2:O:195:LYS:HD2	1.98	0.46
3:I:148:TRP:CE2	3:I:179:LEU:HB2	2.51	0.46
3:N:118:PHE:N	3:N:133:VAL:O	2.48	0.46
2:D:51:ILE:HG23	2:D:70:LEU:HD12	1.98	0.45
2:F:147:ASP:HA	2:F:179:TYR:HB3	1.98	0.45
1:B:98:GLY:HA3	1:B:99:GLY:HA3	1.73	0.45
2:P:32:TYR:HB3	2:P:98:TYR:HB3	1.98	0.45
3:N:132:VAL:HB	3:N:179:LEU:HB3	1.97	0.45
2:D:147:ASP:HA	2:D:179:TYR:HB3	1.98	0.45
2:D:203:HIS:CE1	2:D:205:PRO:HG2	2.51	0.45
2:F:61:ASN:HD22	2:F:62:GLN:H	1.64	0.45
2:F:127:LEU:HD12	3:H:118:PHE:HD1	1.81	0.45
2:F:192:LEU:HD22	2:F:195:LYS:HD2	1.98	0.45
2:F:203:HIS:CE1	2:F:205:PRO:HG2	2.51	0.45
3:L:20:THR:HA	3:L:74:THR:HA	1.98	0.45
2:G:51:ILE:HG23	2:G:70:LEU:HD12	1.98	0.45
2:F:32:TYR:HB3	2:F:98:TYR:HB3	1.98	0.45
1:J:31:LEU:HD12	1:J:97:LEU:HD13	1.99	0.45
2:P:147:ASP:HA	2:P:179:TYR:HB3	1.98	0.45
2:P:203:HIS:CE1	2:P:205:PRO:HG2	2.51	0.45
3:M:131:SER:HA	3:M:180:THR:HA	1.98	0.45
3:N:148:TRP:CE2	3:N:179:LEU:HB2	2.51	0.45
2:G:192:LEU:HD22	2:G:195:LYS:HD2	1.98	0.45
1:C:67:VAL:HG13	1:C:140:LEU:HD21	1.99	0.45
2:K:32:TYR:HB3	2:K:98:TYR:HB3	1.98	0.45
2:P:127:LEU:HD12	3:N:118:PHE:HD1	1.81	0.45
3:I:20:THR:HA	3:I:74:THR:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:132:VAL:HB	3:H:179:LEU:HB3	1.97	0.45
1:B:16:SER:HB3	1:B:25:GLU:HG3	1.98	0.45
1:C:228:HIS:NE2	1:C:274:ASP:OD2	2.44	0.45
1:J:180:ARG:HB3	1:J:200:MET:HG3	1.99	0.45
2:K:192:LEU:HD22	2:K:195:LYS:HD2	1.98	0.45
2:K:203:HIS:CE1	2:K:205:PRO:HG2	2.51	0.45
2:O:51:ILE:HG23	2:O:70:LEU:HD12	1.98	0.45
1:Q:203:VAL:HA	1:Q:211:VAL:HG21	1.99	0.45
3:N:20:THR:HA	3:N:74:THR:HA	1.98	0.45
3:E:131:SER:HA	3:E:180:THR:HA	1.98	0.45
2:G:101:TYR:O	3:I:34:HIS:NE2	2.50	0.45
2:K:61:ASN:HD22	2:K:62:GLN:H	1.64	0.45
2:O:32:TYR:HB3	2:O:98:TYR:HB3	1.97	0.45
2:P:61:ASN:HD22	2:P:62:GLN:H	1.64	0.45
1:Q:180:ARG:HB3	1:Q:200:MET:HG3	1.99	0.45
3:N:108:ARG:NE	3:N:109:THR:O	2.42	0.45
2:G:32:TYR:HB3	2:G:98:TYR:HB3	1.98	0.45
2:G:61:ASN:HD22	2:G:62:GLN:H	1.63	0.45
2:G:203:HIS:CE1	2:G:205:PRO:HG2	2.51	0.45
2:F:41:PRO:HD3	2:F:92:ALA:HA	1.99	0.45
3:H:131:SER:HA	3:H:180:THR:HA	1.98	0.45
3:N:131:SER:HA	3:N:180:THR:HA	1.98	0.45
2:K:104:ASP:HB3	3:L:46:LEU:HD23	1.99	0.45
2:P:192:LEU:HD22	2:P:195:LYS:HD2	1.98	0.45
1:R:98:GLY:HA3	1:R:99:GLY:HA3	1.70	0.45
1:A:175:VAL:HG11	1:A:215:THR:HG23	1.99	0.45
3:E:118:PHE:N	3:E:133:VAL:O	2.49	0.45
1:B:175:VAL:HG11	1:B:215:THR:HG23	1.98	0.45
1:R:203:VAL:HA	1:R:211:VAL:HG21	1.99	0.45
3:L:131:SER:HA	3:L:180:THR:HA	1.98	0.45
1:A:16:SER:HB3	1:A:25:GLU:HG3	1.99	0.45
1:J:203:VAL:HA	1:J:211:VAL:HG21	1.98	0.45
2:P:51:ILE:HG23	2:P:70:LEU:HD12	1.98	0.45
3:I:131:SER:HA	3:I:180:THR:HA	1.98	0.45
2:G:41:PRO:HD3	2:G:92:ALA:HA	1.99	0.44
1:J:301:LEU:HB3	1:J:306:LEU:HD13	1.99	0.44
2:O:41:PRO:HD3	2:O:92:ALA:HA	1.99	0.44
3:M:91:SER:O	3:M:96:ARG:NE	2.51	0.44
2:G:52:SER:OG	2:G:55:ASN:OD1	2.32	0.44
2:G:100:LEU:O	3:I:96:ARG:NH1	2.51	0.44
2:K:51:ILE:HG23	2:K:70:LEU:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:52:SER:OG	2:K:55:ASN:OD1	2.32	0.44
2:O:173:LEU:HA	2:O:180:SER:HA	2.00	0.44
3:I:164:THR:OG1	3:I:174:SER:N	2.51	0.44
3:M:164:THR:OG1	3:M:174:SER:N	2.51	0.44
1:A:3:ALA:O	1:A:7:THR:OG1	2.35	0.44
3:H:187:GLU:OE1	3:H:211:ARG:NH1	2.51	0.44
3:L:187:GLU:OE1	3:L:211:ARG:NH1	2.51	0.44
2:D:173:LEU:HA	2:D:180:SER:HA	1.99	0.44
2:D:192:LEU:HD22	2:D:195:LYS:HD2	1.98	0.44
2:P:173:LEU:HA	2:P:180:SER:HA	1.99	0.44
3:I:91:SER:O	3:I:96:ARG:NE	2.51	0.44
3:L:70:ASP:OD1	3:L:70:ASP:N	2.51	0.44
3:N:164:THR:OG1	3:N:174:SER:N	2.51	0.44
1:C:232:ASP:OD1	1:C:233:VAL:N	2.51	0.44
1:J:101:HIS:HB3	1:J:144:PRO:HG3	2.00	0.44
3:I:70:ASP:OD1	3:I:70:ASP:N	2.51	0.44
3:I:187:GLU:OE1	3:I:211:ARG:NH1	2.51	0.44
3:M:11:LEU:O	3:M:105:GLU:N	2.50	0.44
2:F:137:SER:O	2:F:190:SER:N	2.51	0.44
1:C:264:ILE:O	1:C:267:THR:OG1	2.25	0.44
1:C:284:LYS:N	1:C:288:GLU:OE1	2.40	0.44
2:O:101:TYR:O	3:M:34:HIS:NE2	2.50	0.44
3:E:91:SER:O	3:E:96:ARG:NE	2.51	0.44
2:P:41:PRO:HD3	2:P:92:ALA:HA	1.99	0.44
1:Q:31:LEU:HD12	1:Q:97:LEU:HD13	1.99	0.44
3:I:61:ARG:HB3	3:I:77:SER:HB3	2.00	0.44
3:M:61:ARG:HB3	3:M:77:SER:HB3	2.00	0.44
3:E:164:THR:OG1	3:E:174:SER:N	2.51	0.44
2:G:137:SER:O	2:G:190:SER:N	2.51	0.44
2:F:51:ILE:HG23	2:F:70:LEU:HD12	1.98	0.44
2:F:173:LEU:HA	2:F:180:SER:HA	2.00	0.44
2:K:157:TRP:HE1	2:K:184:VAL:HG12	1.83	0.44
2:G:157:TRP:HE1	2:G:184:VAL:HG12	1.84	0.43
1:J:17:LYS:NZ	1:J:57:ASP:OD1	2.41	0.43
2:K:41:PRO:HD3	2:K:92:ALA:HA	1.99	0.43
2:K:173:LEU:HA	2:K:180:SER:HA	1.99	0.43
1:R:31:LEU:HD12	1:R:97:LEU:HD13	1.99	0.43
3:L:61:ARG:HB3	3:L:77:SER:HB3	2.00	0.43
3:M:20:THR:HA	3:M:74:THR:HA	1.98	0.43
3:N:91:SER:O	3:N:96:ARG:NE	2.51	0.43
1:A:98:GLY:HA3	1:A:99:GLY:HA3	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:PRO:HD3	2:D:92:ALA:HA	1.99	0.43
2:D:104:ASP:HB3	3:E:46:LEU:HD23	1.99	0.43
2:D:137:SER:O	2:D:190:SER:N	2.51	0.43
2:G:4:LEU:HD23	2:G:4:LEU:HA	1.87	0.43
2:G:60:TYR:OH	2:G:70:LEU:N	2.47	0.43
2:F:76:THR:O	2:F:78:THR:N	2.51	0.43
1:Q:16:SER:HB2	1:Q:19:GLN:HE21	1.84	0.43
3:H:11:LEU:O	3:H:105:GLU:N	2.50	0.43
3:H:61:ARG:HB3	3:H:77:SER:HB3	2.00	0.43
3:E:187:GLU:OE1	3:E:211:ARG:NH1	2.51	0.43
2:F:215:GLU:HA	2:O:218:TYR:CE2	2.53	0.43
1:B:30:VAL:HA	1:B:33:LYS:HG2	1.98	0.43
1:B:232:ASP:OD1	1:B:233:VAL:N	2.51	0.43
2:O:100:LEU:O	3:M:96:ARG:NH1	2.51	0.43
2:O:137:SER:O	2:O:190:SER:N	2.51	0.43
3:E:61:ARG:HB3	3:E:77:SER:HB3	2.00	0.43
2:K:76:THR:O	2:K:78:THR:N	2.51	0.43
2:P:137:SER:O	2:P:190:SER:N	2.51	0.43
3:H:20:THR:HA	3:H:74:THR:HA	1.98	0.43
3:N:61:ARG:HB3	3:N:77:SER:HB3	2.00	0.43
2:G:76:THR:O	2:G:78:THR:N	2.51	0.43
2:K:137:SER:O	2:K:190:SER:N	2.51	0.43
1:Q:84:VAL:HG21	1:Q:107:SER:HA	2.00	0.43
3:H:70:ASP:OD1	3:H:70:ASP:N	2.51	0.43
3:L:118:PHE:N	3:L:133:VAL:O	2.49	0.43
3:M:187:GLU:OE1	3:M:211:ARG:NH1	2.51	0.43
2:D:76:THR:O	2:D:78:THR:N	2.51	0.43
1:Q:17:LYS:NZ	1:Q:57:ASP:OD1	2.41	0.43
3:N:34:HIS:ND1	3:N:49:LYS:O	2.52	0.43
3:N:187:GLU:OE1	3:N:211:ARG:NH1	2.51	0.43
2:F:157:TRP:HE1	2:F:184:VAL:HG12	1.83	0.43
3:H:91:SER:O	3:H:96:ARG:NE	2.51	0.43
3:L:164:THR:OG1	3:L:174:SER:N	2.51	0.43
2:F:174:GLN:HB3	2:F:176:SER:H	1.84	0.43
2:O:174:GLN:HB3	2:O:176:SER:H	1.84	0.43
1:R:301:LEU:HB3	1:R:306:LEU:HD13	2.00	0.43
3:I:11:LEU:O	3:I:105:GLU:N	2.51	0.43
3:H:37:GLN:HB2	3:H:47:LEU:HD11	2.01	0.43
3:H:118:PHE:N	3:H:133:VAL:O	2.49	0.43
3:L:91:SER:O	3:L:96:ARG:NE	2.51	0.43
3:M:34:HIS:ND1	3:M:49:LYS:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:118:PHE:N	3:M:133:VAL:O	2.49	0.43
1:C:19:GLN:NE2	1:C:21:ARG:O	2.45	0.43
2:O:157:TRP:HE1	2:O:184:VAL:HG12	1.83	0.43
2:O:201:VAL:HB	2:O:210:VAL:HB	2.01	0.43
2:P:12:LYS:O	2:P:115:SER:N	2.52	0.43
2:P:76:THR:O	2:P:78:THR:N	2.51	0.43
3:H:34:HIS:ND1	3:H:49:LYS:O	2.52	0.43
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.01	0.43
3:M:6:GLN:HE22	3:M:87:TYR:HA	1.84	0.43
3:M:151:ASP:N	3:M:191:VAL:O	2.48	0.43
3:E:37:GLN:HB2	3:E:47:LEU:HD11	2.01	0.43
2:F:52:SER:OG	2:F:55:ASN:OD1	2.32	0.43
1:B:140:LEU:HA	1:B:140:LEU:HD23	1.84	0.43
2:K:12:LYS:O	2:K:115:SER:N	2.52	0.43
3:I:37:GLN:HB2	3:I:47:LEU:HD11	2.01	0.43
3:H:6:GLN:HE22	3:H:87:TYR:HA	1.84	0.43
1:A:190:LEU:HD12	1:A:195:ILE:HB	2.00	0.42
1:A:224:LYS:HD2	1:A:269:LEU:HD11	2.01	0.42
2:D:157:TRP:HE1	2:D:184:VAL:HG12	1.83	0.42
2:G:173:LEU:HA	2:G:180:SER:HA	1.99	0.42
2:G:174:GLN:HB3	2:G:176:SER:H	1.84	0.42
2:F:201:VAL:HB	2:F:210:VAL:HB	2.01	0.42
2:O:60:TYR:OH	2:O:70:LEU:N	2.47	0.42
2:O:76:THR:O	2:O:78:THR:N	2.51	0.42
2:F:60:TYR:OH	2:F:70:LEU:N	2.47	0.42
1:J:232:ASP:OD1	1:J:233:VAL:N	2.51	0.42
2:P:173:LEU:HD23	2:P:180:SER:HB3	2.01	0.42
1:A:67:VAL:HG13	1:A:140:LEU:HD21	2.01	0.42
2:D:12:LYS:O	2:D:115:SER:N	2.52	0.42
3:E:34:HIS:ND1	3:E:49:LYS:O	2.52	0.42
2:G:173:LEU:HD23	2:G:180:SER:HB3	2.01	0.42
1:B:301:LEU:HB3	1:B:306:LEU:HD13	2.01	0.42
1:C:16:SER:HB2	1:C:19:GLN:HE21	1.84	0.42
2:O:12:LYS:O	2:O:115:SER:N	2.52	0.42
1:R:101:HIS:HB3	1:R:144:PRO:HG3	2.01	0.42
3:I:210:ASN:HB2	3:I:213:GLU:HB2	2.02	0.42
3:N:6:GLN:HE22	3:N:87:TYR:HA	1.84	0.42
1:A:31:LEU:HD12	1:A:97:LEU:HD13	2.02	0.42
3:E:210:ASN:HB2	3:E:213:GLU:HB2	2.02	0.42
2:G:218:TYR:CE2	2:P:215:GLU:HA	2.53	0.42
2:K:174:GLN:HB3	2:K:176:SER:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:174:GLN:HB3	2:P:176:SER:H	1.84	0.42
3:L:11:LEU:O	3:L:105:GLU:N	2.51	0.42
2:D:156:SER:O	2:D:200:ASN:N	2.53	0.42
2:G:12:LYS:O	2:G:115:SER:N	2.52	0.42
1:B:124:ASP:OD1	1:B:125:ALA:N	2.53	0.42
3:L:34:HIS:ND1	3:L:49:LYS:O	2.52	0.42
2:F:173:LEU:HD23	2:F:180:SER:HB3	2.01	0.42
1:B:19:GLN:NE2	1:B:21:ARG:O	2.47	0.42
1:B:104:ALA:HA	1:B:107:SER:HB3	2.02	0.42
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.84	0.42
3:N:11:LEU:O	3:N:105:GLU:N	2.50	0.42
1:A:16:SER:HB2	1:A:19:GLN:HE21	1.84	0.42
2:F:12:LYS:O	2:F:115:SER:N	2.52	0.42
2:F:156:SER:O	2:F:200:ASN:N	2.53	0.42
1:J:84:VAL:HG21	1:J:107:SER:HA	2.02	0.42
1:Q:232:ASP:OD1	1:Q:233:VAL:N	2.52	0.42
3:I:6:GLN:HE22	3:I:87:TYR:HA	1.84	0.42
3:I:118:PHE:N	3:I:133:VAL:O	2.49	0.42
3:L:210:ASN:HB2	3:L:213:GLU:HB2	2.02	0.42
3:N:210:ASN:HB2	3:N:213:GLU:HB2	2.02	0.42
1:B:317:TYR:HD2	1:C:185:GLY:HA2	1.85	0.42
2:K:201:VAL:HB	2:K:210:VAL:HB	2.01	0.42
1:Q:7:THR:O	1:Q:93:ILE:N	2.49	0.42
1:A:288:GLU:HG2	1:A:291:ARG:HH21	1.85	0.42
2:D:174:GLN:HB3	2:D:176:SER:H	1.83	0.42
2:F:103:PHE:HD1	2:F:103:PHE:HA	1.80	0.42
1:Q:101:HIS:HB3	1:Q:144:PRO:HG3	2.02	0.42
3:I:151:ASP:N	3:I:191:VAL:O	2.48	0.42
1:A:258:LEU:HD13	1:A:308:ARG:HD3	2.00	0.42
1:C:301:LEU:HB3	1:C:306:LEU:HD13	2.02	0.42
2:O:52:SER:OG	2:O:55:ASN:OD1	2.32	0.42
2:P:106:TRP:CE3	3:N:44:PRO:HD2	2.55	0.42
3:N:37:GLN:HB2	3:N:47:LEU:HD11	2.01	0.42
3:E:6:GLN:HE22	3:E:87:TYR:HA	1.84	0.41
2:F:172:VAL:O	2:F:181:LEU:N	2.45	0.41
2:K:173:LEU:HD23	2:K:180:SER:HB3	2.01	0.41
2:P:60:TYR:OH	2:P:70:LEU:N	2.47	0.41
2:P:156:SER:O	2:P:200:ASN:N	2.53	0.41
1:Q:7:THR:HG23	1:Q:46:ASP:HB3	2.02	0.41
3:H:96:ARG:HA	3:H:96:ARG:HD3	1.89	0.41
1:A:301:LEU:HB3	1:A:306:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:VAL:HB	2:D:210:VAL:HB	2.01	0.41
2:G:103:PHE:HD1	2:G:103:PHE:HA	1.80	0.41
2:O:173:LEU:HD23	2:O:180:SER:HB3	2.01	0.41
2:P:157:TRP:HE1	2:P:184:VAL:HG12	1.83	0.41
3:I:113:PRO:HD2	3:I:201:LEU:HG	2.03	0.41
2:F:106:TRP:CE3	3:H:44:PRO:HD2	2.55	0.41
1:B:209:GLY:HA2	1:B:259:TYR:CE2	2.56	0.41
1:J:236:LEU:HD23	1:J:252:LEU:HB2	2.02	0.41
2:P:201:VAL:HB	2:P:210:VAL:HB	2.01	0.41
1:R:242:PRO:HG3	1:R:291:ARG:NH2	2.35	0.41
3:H:164:THR:OG1	3:H:174:SER:N	2.51	0.41
3:M:37:GLN:HB2	3:M:47:LEU:HD11	2.01	0.41
3:N:113:PRO:HD2	3:N:201:LEU:HG	2.03	0.41
3:E:11:LEU:O	3:E:105:GLU:N	2.50	0.41
2:F:172:VAL:HG21	3:H:160:GLN:HB3	2.02	0.41
1:Q:242:PRO:HG3	1:Q:291:ARG:HH22	1.85	0.41
3:I:34:HIS:ND1	3:I:49:LYS:O	2.52	0.41
3:E:113:PRO:HD2	3:E:201:LEU:HG	2.03	0.41
1:B:16:SER:HB2	1:B:19:GLN:HE21	1.86	0.41
1:C:104:ALA:HA	1:C:107:SER:HB3	2.02	0.41
2:O:156:SER:O	2:O:200:ASN:N	2.53	0.41
2:P:52:SER:OG	2:P:55:ASN:OD1	2.32	0.41
3:L:113:PRO:HD2	3:L:201:LEU:HG	2.02	0.41
3:M:210:ASN:HB2	3:M:213:GLU:HB2	2.02	0.41
2:D:173:LEU:HD23	2:D:180:SER:HB3	2.01	0.41
1:C:224:LYS:HD2	1:C:269:LEU:HD11	2.03	0.41
1:J:123:VAL:HG22	1:J:177:ILE:HB	2.03	0.41
1:Q:146:SER:HB2	1:Q:156:ILE:HD11	2.02	0.41
3:L:32:ASP:HA	3:L:50:TYR:HD1	1.85	0.41
1:A:202:GLU:HG3	1:A:205:ARG:HH12	1.86	0.41
1:C:175:VAL:HG11	1:C:215:THR:HG23	2.02	0.41
3:H:210:ASN:HB2	3:H:213:GLU:HB2	2.02	0.41
1:A:124:ASP:OD1	1:A:125:ALA:N	2.54	0.41
1:B:190:LEU:HD12	1:B:195:ILE:HB	2.03	0.41
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.93	0.41
1:J:7:THR:HG23	1:J:46:ASP:HB3	2.01	0.41
1:J:202:GLU:HG3	1:J:205:ARG:NH1	2.36	0.41
2:P:127:LEU:HA	2:P:214:VAL:HG21	2.03	0.41
1:Q:123:VAL:HG22	1:Q:177:ILE:HB	2.02	0.41
1:R:232:ASP:OD1	1:R:233:VAL:N	2.53	0.41
1:A:104:ALA:HA	1:A:107:SER:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:HE22	2:D:95:TYR:HA	1.86	0.41
2:G:156:SER:O	2:G:200:ASN:N	2.53	0.41
1:C:43:GLN:O	1:C:45:CYS:N	2.54	0.41
2:K:127:LEU:HA	2:K:214:VAL:HG21	2.03	0.41
1:R:7:THR:HG23	1:R:46:ASP:HB3	2.02	0.41
1:R:30:VAL:HA	1:R:33:LYS:HG2	2.03	0.41
1:R:202:GLU:HG3	1:R:205:ARG:NH1	2.36	0.41
3:I:32:ASP:HA	3:I:50:TYR:HD1	1.85	0.41
3:H:32:ASP:HA	3:H:50:TYR:HD1	1.85	0.41
3:L:94:TRP:HA	3:L:95:PRO:HA	1.89	0.41
3:M:32:ASP:HA	3:M:50:TYR:HD1	1.85	0.41
3:M:113:PRO:HD2	3:M:201:LEU:HG	2.03	0.41
1:A:43:GLN:O	1:A:45:CYS:N	2.54	0.41
1:A:209:GLY:HA2	1:A:259:TYR:CE2	2.56	0.41
2:D:127:LEU:HA	2:D:214:VAL:HG21	2.03	0.41
2:G:33:TYR:HD1	2:G:52:SER:HA	1.86	0.41
2:G:6:GLN:HE22	2:G:95:TYR:HA	1.86	0.40
2:G:201:VAL:HB	2:G:210:VAL:HB	2.01	0.40
1:B:43:GLN:O	1:B:45:CYS:N	2.54	0.40
1:C:188:TYR:O	1:C:192:THR:OG1	2.26	0.40
1:R:84:VAL:HG21	1:R:107:SER:HA	2.02	0.40
3:M:94:TRP:HA	3:M:95:PRO:HA	1.89	0.40
3:M:96:ARG:HA	3:M:96:ARG:HD3	1.89	0.40
3:E:32:ASP:HA	3:E:50:TYR:HD1	1.85	0.40
2:F:7:SER:HA	2:F:8:GLY:HA2	1.91	0.40
2:F:33:TYR:HD1	2:F:52:SER:HA	1.86	0.40
1:B:67:VAL:HG13	1:B:140:LEU:HD21	2.03	0.40
1:C:190:LEU:HD12	1:C:195:ILE:HB	2.03	0.40
2:O:127:LEU:HA	2:O:214:VAL:HG21	2.03	0.40
2:P:6:GLN:HE22	2:P:95:TYR:HA	1.86	0.40
2:P:172:VAL:HG21	3:N:160:GLN:HB3	2.02	0.40
2:F:127:LEU:HA	2:F:214:VAL:HG21	2.03	0.40
1:J:202:GLU:HG3	1:J:205:ARG:HH12	1.86	0.40
3:H:113:PRO:HD2	3:H:201:LEU:HG	2.03	0.40
3:L:151:ASP:N	3:L:191:VAL:O	2.48	0.40
3:N:150:VAL:HG13	3:N:192:TYR:HE1	1.87	0.40
2:D:33:TYR:HD1	2:D:52:SER:HA	1.87	0.40
2:P:33:TYR:HD1	2:P:52:SER:HA	1.87	0.40
1:Q:202:GLU:HG3	1:Q:205:ARG:NH1	2.36	0.40
1:R:146:SER:HB2	1:R:156:ILE:HD11	2.02	0.40
1:R:202:GLU:HG3	1:R:205:ARG:HH12	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:VAL:HG13	3:H:192:TYR:HE1	1.87	0.40
3:N:32:ASP:HA	3:N:50:TYR:HD1	1.85	0.40
3:N:75:ILE:HG22	3:N:78:LEU:HA	2.04	0.40
1:C:209:GLY:HA2	1:C:259:TYR:CE2	2.56	0.40
1:J:242:PRO:HG3	1:J:291:ARG:NH2	2.36	0.40
2:K:33:TYR:HD1	2:K:52:SER:HA	1.86	0.40
2:O:4:LEU:HD23	2:O:4:LEU:HA	1.87	0.40
3:M:75:ILE:HG22	3:M:78:LEU:HA	2.04	0.40
3:N:117:ILE:HD12	3:N:194:CYS:HB2	2.04	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 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	315/322 (98%)	297 (94%)	18 (6%)	0	100	100
1	B	315/322 (98%)	298 (95%)	17 (5%)	0	100	100
1	C	315/322 (98%)	298 (95%)	17 (5%)	0	100	100
1	J	315/322 (98%)	298 (95%)	17 (5%)	0	100	100
1	Q	315/322 (98%)	299 (95%)	16 (5%)	0	100	100
1	R	315/322 (98%)	298 (95%)	17 (5%)	0	100	100
2	D	203/443 (46%)	178 (88%)	25 (12%)	0	100	100
2	F	203/443 (46%)	179 (88%)	24 (12%)	0	100	100
2	G	203/443 (46%)	179 (88%)	24 (12%)	0	100	100
2	K	203/443 (46%)	178 (88%)	25 (12%)	0	100	100
2	O	203/443 (46%)	179 (88%)	24 (12%)	0	100	100
2	P	203/443 (46%)	178 (88%)	25 (12%)	0	100	100
3	E	210/214 (98%)	170 (81%)	39 (19%)	1 (0%)	29	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	210/214 (98%)	170 (81%)	39 (19%)	1 (0%)	29	65
3	I	210/214 (98%)	172 (82%)	37 (18%)	1 (0%)	29	65
3	L	210/214 (98%)	170 (81%)	39 (19%)	1 (0%)	29	65
3	M	210/214 (98%)	170 (81%)	39 (19%)	1 (0%)	29	65
3	N	210/214 (98%)	170 (81%)	39 (19%)	1 (0%)	29	65
All	All	4368/5874 (74%)	3881 (89%)	481 (11%)	6 (0%)	54	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	59	PRO
3	I	59	PRO
3	H	59	PRO
3	L	59	PRO
3	M	59	PRO
3	N	59	PRO

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 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	265/270 (98%)	265 (100%)	0	100	100
1	B	265/270 (98%)	265 (100%)	0	100	100
1	C	265/270 (98%)	265 (100%)	0	100	100
1	J	265/270 (98%)	265 (100%)	0	100	100
1	Q	265/270 (98%)	265 (100%)	0	100	100
1	R	265/270 (98%)	265 (100%)	0	100	100
2	D	176/396 (44%)	174 (99%)	2 (1%)	73	85
2	F	176/396 (44%)	174 (99%)	2 (1%)	73	85
2	G	176/396 (44%)	174 (99%)	2 (1%)	73	85
2	K	176/396 (44%)	174 (99%)	2 (1%)	73	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	176/396 (44%)	174 (99%)	2 (1%)	73	85
2	P	176/396 (44%)	174 (99%)	2 (1%)	73	85
3	E	186/188 (99%)	184 (99%)	2 (1%)	73	85
3	H	186/188 (99%)	184 (99%)	2 (1%)	73	85
3	I	186/188 (99%)	184 (99%)	2 (1%)	73	85
3	L	186/188 (99%)	184 (99%)	2 (1%)	73	85
3	M	186/188 (99%)	184 (99%)	2 (1%)	73	85
3	N	186/188 (99%)	184 (99%)	2 (1%)	73	85
All	All	3762/5124 (73%)	3738 (99%)	24 (1%)	86	92

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

Mol	Chain	Res	Type
2	D	61	ASN
2	D	65	LYS
3	E	108	ARG
3	E	137	ASN
2	G	61	ASN
2	G	65	LYS
2	F	61	ASN
2	F	65	LYS
2	K	61	ASN
2	K	65	LYS
2	O	61	ASN
2	O	65	LYS
2	P	61	ASN
2	P	65	LYS
3	I	108	ARG
3	I	137	ASN
3	H	108	ARG
3	H	137	ASN
3	L	108	ARG
3	L	137	ASN
3	M	108	ARG
3	M	137	ASN
3	N	108	ARG
3	N	137	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	141	HIS
1	A	319	ASN
2	D	61	ASN
3	E	92	ASN
3	E	137	ASN
3	E	189	HIS
2	G	61	ASN
2	F	61	ASN
1	B	141	HIS
1	B	319	ASN
1	C	126	HIS
1	C	141	HIS
1	C	319	ASN
1	J	90	ASN
1	J	141	HIS
1	J	143	GLN
1	J	319	ASN
2	K	61	ASN
2	O	61	ASN
2	P	61	ASN
1	Q	90	ASN
1	Q	141	HIS
1	Q	143	GLN
1	Q	319	ASN
1	R	90	ASN
1	R	141	HIS
1	R	143	GLN
1	R	319	ASN
3	I	92	ASN
3	I	137	ASN
3	I	189	HIS
3	H	27	GLN
3	H	92	ASN
3	H	137	ASN
3	H	160	GLN
3	H	189	HIS
3	L	92	ASN
3	L	137	ASN
3	L	189	HIS
3	M	92	ASN
3	M	137	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	189	HIS
3	N	92	ASN
3	N	137	ASN
3	N	160	GLN
3	N	189	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	O	1
2	P	1
2	D	1
2	G	1
2	F	1
2	K	1
3	E	1
3	I	1
3	H	1
3	L	1
3	M	1
3	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	114:VAL	C	115:SER	N	3.84
1	P	114:VAL	C	115:SER	N	3.84
1	D	114:VAL	C	115:SER	N	3.83
1	G	114:VAL	C	115:SER	N	3.83
1	F	114:VAL	C	115:SER	N	3.83
1	K	114:VAL	C	115:SER	N	3.83
1	E	107:LYS	C	108:ARG	N	3.17
1	I	107:LYS	C	108:ARG	N	3.17
1	H	107:LYS	C	108:ARG	N	3.17
1	L	107:LYS	C	108:ARG	N	3.17
1	M	107:LYS	C	108:ARG	N	3.17
1	N	107:LYS	C	108:ARG	N	3.17

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23298. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.