Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 01:21 AM EST

PDB ID	:	7LEX
EMDB ID	:	EMD-23293
Title	:	Trimeric human Arginase 1 in complex with mAb1 - 2 hArg:3 mAb1 complex
Authors	:	Gomez-Llorente, Y.; Scapin, G.; Palte, R.L.
Deposited on	:	2021-01-15
Resolution	:	3.60 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 ⓘ 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:

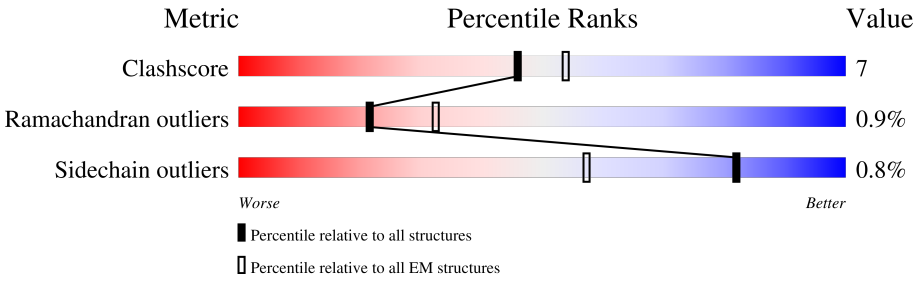
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	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	86% 13% •
1	B	322	86% 13% •
1	C	322	85% 13% •
1	J	322	85% 13% •
1	M	322	86% 12% •
1	N	322	86% 12% •
2	D	455	39% 10% • 50%
2	F	455	39% 10% • 50%
2	G	455	39% 11% • 50%

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Mol	Chain	Length	Quality of chain
2	K	455	39% 10% 50%
2	Q	455	39% 10% 50%
2	R	455	39% 11% 50%
3	E	214	77% 22%
3	H	214	78% 21%
3	I	214	77% 22%
3	L	214	76% 23%
3	O	214	78% 21%
3	P	214	78% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34596 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
1	A	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		
1	B	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		
1	C	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		
1	J	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		
1	M	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		
1	N	317	Total	C	N	O	S	0	0
			2409	1535	411	457	6		

- Molecule 2 is a protein called mAb1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		
2	F	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		
2	G	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		
2	K	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		
2	Q	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		
2	R	228	Total	C	N	O	S	0	0
			1717	1082	286	341	8		

- Molecule 3 is a protein called mAb1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		

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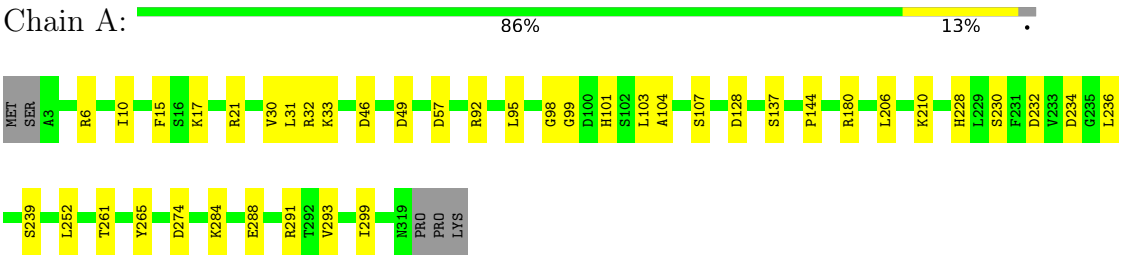
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		
3	I	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		
3	L	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		
3	O	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		
3	P	214	Total	C	N	O	S	0	0
			1640	1020	279	334	7		

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.

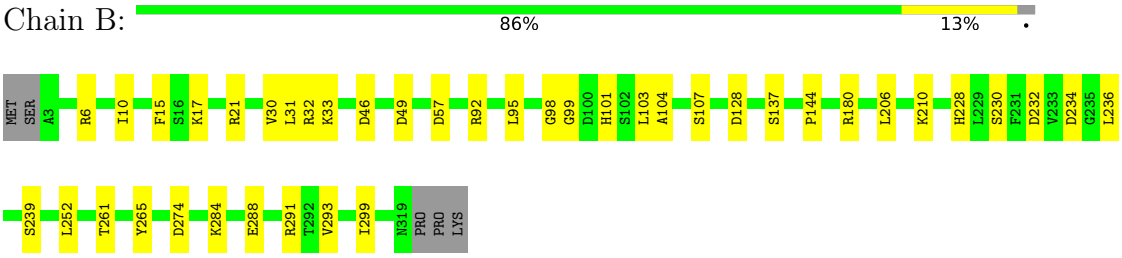
• Molecule 1: Arginase-1

Chain A:



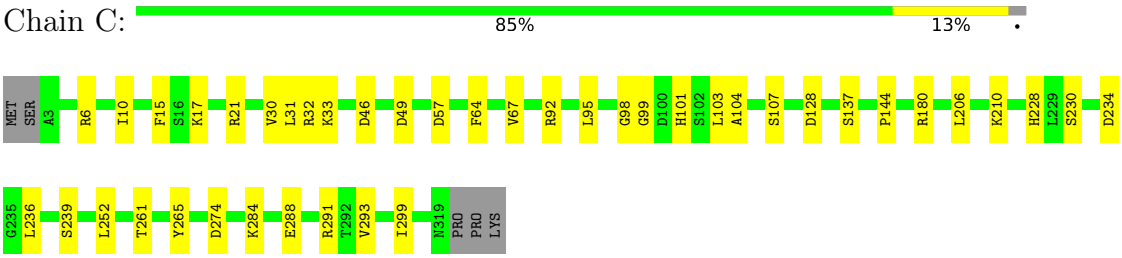
• Molecule 1: Arginase-1

Chain B:



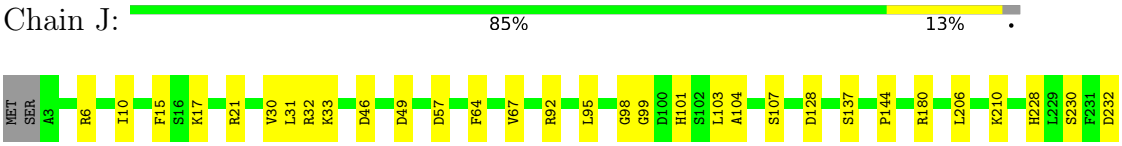
• Molecule 1: Arginase-1

Chain C:



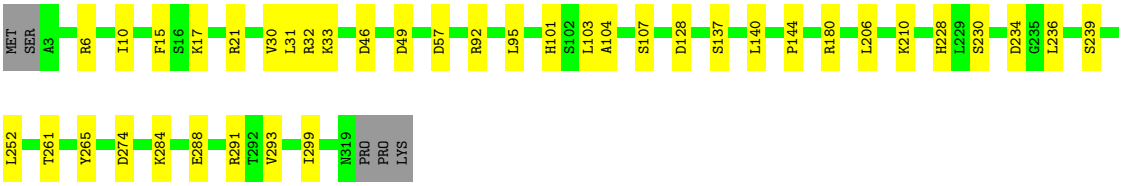
• Molecule 1: Arginase-1

Chain J:



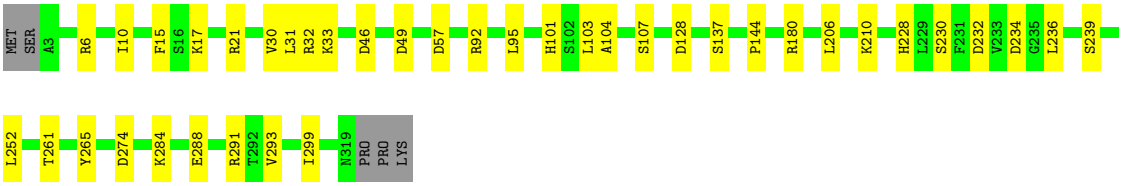
• Molecule 1: Arginase-1

Chain M:



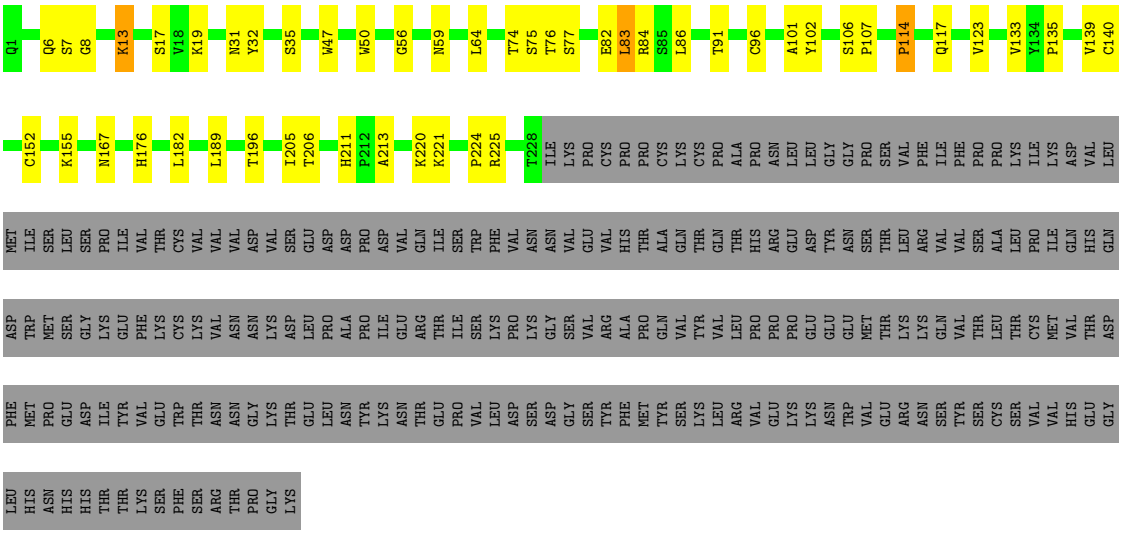
• Molecule 1: Arginase-1

Chain N:



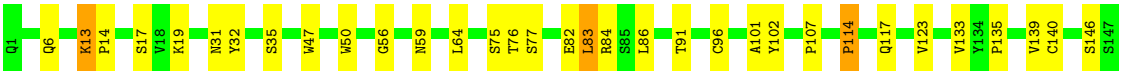
• Molecule 2: mAb1 heavy chain

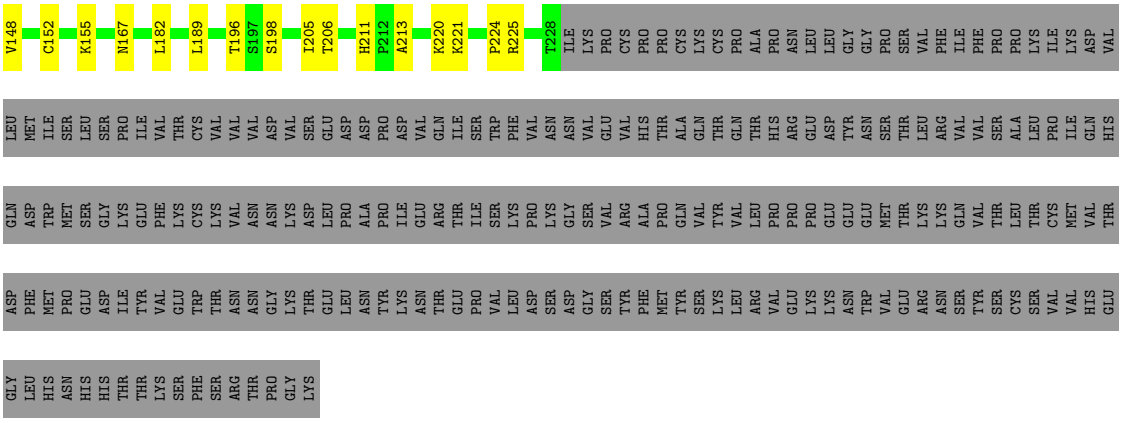
Chain D:



• Molecule 2: mAb1 heavy chain

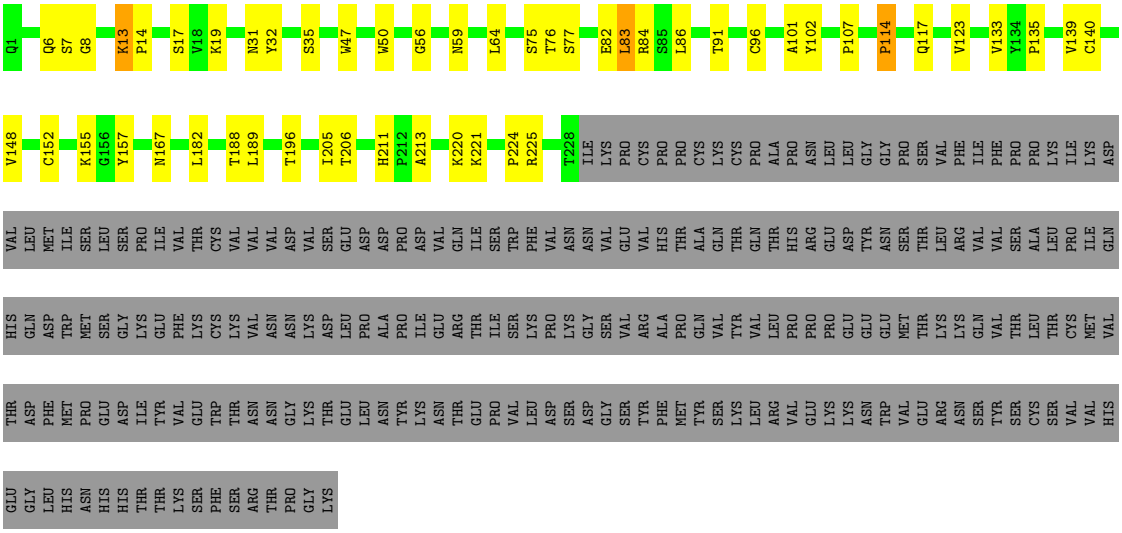
Chain F:





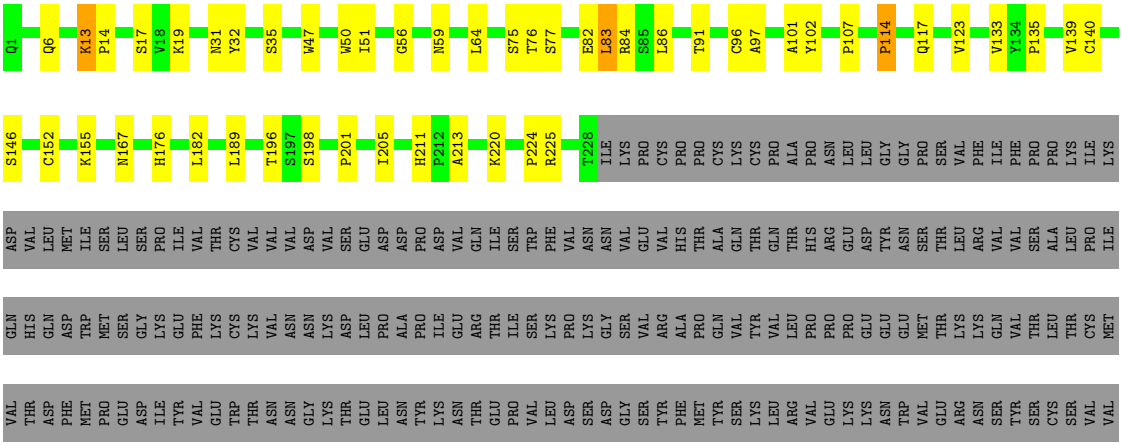
• Molecule 2: mAb1 heavy chain

Chain G:



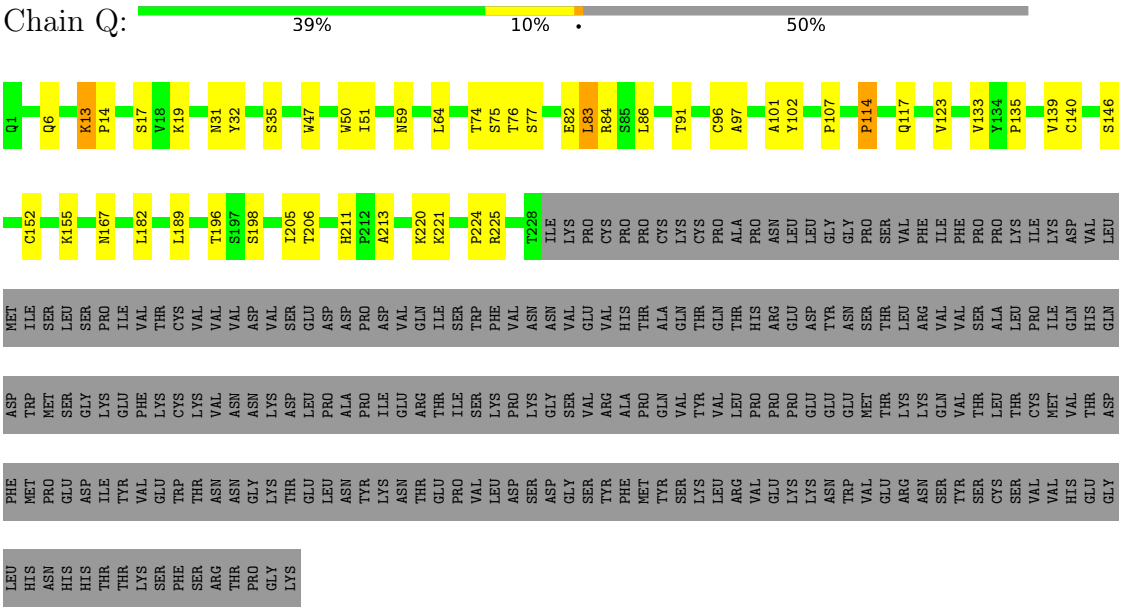
• Molecule 2: mAb1 heavy chain

Chain K:



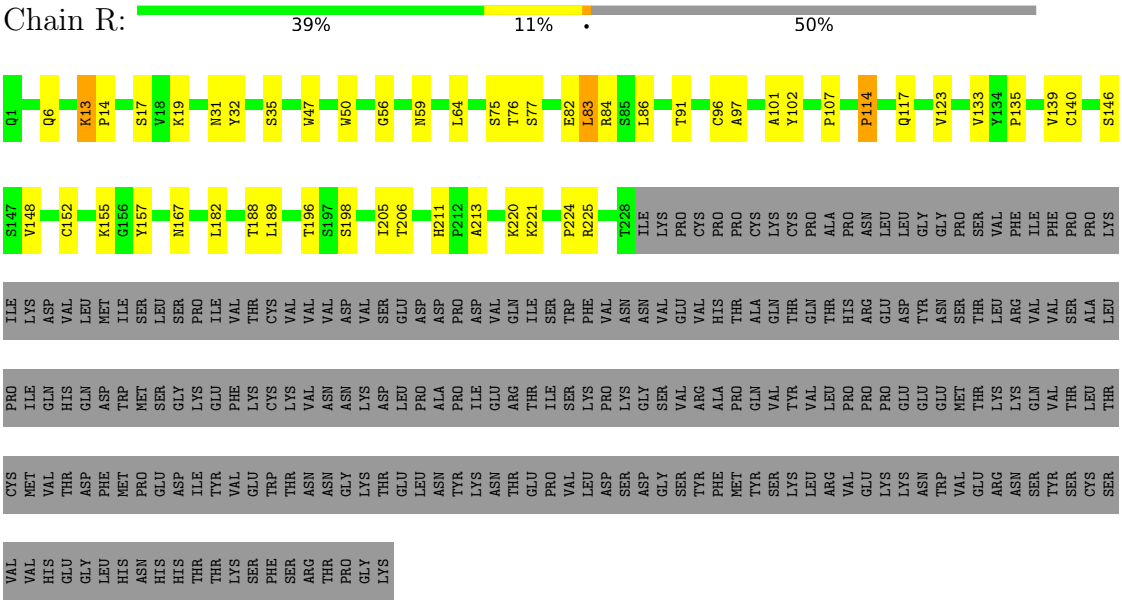
• Molecule 2: mAb1 heavy chain

Chain Q:



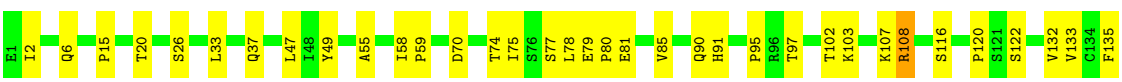
• Molecule 2: mAb1 heavy chain

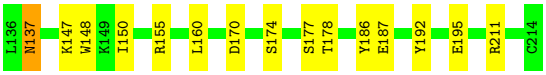
Chain R:



• Molecule 3: mAb1 light chain

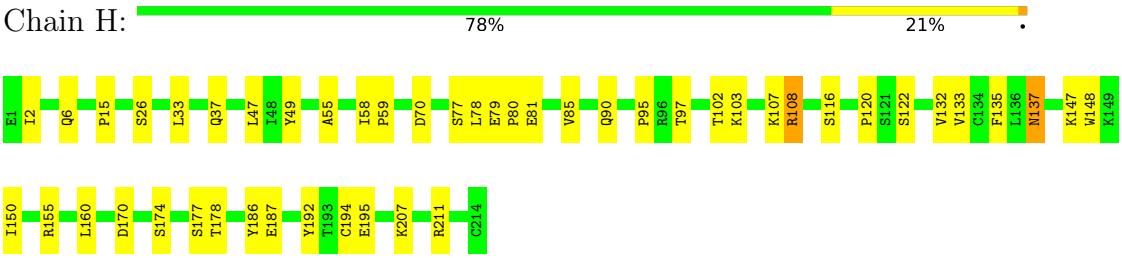
Chain E:





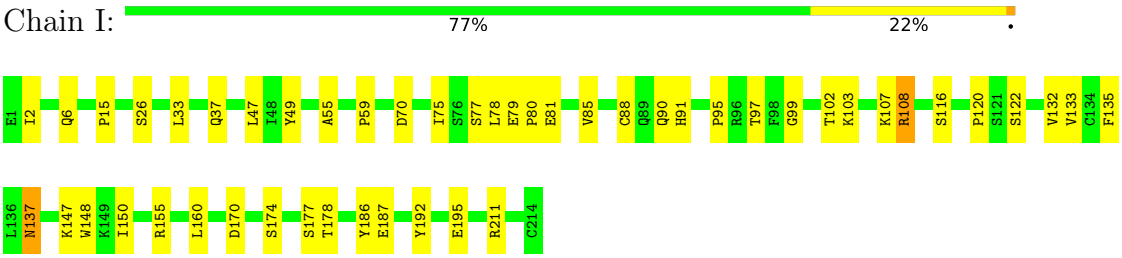
• Molecule 3: mAb1 light chain

Chain H:



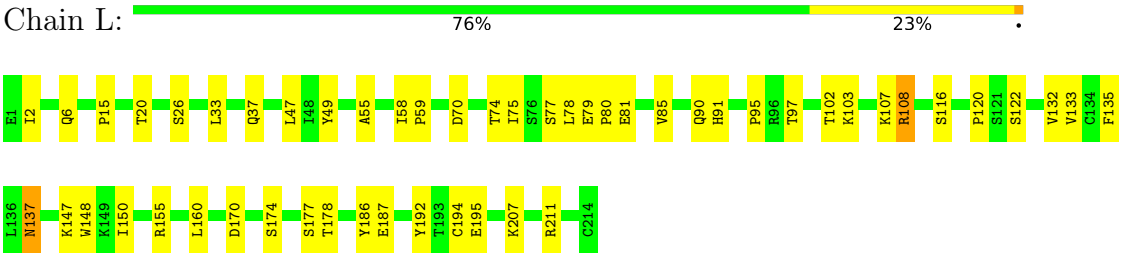
• Molecule 3: mAb1 light chain

Chain I:



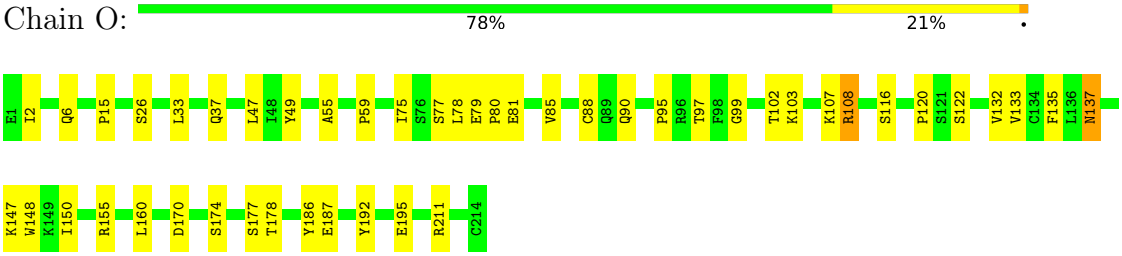
• Molecule 3: mAb1 light chain

Chain L:



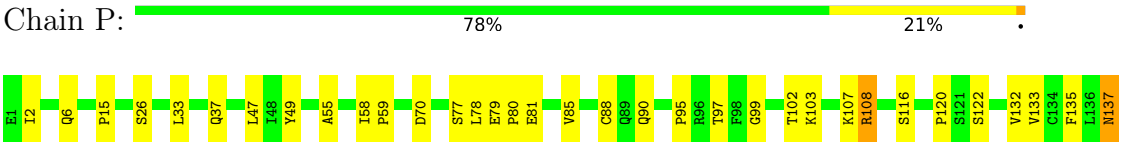
• Molecule 3: mAb1 light chain

Chain O:



• Molecule 3: mAb1 light chain

Chain P:




K147
W148
K149
I150
R155
L160
D170
S174
S177
T178
Y186
E187
Y192
E195
R211
C214

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37385	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 ($e^-/Å^2$)	45.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.36	0/2459	0.54	0/3336
1	B	0.36	0/2459	0.54	0/3336
1	C	0.36	0/2459	0.54	0/3336
1	J	0.36	0/2459	0.54	0/3336
1	M	0.36	0/2459	0.54	0/3336
1	N	0.36	0/2459	0.54	0/3336
2	D	0.36	0/1761	0.66	2/2407 (0.1%)
2	F	0.36	0/1761	0.66	2/2407 (0.1%)
2	G	0.36	0/1761	0.66	2/2407 (0.1%)
2	K	0.36	0/1761	0.66	2/2407 (0.1%)
2	Q	0.36	0/1761	0.66	2/2407 (0.1%)
2	R	0.36	0/1761	0.66	2/2407 (0.1%)
3	E	0.32	0/1676	0.64	1/2276 (0.0%)
3	H	0.32	0/1676	0.64	1/2276 (0.0%)
3	I	0.32	0/1676	0.64	1/2276 (0.0%)
3	L	0.32	0/1676	0.64	1/2276 (0.0%)
3	O	0.31	0/1676	0.64	1/2276 (0.0%)
3	P	0.32	0/1676	0.64	1/2276 (0.0%)
All	All	0.35	0/35376	0.61	18/48114 (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	3
2	F	0	3
2	G	0	3
2	K	0	3
2	Q	0	3
2	R	0	3
3	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	P	0	2
All	All	0	30

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	64	LEU	CA-CB-CG	7.06	131.54	115.30
2	K	64	LEU	CA-CB-CG	7.04	131.49	115.30
2	Q	64	LEU	CA-CB-CG	7.03	131.48	115.30
2	F	64	LEU	CA-CB-CG	7.03	131.46	115.30
2	D	64	LEU	CA-CB-CG	7.01	131.43	115.30
2	R	64	LEU	CA-CB-CG	7.00	131.39	115.30
3	P	33	LEU	CA-CB-CG	5.47	127.88	115.30
3	I	33	LEU	CA-CB-CG	5.47	127.88	115.30
3	O	33	LEU	CA-CB-CG	5.46	127.86	115.30
3	L	33	LEU	CA-CB-CG	5.45	127.84	115.30
3	H	33	LEU	CA-CB-CG	5.45	127.83	115.30
3	E	33	LEU	CA-CB-CG	5.43	127.80	115.30
2	G	182	LEU	CA-CB-CG	5.08	127.00	115.30
2	K	182	LEU	CA-CB-CG	5.08	126.98	115.30
2	Q	182	LEU	CA-CB-CG	5.06	126.94	115.30
2	R	182	LEU	CA-CB-CG	5.05	126.91	115.30
2	D	182	LEU	CA-CB-CG	5.04	126.88	115.30
2	F	182	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	114	PRO	Peptide
2	D	13	LYS	Peptide
2	D	76	THR	Peptide
3	E	77	SER	Peptide
3	E	95	PRO	Peptide
2	F	114	PRO	Peptide
2	F	13	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	F	76	THR	Peptide
2	G	114	PRO	Peptide
2	G	13	LYS	Peptide
2	G	76	THR	Peptide
3	H	77	SER	Peptide
3	H	95	PRO	Peptide
3	I	77	SER	Peptide
3	I	95	PRO	Peptide
2	K	114	PRO	Peptide
2	K	13	LYS	Peptide
2	K	76	THR	Peptide
3	L	77	SER	Peptide
3	L	95	PRO	Peptide
3	O	77	SER	Peptide
3	O	95	PRO	Peptide
3	P	77	SER	Peptide
3	P	95	PRO	Peptide
2	Q	114	PRO	Peptide
2	Q	13	LYS	Peptide
2	Q	76	THR	Peptide
2	R	114	PRO	Peptide
2	R	13	LYS	Peptide
2	R	76	THR	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	24	0
1	B	2409	0	2456	24	0
1	C	2409	0	2456	24	0
1	J	2409	0	2456	25	0
1	M	2409	0	2456	23	0
1	N	2409	0	2456	23	0
2	D	1717	0	1651	29	0
2	F	1717	0	1651	26	0
2	G	1717	0	1651	29	0
2	K	1717	0	1651	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1717	0	1651	28	0
2	R	1717	0	1651	29	0
3	E	1640	0	1571	30	0
3	H	1640	0	1571	27	0
3	I	1640	0	1571	28	0
3	L	1640	0	1571	31	0
3	O	1640	0	1571	26	0
3	P	1640	0	1571	27	0
All	All	34596	0	34068	453	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 7.

All (453) 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:H:107:LYS:C	3:H:108:ARG:N	2.25	0.91
3:O:107:LYS:C	3:O:108:ARG:N	2.25	0.90
3:P:107:LYS:C	3:P:108:ARG:N	2.25	0.90
3:E:107:LYS:C	3:E:108:ARG:N	2.25	0.90
3:I:107:LYS:C	3:I:108:ARG:N	2.25	0.90
3:L:107:LYS:C	3:L:108:ARG:N	2.25	0.90
3:E:148:TRP:HE1	3:E:177:SER:HG	1.29	0.80
3:I:148:TRP:HE1	3:I:177:SER:HG	1.30	0.79
3:H:148:TRP:HE1	3:H:177:SER:HG	1.28	0.78
3:O:148:TRP:HE1	3:O:177:SER:HG	1.32	0.77
3:L:148:TRP:HE1	3:L:177:SER:HG	1.32	0.77
3:P:148:TRP:HE1	3:P:177:SER:HG	1.32	0.77
3:L:122:SER:H	2:K:225:ARG:HH22	1.34	0.76
2:D:225:ARG:HH22	3:E:122:SER:H	1.34	0.76
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.76	0.68
1:M:128:ASP:HB3	1:M:144:PRO:HD2	1.75	0.68
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.76	0.68
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.75	0.68
1:N:128:ASP:HB3	1:N:144:PRO:HD2	1.75	0.67
1:J:128:ASP:HB3	1:J:144:PRO:HD2	1.75	0.67
3:H:122:SER:H	2:F:225:ARG:HH22	1.42	0.66
1:A:180:ARG:NH1	1:A:234:ASP:O	2.29	0.66
1:N:180:ARG:NH1	1:N:234:ASP:O	2.29	0.65
1:C:180:ARG:NH1	1:C:234:ASP:O	2.29	0.65
1:J:180:ARG:NH1	1:J:234:ASP:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:NH1	1:B:234:ASP:O	2.29	0.64
3:O:122:SER:H	2:Q:225:ARG:HH22	1.42	0.64
1:M:180:ARG:NH1	1:M:234:ASP:O	2.29	0.64
3:L:108:ARG:NH1	3:L:170:ASP:O	2.32	0.63
3:P:108:ARG:NH1	3:P:170:ASP:O	2.32	0.63
3:I:108:ARG:NH1	3:I:170:ASP:O	2.32	0.63
3:E:108:ARG:NH1	3:E:170:ASP:O	2.32	0.63
3:H:108:ARG:NH1	3:H:170:ASP:O	2.32	0.63
1:N:137:SER:HA	2:Q:107:PRO:HA	1.81	0.62
3:P:122:SER:H	2:R:225:ARG:HH22	1.46	0.62
3:O:108:ARG:NH1	3:O:170:ASP:O	2.32	0.62
1:C:137:SER:HA	2:F:107:PRO:HA	1.81	0.62
3:I:122:SER:H	2:G:225:ARG:HH22	1.46	0.62
1:J:137:SER:HA	2:R:107:PRO:HA	1.81	0.62
1:A:137:SER:HA	2:G:107:PRO:HA	1.81	0.61
2:D:107:PRO:HA	1:B:137:SER:HA	1.84	0.59
1:C:239:SER:O	1:C:291:ARG:NH1	2.35	0.59
1:N:239:SER:O	1:N:291:ARG:NH1	2.35	0.59
1:B:239:SER:O	1:B:291:ARG:NH1	2.36	0.59
1:A:239:SER:O	1:A:291:ARG:NH1	2.36	0.59
3:L:147:LYS:HB2	3:L:195:GLU:HB3	1.85	0.59
1:M:137:SER:HA	2:K:107:PRO:HA	1.84	0.59
3:E:147:LYS:HB2	3:E:195:GLU:HB3	1.85	0.59
3:I:147:LYS:HB2	3:I:195:GLU:HB3	1.85	0.58
2:G:133:VAL:HG12	2:G:135:PRO:HD3	1.85	0.58
2:Q:6:GLN:NE2	2:Q:96:CYS:SG	2.76	0.58
1:J:239:SER:O	1:J:291:ARG:NH1	2.36	0.58
3:O:147:LYS:HB2	3:O:195:GLU:HB3	1.85	0.58
2:G:6:GLN:NE2	2:G:96:CYS:SG	2.76	0.58
2:K:133:VAL:HG12	2:K:135:PRO:HD3	1.85	0.58
1:M:239:SER:O	1:M:291:ARG:NH1	2.36	0.58
2:F:6:GLN:NE2	2:F:96:CYS:SG	2.76	0.58
2:R:133:VAL:HG12	2:R:135:PRO:HD3	1.85	0.58
2:D:133:VAL:HG12	2:D:135:PRO:HD3	1.85	0.58
3:I:133:VAL:HG22	3:I:178:THR:HA	1.86	0.58
2:K:6:GLN:NE2	2:K:96:CYS:SG	2.76	0.58
3:H:133:VAL:HG22	3:H:178:THR:HA	1.86	0.57
3:H:147:LYS:HB2	3:H:195:GLU:HB3	1.85	0.57
3:P:147:LYS:HB2	3:P:195:GLU:HB3	1.85	0.57
2:F:133:VAL:HG12	2:F:135:PRO:HD3	1.85	0.57
3:P:133:VAL:HG22	3:P:178:THR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:6:GLN:NE2	2:R:96:CYS:SG	2.76	0.57
2:D:6:GLN:NE2	2:D:96:CYS:SG	2.76	0.57
2:Q:133:VAL:HG12	2:Q:135:PRO:HD3	1.85	0.57
1:J:261:THR:HG21	1:J:299:ILE:HG23	1.87	0.57
1:B:10:ILE:HG12	1:B:95:LEU:HD23	1.87	0.56
3:L:133:VAL:HG22	3:L:178:THR:HA	1.86	0.56
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.87	0.56
1:A:10:ILE:HG12	1:A:95:LEU:HD23	1.87	0.56
1:C:10:ILE:HG12	1:C:95:LEU:HD23	1.87	0.56
1:C:261:THR:HG21	1:C:299:ILE:HG23	1.87	0.56
3:O:133:VAL:HG22	3:O:178:THR:HA	1.86	0.56
3:E:133:VAL:HG22	3:E:178:THR:HA	1.86	0.56
1:N:10:ILE:HG12	1:N:95:LEU:HD23	1.87	0.56
1:M:261:THR:HG21	1:M:299:ILE:HG23	1.87	0.56
1:J:10:ILE:HG12	1:J:95:LEU:HD23	1.87	0.55
3:P:137:ASN:ND2	3:P:174:SER:OG	2.39	0.55
3:H:137:ASN:ND2	3:H:174:SER:OG	2.39	0.55
3:I:137:ASN:ND2	3:I:174:SER:OG	2.40	0.55
1:M:10:ILE:HG12	1:M:95:LEU:HD23	1.87	0.55
3:E:137:ASN:ND2	3:E:174:SER:OG	2.40	0.55
3:O:137:ASN:ND2	3:O:174:SER:OG	2.39	0.55
3:E:2:ILE:HB	3:E:90:GLN:HE22	1.72	0.55
3:E:160:LEU:HB2	3:E:178:THR:HB	1.89	0.54
3:H:2:ILE:HB	3:H:90:GLN:HE22	1.72	0.54
1:J:6:ARG:NH1	1:J:265:TYR:OH	2.41	0.54
3:L:137:ASN:ND2	3:L:174:SER:OG	2.39	0.54
3:L:160:LEU:HB2	3:L:178:THR:HB	1.89	0.54
3:O:2:ILE:HB	3:O:90:GLN:HE22	1.72	0.54
1:A:6:ARG:NH1	1:A:265:TYR:OH	2.40	0.54
1:N:261:THR:HG21	1:N:299:ILE:HG23	1.87	0.54
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.87	0.54
1:A:228:HIS:NE2	1:A:274:ASP:OD2	2.40	0.54
1:N:6:ARG:NH1	1:N:265:TYR:OH	2.40	0.54
3:O:2:ILE:HG23	3:O:26:SER:HB3	1.90	0.54
1:B:6:ARG:NH1	1:B:265:TYR:OH	2.41	0.54
3:E:85:VAL:HG22	3:E:103:LYS:HG2	1.90	0.54
3:L:2:ILE:HB	3:L:90:GLN:HE22	1.73	0.54
3:O:160:LEU:HB2	3:O:178:THR:HB	1.90	0.54
3:P:85:VAL:HG22	3:P:103:LYS:HG2	1.90	0.54
3:I:2:ILE:HG23	3:I:26:SER:HB3	1.90	0.53
3:I:85:VAL:HG22	3:I:103:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ARG:NH1	1:C:265:TYR:OH	2.40	0.53
3:H:160:LEU:HB2	3:H:178:THR:HB	1.89	0.53
1:M:6:ARG:NH1	1:M:265:TYR:OH	2.41	0.53
3:P:160:LEU:HB2	3:P:178:THR:HB	1.89	0.53
3:I:2:ILE:HB	3:I:90:GLN:HE22	1.72	0.53
3:I:160:LEU:HB2	3:I:178:THR:HB	1.89	0.53
1:B:32:ARG:O	2:F:75:SER:OG	2.27	0.53
1:M:228:HIS:NE2	1:M:274:ASP:OD2	2.40	0.53
3:P:2:ILE:HG23	3:P:26:SER:HB3	1.90	0.53
1:A:17:LYS:NZ	1:A:57:ASP:OD1	2.42	0.53
3:H:85:VAL:HG22	3:H:103:LYS:HG2	1.90	0.53
1:N:17:LYS:NZ	1:N:57:ASP:OD1	2.42	0.53
3:O:85:VAL:HG22	3:O:103:LYS:HG2	1.90	0.52
3:H:2:ILE:HG23	3:H:26:SER:HB3	1.90	0.52
3:E:2:ILE:HG23	3:E:26:SER:HB3	1.90	0.52
3:L:85:VAL:HG22	3:L:103:LYS:HG2	1.90	0.52
1:C:17:LYS:NZ	1:C:57:ASP:OD1	2.42	0.52
2:F:140:CYS:HG	2:F:196:THR:HG1	1.56	0.52
2:F:167:ASN:HD21	2:F:205:ILE:HA	1.75	0.52
3:L:2:ILE:HG23	3:L:26:SER:HB3	1.90	0.52
2:K:139:VAL:HB	2:K:224:PRO:HD3	1.92	0.52
1:M:32:ARG:O	2:Q:75:SER:OG	2.27	0.52
3:P:2:ILE:HB	3:P:90:GLN:HE22	1.72	0.52
2:Q:139:VAL:HB	2:Q:224:PRO:HD3	1.92	0.52
1:A:101:HIS:ND1	1:A:128:ASP:OD2	2.42	0.52
3:H:15:PRO:HA	3:H:78:LEU:HD12	1.92	0.52
1:J:17:LYS:NZ	1:J:57:ASP:OD1	2.42	0.52
1:M:17:LYS:NZ	1:M:57:ASP:OD1	2.42	0.52
2:G:167:ASN:HD21	2:G:205:ILE:HA	1.75	0.52
2:D:139:VAL:HB	2:D:224:PRO:HD3	1.92	0.51
2:D:167:ASN:HD21	2:D:205:ILE:HA	1.75	0.51
1:C:228:HIS:NE2	1:C:274:ASP:OD2	2.40	0.51
3:I:186:TYR:O	3:I:192:TYR:OH	2.29	0.51
2:K:6:GLN:H	2:K:117:GLN:HE22	1.59	0.51
2:R:167:ASN:HD21	2:R:205:ILE:HA	1.75	0.51
3:H:186:TYR:O	3:H:192:TYR:OH	2.29	0.51
3:L:186:TYR:O	3:L:192:TYR:OH	2.29	0.51
2:K:167:ASN:HD21	2:K:205:ILE:HA	1.75	0.51
2:Q:6:GLN:H	2:Q:117:GLN:HE22	1.59	0.51
2:G:139:VAL:HB	2:G:224:PRO:HD3	1.92	0.51
1:B:17:LYS:NZ	1:B:57:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:ND1	1:C:128:ASP:OD2	2.43	0.51
2:Q:167:ASN:HD21	2:Q:205:ILE:HA	1.75	0.51
1:B:228:HIS:NE2	1:B:274:ASP:OD2	2.40	0.51
2:D:86:LEU:HB3	2:D:123:VAL:HG11	1.93	0.51
3:O:15:PRO:HA	3:O:78:LEU:HD12	1.92	0.51
3:P:186:TYR:O	3:P:192:TYR:OH	2.29	0.51
2:D:6:GLN:H	2:D:117:GLN:HE22	1.59	0.51
3:O:186:TYR:O	3:O:192:TYR:OH	2.29	0.51
3:P:15:PRO:HA	3:P:78:LEU:HD12	1.92	0.51
2:G:6:GLN:H	2:G:117:GLN:HE22	1.59	0.51
3:E:79:GLU:HG3	3:E:81:GLU:HG2	1.94	0.50
2:R:139:VAL:HB	2:R:224:PRO:HD3	1.92	0.50
2:G:86:LEU:HB3	2:G:123:VAL:HG11	1.93	0.50
2:R:140:CYS:SG	2:R:196:THR:OG1	2.70	0.50
3:I:79:GLU:HG3	3:I:81:GLU:HG2	1.94	0.50
2:K:86:LEU:HB3	2:K:123:VAL:HG11	1.93	0.50
3:E:186:TYR:O	3:E:192:TYR:OH	2.29	0.50
3:P:79:GLU:HG3	3:P:81:GLU:HG2	1.94	0.50
2:F:139:VAL:HB	2:F:224:PRO:HD3	1.92	0.50
3:E:15:PRO:HA	3:E:78:LEU:HD12	1.93	0.50
1:J:228:HIS:NE2	1:J:274:ASP:OD2	2.40	0.50
1:J:230:SER:HA	1:J:274:ASP:HB2	1.94	0.50
3:L:79:GLU:HG3	3:L:81:GLU:HG2	1.94	0.50
1:M:230:SER:HA	1:M:274:ASP:HB2	1.94	0.50
3:L:15:PRO:HA	3:L:78:LEU:HD12	1.93	0.50
2:F:6:GLN:H	2:F:117:GLN:HE22	1.59	0.50
2:F:86:LEU:HB3	2:F:123:VAL:HG11	1.93	0.50
2:R:6:GLN:H	2:R:117:GLN:HE22	1.59	0.50
3:I:15:PRO:HA	3:I:78:LEU:HD12	1.92	0.50
1:N:32:ARG:O	2:R:75:SER:OG	2.30	0.50
1:A:230:SER:HA	1:A:274:ASP:HB2	1.94	0.49
2:F:91:THR:HG22	2:F:123:VAL:H	1.77	0.49
2:R:86:LEU:HB3	2:R:123:VAL:HG11	1.93	0.49
1:M:21:ARG:HD3	2:K:102:TYR:CG	2.47	0.49
1:J:101:HIS:ND1	1:J:128:ASP:OD2	2.42	0.49
2:Q:91:THR:HG22	2:Q:123:VAL:H	1.77	0.49
1:A:15:PHE:HB3	1:A:103:LEU:HD11	1.94	0.49
2:D:91:THR:HG22	2:D:123:VAL:H	1.78	0.49
2:D:102:TYR:CG	1:B:21:ARG:HD3	2.47	0.49
1:J:15:PHE:HB3	1:J:103:LEU:HD11	1.94	0.49
3:L:91:HIS:NE2	2:K:102:TYR:OH	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:91:THR:HG22	2:K:123:VAL:H	1.77	0.49
1:B:230:SER:HA	1:B:274:ASP:HB2	1.94	0.49
1:C:32:ARG:O	2:G:75:SER:OG	2.30	0.49
3:H:79:GLU:HG3	3:H:81:GLU:HG2	1.94	0.49
2:R:91:THR:HG22	2:R:123:VAL:H	1.78	0.49
3:L:137:ASN:HD21	2:K:176:HIS:CD2	2.31	0.49
1:N:101:HIS:ND1	1:N:128:ASP:OD2	2.42	0.49
3:O:79:GLU:HG3	3:O:81:GLU:HG2	1.94	0.49
2:Q:86:LEU:HB3	2:Q:123:VAL:HG11	1.93	0.49
1:N:15:PHE:HB3	1:N:103:LEU:HD11	1.95	0.49
1:C:15:PHE:HB3	1:C:103:LEU:HD11	1.95	0.48
2:G:91:THR:HG22	2:G:123:VAL:H	1.78	0.48
1:M:15:PHE:HB3	1:M:103:LEU:HD11	1.95	0.48
3:L:187:GLU:OE1	3:L:211:ARG:NH1	2.47	0.48
1:N:228:HIS:NE2	1:N:274:ASP:OD2	2.40	0.48
2:D:102:TYR:OH	3:E:91:HIS:NE2	2.44	0.48
1:J:30:VAL:HA	1:J:33:LYS:HG2	1.96	0.48
1:N:21:ARG:HD3	2:Q:102:TYR:CG	2.49	0.48
3:P:187:GLU:OE1	3:P:211:ARG:NH1	2.47	0.48
3:E:187:GLU:OE1	3:E:211:ARG:NH1	2.47	0.48
1:M:101:HIS:ND1	1:M:128:ASP:OD2	2.42	0.48
2:F:35:SER:HB2	2:F:47:TRP:HE1	1.79	0.48
1:A:30:VAL:HA	1:A:33:LYS:HG2	1.96	0.48
2:D:176:HIS:CD2	3:E:137:ASN:HD21	2.31	0.48
1:C:30:VAL:HA	1:C:33:LYS:HG2	1.96	0.48
1:N:230:SER:HA	1:N:274:ASP:HB2	1.94	0.48
3:O:148:TRP:HB3	3:O:155:ARG:HD2	1.96	0.48
1:B:15:PHE:HB3	1:B:103:LEU:HD11	1.95	0.48
1:N:30:VAL:HA	1:N:33:LYS:HG2	1.96	0.48
1:C:21:ARG:HD3	2:F:102:TYR:CG	2.49	0.48
3:H:148:TRP:HB3	3:H:155:ARG:HD2	1.96	0.48
3:H:187:GLU:OE1	3:H:211:ARG:NH1	2.47	0.48
3:P:148:TRP:HB3	3:P:155:ARG:HD2	1.96	0.48
1:C:230:SER:HA	1:C:274:ASP:HB2	1.94	0.48
2:R:35:SER:HB2	2:R:47:TRP:HE1	1.79	0.48
3:L:148:TRP:HB3	3:L:155:ARG:HD2	1.96	0.47
3:L:160:LEU:O	3:L:178:THR:N	2.45	0.47
3:H:160:LEU:O	3:H:178:THR:N	2.45	0.47
2:K:35:SER:HB2	2:K:47:TRP:HE1	1.79	0.47
2:R:135:PRO:HB3	2:R:152:CYS:HA	1.97	0.47
2:Q:35:SER:HB2	2:Q:47:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:35:SER:HB2	2:G:47:TRP:HE1	1.79	0.47
3:I:187:GLU:OE1	3:I:211:ARG:NH1	2.47	0.47
3:O:6:GLN:OE1	3:O:102:THR:OG1	2.33	0.47
3:O:187:GLU:OE1	3:O:211:ARG:NH1	2.47	0.47
3:P:6:GLN:OE1	3:P:102:THR:OG1	2.33	0.47
1:A:32:ARG:O	2:D:75:SER:OG	2.31	0.47
2:D:35:SER:HB2	2:D:47:TRP:HE1	1.79	0.47
2:D:140:CYS:HG	2:D:196:THR:HG1	1.52	0.47
3:E:148:TRP:HB3	3:E:155:ARG:HD2	1.96	0.47
1:B:30:VAL:HA	1:B:33:LYS:HG2	1.96	0.47
3:I:6:GLN:OE1	3:I:102:THR:OG1	2.33	0.47
2:Q:74:THR:O	2:Q:74:THR:OG1	2.33	0.47
1:J:32:ARG:O	2:K:75:SER:OG	2.31	0.47
1:M:30:VAL:HA	1:M:33:LYS:HG2	1.96	0.47
1:M:104:ALA:HA	1:M:107:SER:HB3	1.97	0.47
1:N:46:ASP:O	1:N:92:ARG:NH1	2.48	0.47
2:G:135:PRO:HB3	2:G:152:CYS:HA	1.97	0.47
1:M:46:ASP:O	1:M:92:ARG:NH1	2.48	0.47
1:A:46:ASP:O	1:A:92:ARG:NH1	2.48	0.46
2:D:83:LEU:HD12	2:D:86:LEU:HG	1.98	0.46
1:J:46:ASP:O	1:J:92:ARG:NH1	2.48	0.46
2:D:135:PRO:HB3	2:D:152:CYS:HA	1.97	0.46
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.97	0.46
2:K:135:PRO:HB3	2:K:152:CYS:HA	1.97	0.46
2:Q:83:LEU:HD12	2:Q:86:LEU:HG	1.98	0.46
3:E:70:ASP:OD1	3:E:70:ASP:N	2.49	0.46
3:I:148:TRP:HB3	3:I:155:ARG:HD2	1.96	0.46
2:G:140:CYS:SG	2:G:196:THR:OG1	2.70	0.46
1:B:284:LYS:N	1:B:288:GLU:OE1	2.43	0.46
1:C:104:ALA:HA	1:C:107:SER:HB3	1.97	0.46
3:L:70:ASP:OD1	3:L:70:ASP:N	2.48	0.46
1:N:104:ALA:HA	1:N:107:SER:HB3	1.97	0.46
2:F:83:LEU:HD12	2:F:86:LEU:HG	1.98	0.46
2:Q:135:PRO:HB3	2:Q:152:CYS:HA	1.97	0.46
3:P:90:GLN:NE2	3:P:97:THR:OG1	2.49	0.46
1:J:284:LYS:N	1:J:288:GLU:OE1	2.43	0.46
3:L:6:GLN:OE1	3:L:102:THR:OG1	2.33	0.46
1:A:104:ALA:HA	1:A:107:SER:HB3	1.97	0.46
3:I:90:GLN:NE2	3:I:97:THR:OG1	2.49	0.46
2:F:135:PRO:HB3	2:F:152:CYS:HA	1.97	0.46
2:G:83:LEU:HD12	2:G:86:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ASP:O	1:C:92:ARG:NH1	2.48	0.46
3:I:70:ASP:OD1	3:I:70:ASP:N	2.48	0.46
1:J:98:GLY:HA3	1:J:99:GLY:HA3	1.75	0.46
3:O:120:PRO:HD3	3:O:132:VAL:HG22	1.98	0.46
2:K:83:LEU:HD12	2:K:86:LEU:HG	1.98	0.46
3:E:160:LEU:O	3:E:178:THR:N	2.45	0.45
3:E:6:GLN:OE1	3:E:102:THR:OG1	2.33	0.45
3:E:120:PRO:HD3	3:E:132:VAL:HG22	1.98	0.45
1:B:46:ASP:O	1:B:92:ARG:NH1	2.48	0.45
3:H:6:GLN:OE1	3:H:102:THR:OG1	2.33	0.45
3:O:90:GLN:NE2	3:O:97:THR:OG1	2.49	0.45
3:P:70:ASP:OD1	3:P:70:ASP:N	2.49	0.45
1:B:104:ALA:HA	1:B:107:SER:HB3	1.97	0.45
3:H:90:GLN:NE2	3:H:97:THR:OG1	2.49	0.45
3:E:90:GLN:NE2	3:E:97:THR:OG1	2.49	0.45
1:B:101:HIS:ND1	1:B:128:ASP:OD2	2.42	0.45
1:M:206:LEU:HB3	1:M:210:LYS:HB3	1.99	0.45
1:N:206:LEU:HB3	1:N:210:LYS:HB3	1.99	0.45
3:O:116:SER:O	3:O:135:PHE:N	2.50	0.45
3:P:120:PRO:HD3	3:P:132:VAL:HG22	1.98	0.45
2:R:83:LEU:HD12	2:R:86:LEU:HG	1.98	0.45
1:J:104:ALA:HA	1:J:107:SER:HB3	1.97	0.45
3:O:49:TYR:HD1	3:O:55:ALA:HB2	1.82	0.45
2:D:19:LYS:HB2	2:D:82:GLU:HG2	2.00	0.44
3:I:120:PRO:HD3	3:I:132:VAL:HG22	1.98	0.44
2:D:32:TYR:HA	2:D:101:ALA:H	1.83	0.44
1:B:98:GLY:HA3	1:B:99:GLY:HA3	1.74	0.44
3:L:90:GLN:NE2	3:L:97:THR:OG1	2.49	0.44
2:K:17:SER:HA	2:K:86:LEU:HD11	2.00	0.44
2:Q:17:SER:HA	2:Q:86:LEU:HD11	1.99	0.44
3:P:49:TYR:HD1	3:P:55:ALA:HB2	1.82	0.44
3:E:49:TYR:HD1	3:E:55:ALA:HB2	1.83	0.44
2:F:17:SER:HA	2:F:86:LEU:HD11	2.00	0.44
2:R:32:TYR:HA	2:R:101:ALA:H	1.82	0.44
2:G:19:LYS:HB2	2:G:82:GLU:HG2	1.99	0.44
2:R:148:VAL:N	2:R:196:THR:O	2.45	0.44
3:L:49:TYR:HD1	3:L:55:ALA:HB2	1.82	0.44
2:G:32:TYR:HA	2:G:101:ALA:H	1.83	0.44
2:K:19:LYS:HB2	2:K:82:GLU:HG2	1.99	0.44
2:D:17:SER:HA	2:D:86:LEU:HD11	1.99	0.44
3:H:120:PRO:HD3	3:H:132:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:19:LYS:HB2	2:Q:82:GLU:HG2	2.00	0.44
1:B:206:LEU:HB3	1:B:210:LYS:HB3	1.99	0.44
1:C:206:LEU:HB3	1:C:210:LYS:HB3	1.99	0.44
3:H:49:TYR:HD1	3:H:55:ALA:HB2	1.83	0.44
3:H:58:ILE:HD12	3:H:58:ILE:HA	1.86	0.44
3:P:37:GLN:HB2	3:P:47:LEU:HD21	2.00	0.44
2:K:35:SER:N	2:K:97:ALA:O	2.44	0.44
2:Q:140:CYS:SG	2:Q:196:THR:OG1	2.70	0.44
3:E:150:ILE:HA	3:E:155:ARG:HH21	1.83	0.44
3:I:49:TYR:HD1	3:I:55:ALA:HB2	1.83	0.44
3:O:37:GLN:HB2	3:O:47:LEU:HD21	2.00	0.44
2:Q:32:TYR:HA	2:Q:101:ALA:H	1.83	0.44
3:P:160:LEU:O	3:P:178:THR:N	2.45	0.43
2:F:19:LYS:HB2	2:F:82:GLU:HG2	2.00	0.43
3:E:116:SER:O	3:E:135:PHE:N	2.50	0.43
3:O:150:ILE:HA	3:O:155:ARG:HH21	1.83	0.43
2:K:32:TYR:HA	2:K:101:ALA:H	1.83	0.43
2:K:140:CYS:HG	2:K:196:THR:HG1	1.56	0.43
2:R:19:LYS:HB2	2:R:82:GLU:HG2	2.00	0.43
3:I:116:SER:O	3:I:135:PHE:N	2.50	0.43
1:A:206:LEU:HB3	1:A:210:LYS:HB3	1.99	0.43
3:H:37:GLN:HB2	3:H:47:LEU:HD21	2.00	0.43
2:R:17:SER:HA	2:R:86:LEU:HD11	1.99	0.43
2:D:101:ALA:O	2:D:106:SER:OG	2.28	0.43
3:H:70:ASP:OD1	3:H:70:ASP:N	2.49	0.43
3:I:150:ILE:HA	3:I:155:ARG:HH21	1.83	0.43
1:J:206:LEU:HB3	1:J:210:LYS:HB3	1.99	0.43
2:Q:51:ILE:H	2:Q:51:ILE:HG13	1.72	0.43
2:R:35:SER:N	2:R:97:ALA:O	2.44	0.43
1:N:236:LEU:HD23	1:N:252:LEU:HB2	2.01	0.43
3:H:150:ILE:HA	3:H:155:ARG:HH21	1.83	0.43
3:P:116:SER:O	3:P:135:PHE:N	2.50	0.43
2:F:148:VAL:N	2:F:196:THR:O	2.45	0.43
2:G:17:SER:HA	2:G:86:LEU:HD11	1.99	0.43
2:G:148:VAL:N	2:G:196:THR:O	2.45	0.43
3:E:37:GLN:HB2	3:E:47:LEU:HD21	2.00	0.42
3:L:150:ILE:HA	3:L:155:ARG:HH21	1.84	0.42
3:I:160:LEU:O	3:I:178:THR:N	2.45	0.42
3:L:58:ILE:HD12	3:L:58:ILE:HA	1.86	0.42
3:H:194:CYS:N	3:H:207:LYS:O	2.51	0.42
1:M:31:LEU:HD23	1:M:293:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLY:HA3	1:C:99:GLY:HA3	1.75	0.42
2:R:155:LYS:HA	2:R:189:LEU:HD23	2.02	0.42
2:D:211:HIS:CE1	2:D:213:ALA:HB3	2.55	0.42
3:I:37:GLN:HB2	3:I:47:LEU:HD21	2.00	0.42
3:P:150:ILE:HA	3:P:155:ARG:HH21	1.83	0.42
1:A:236:LEU:HD23	1:A:252:LEU:HB2	2.01	0.42
2:G:206:THR:HG22	2:G:221:LYS:HA	2.02	0.42
1:B:236:LEU:HD23	1:B:252:LEU:HB2	2.01	0.42
1:C:236:LEU:HD23	1:C:252:LEU:HB2	2.01	0.42
1:C:284:LYS:N	1:C:288:GLU:OE1	2.43	0.42
2:F:32:TYR:HA	2:F:101:ALA:H	1.83	0.42
2:F:155:LYS:HA	2:F:189:LEU:HD23	2.02	0.42
2:D:155:LYS:HA	2:D:189:LEU:HD23	2.01	0.42
1:B:31:LEU:HD23	1:B:293:VAL:HG13	2.01	0.42
3:L:37:GLN:HB2	3:L:47:LEU:HD21	2.00	0.42
1:J:236:LEU:HD23	1:J:252:LEU:HB2	2.01	0.42
2:Q:206:THR:HG22	2:Q:221:LYS:HA	2.02	0.42
2:Q:211:HIS:CE1	2:Q:213:ALA:HB3	2.55	0.42
1:A:32:ARG:NH2	1:A:49:ASP:OD1	2.53	0.42
1:B:32:ARG:NH2	1:B:49:ASP:OD1	2.53	0.42
1:C:31:LEU:HD23	1:C:293:VAL:HG13	2.01	0.42
3:L:116:SER:O	3:L:135:PHE:N	2.50	0.42
3:O:160:LEU:O	3:O:178:THR:N	2.45	0.42
1:A:98:GLY:HA3	1:A:99:GLY:HA3	1.75	0.41
3:I:91:HIS:NE2	2:G:102:TYR:OH	2.53	0.41
1:J:21:ARG:HD3	2:R:102:TYR:CG	2.55	0.41
2:F:50:TRP:HZ2	2:F:101:ALA:HA	1.85	0.41
2:F:135:PRO:HG3	2:F:220:LYS:HG2	2.02	0.41
2:G:50:TRP:HZ2	2:G:101:ALA:HA	1.85	0.41
2:K:135:PRO:HG3	2:K:220:LYS:HG2	2.02	0.41
2:K:211:HIS:CE1	2:K:213:ALA:HB3	2.55	0.41
2:R:206:THR:HG22	2:R:221:LYS:HA	2.02	0.41
1:C:32:ARG:NH2	1:C:49:ASP:OD1	2.53	0.41
1:J:31:LEU:HD23	1:J:293:VAL:HG13	2.01	0.41
1:N:32:ARG:NH2	1:N:49:ASP:OD1	2.53	0.41
2:F:206:THR:HG22	2:F:221:LYS:HA	2.02	0.41
2:K:83:LEU:HD13	2:K:84:ARG:H	1.85	0.41
2:R:135:PRO:HG3	2:R:220:LYS:HG2	2.02	0.41
3:H:116:SER:O	3:H:135:PHE:N	2.50	0.41
1:M:236:LEU:HD23	1:M:252:LEU:HB2	2.01	0.41
2:Q:35:SER:N	2:Q:97:ALA:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:146:SER:O	2:F:198:SER:N	2.54	0.41
2:K:146:SER:O	2:K:198:SER:N	2.54	0.41
2:K:155:LYS:HA	2:K:189:LEU:HD23	2.01	0.41
2:Q:135:PRO:HG3	2:Q:220:LYS:HG2	2.02	0.41
3:P:58:ILE:HD12	3:P:58:ILE:HA	1.86	0.41
2:G:7:SER:HA	2:G:8:GLY:HA2	1.88	0.41
2:G:83:LEU:HD13	2:G:84:ARG:H	1.85	0.41
2:K:50:TRP:HZ2	2:K:101:ALA:HA	1.85	0.41
2:Q:50:TRP:HZ2	2:Q:101:ALA:HA	1.85	0.41
1:A:21:ARG:HD3	2:G:102:TYR:CG	2.55	0.41
1:A:31:LEU:HD23	1:A:293:VAL:HG13	2.01	0.41
2:D:74:THR:O	2:D:74:THR:OG1	2.33	0.41
3:E:20:THR:HG22	3:E:74:THR:HG22	2.03	0.41
3:L:20:THR:HG22	3:L:74:THR:HG22	2.03	0.41
1:M:284:LYS:N	1:M:288:GLU:OE1	2.43	0.41
2:F:211:HIS:CE1	2:F:213:ALA:HB3	2.55	0.41
2:G:155:LYS:HA	2:G:189:LEU:HD23	2.01	0.41
2:Q:155:LYS:HA	2:Q:189:LEU:HD23	2.01	0.41
2:D:50:TRP:HZ2	2:D:101:ALA:HA	1.85	0.41
2:D:135:PRO:HG3	2:D:220:LYS:HG2	2.02	0.41
3:L:75:ILE:HG22	3:L:78:LEU:HA	2.03	0.41
2:F:83:LEU:HD13	2:F:84:ARG:H	1.85	0.41
2:K:51:ILE:H	2:K:51:ILE:HG13	1.72	0.41
1:A:101:HIS:CE1	1:A:232:ASP:HB2	2.56	0.41
1:M:32:ARG:NH2	1:M:49:ASP:OD1	2.53	0.41
1:M:140:LEU:HD23	1:M:140:LEU:HA	1.93	0.41
2:R:83:LEU:HD13	2:R:84:ARG:H	1.85	0.41
2:R:211:HIS:CE1	2:R:213:ALA:HB3	2.55	0.41
1:J:32:ARG:NH2	1:J:49:ASP:OD1	2.53	0.41
2:G:211:HIS:CE1	2:G:213:ALA:HB3	2.55	0.41
2:R:146:SER:O	2:R:198:SER:N	2.54	0.41
3:I:88:CYS:O	3:I:99:GLY:N	2.55	0.41
2:R:50:TRP:HZ2	2:R:101:ALA:HA	1.85	0.41
2:D:83:LEU:HD13	2:D:84:ARG:H	1.85	0.40
2:D:206:THR:HG22	2:D:221:LYS:HA	2.02	0.40
1:C:64:PHE:HB3	1:C:67:VAL:HB	2.03	0.40
1:J:101:HIS:CE1	1:J:232:ASP:HB2	2.56	0.40
1:N:101:HIS:CE1	1:N:232:ASP:HB2	2.56	0.40
1:N:284:LYS:N	1:N:288:GLU:OE1	2.43	0.40
3:O:75:ILE:HG22	3:O:78:LEU:HA	2.03	0.40
2:G:140:CYS:HB2	2:G:148:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:146:SER:O	2:Q:198:SER:N	2.54	0.40
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.56	0.40
1:N:31:LEU:HD23	1:N:293:VAL:HG13	2.01	0.40
2:G:135:PRO:HG3	2:G:220:LYS:HG2	2.02	0.40
1:A:284:LYS:N	1:A:288:GLU:OE1	2.43	0.40
3:O:88:CYS:O	3:O:99:GLY:N	2.55	0.40
2:G:157:TYR:O	2:G:188:THR:OG1	2.30	0.40
2:R:140:CYS:HB2	2:R:148:VAL:HG11	2.03	0.40
3:E:58:ILE:HD12	3:E:58:ILE:HA	1.86	0.40
2:K:140:CYS:HA	2:K:201:PRO:HA	2.04	0.40
2:D:7:SER:HA	2:D:8:GLY:HA2	1.88	0.40
3:E:75:ILE:HG22	3:E:78:LEU:HA	2.03	0.40
3:I:75:ILE:HG22	3:I:78:LEU:HA	2.03	0.40
1:J:64:PHE:HB3	1:J:67:VAL:HB	2.03	0.40
3:L:194:CYS:N	3:L:207:LYS:O	2.51	0.40
3:P:88:CYS:O	3:P:99:GLY:N	2.55	0.40
2:Q:83:LEU:HD13	2:Q:84:ARG:H	1.85	0.40
2:R:157:TYR:O	2:R:188:THR:OG1	2.30	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%)	300 (95%)	15 (5%)	0	100	100
1	B	315/322 (98%)	301 (96%)	14 (4%)	0	100	100
1	C	315/322 (98%)	300 (95%)	15 (5%)	0	100	100
1	J	315/322 (98%)	301 (96%)	14 (4%)	0	100	100
1	M	315/322 (98%)	300 (95%)	15 (5%)	0	100	100
1	N	315/322 (98%)	300 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	220/455 (48%)	196 (89%)	20 (9%)	4 (2%)	8	43
2	F	220/455 (48%)	196 (89%)	19 (9%)	5 (2%)	6	38
2	G	220/455 (48%)	197 (90%)	18 (8%)	5 (2%)	6	38
2	K	220/455 (48%)	196 (89%)	19 (9%)	5 (2%)	6	38
2	Q	220/455 (48%)	196 (89%)	20 (9%)	4 (2%)	8	43
2	R	220/455 (48%)	196 (89%)	19 (9%)	5 (2%)	6	38
3	E	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
3	H	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
3	I	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
3	L	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
3	O	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
3	P	210/214 (98%)	177 (84%)	31 (15%)	2 (1%)	15	55
All	All	4470/5946 (75%)	4041 (90%)	389 (9%)	40 (1%)	21	57

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	59	PRO
3	H	59	PRO
3	I	59	PRO
3	L	59	PRO
3	O	59	PRO
3	P	59	PRO
2	G	77	SER
2	K	77	SER
2	Q	77	SER
2	D	77	SER
2	F	77	SER
2	R	77	SER
2	D	13	LYS
2	F	13	LYS
2	G	13	LYS
2	K	13	LYS
2	Q	13	LYS
2	R	13	LYS
3	E	80	PRO
3	H	80	PRO
3	I	80	PRO

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Mol	Chain	Res	Type
3	L	80	PRO
3	O	80	PRO
3	P	80	PRO
2	D	114	PRO
2	F	114	PRO
2	G	114	PRO
2	Q	114	PRO
2	R	114	PRO
2	D	56	GLY
2	F	14	PRO
2	F	56	GLY
2	G	14	PRO
2	G	56	GLY
2	K	14	PRO
2	K	56	GLY
2	K	114	PRO
2	Q	14	PRO
2	R	14	PRO
2	R	56	GLY

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	M	265/270 (98%)	265 (100%)	0	100	100
1	N	265/270 (98%)	265 (100%)	0	100	100
2	D	191/406 (47%)	188 (98%)	3 (2%)	62	83
2	F	191/406 (47%)	188 (98%)	3 (2%)	62	83
2	G	191/406 (47%)	188 (98%)	3 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	191/406 (47%)	188 (98%)	3 (2%)	62	83
2	Q	191/406 (47%)	188 (98%)	3 (2%)	62	83
2	R	191/406 (47%)	188 (98%)	3 (2%)	62	83
3	E	185/187 (99%)	183 (99%)	2 (1%)	73	88
3	H	185/187 (99%)	183 (99%)	2 (1%)	73	88
3	I	185/187 (99%)	183 (99%)	2 (1%)	73	88
3	L	185/187 (99%)	183 (99%)	2 (1%)	73	88
3	O	185/187 (99%)	183 (99%)	2 (1%)	73	88
3	P	185/187 (99%)	183 (99%)	2 (1%)	73	88
All	All	3846/5178 (74%)	3816 (99%)	30 (1%)	82	91

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	31	ASN
2	D	59	ASN
2	D	83	LEU
3	E	108	ARG
3	E	137	ASN
3	H	108	ARG
3	H	137	ASN
3	I	108	ARG
3	I	137	ASN
3	L	108	ARG
3	L	137	ASN
3	O	108	ARG
3	O	137	ASN
3	P	108	ARG
3	P	137	ASN
2	F	31	ASN
2	F	59	ASN
2	F	83	LEU
2	G	31	ASN
2	G	59	ASN
2	G	83	LEU
2	K	31	ASN
2	K	59	ASN
2	K	83	LEU
2	Q	31	ASN

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Mol	Chain	Res	Type
2	Q	59	ASN
2	Q	83	LEU
2	R	31	ASN
2	R	59	ASN
2	R	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
2	D	31	ASN
2	D	59	ASN
3	E	90	GLN
3	E	137	ASN
1	B	126	HIS
1	C	126	HIS
3	H	90	GLN
3	H	137	ASN
3	I	90	GLN
3	I	137	ASN
1	J	126	HIS
3	L	90	GLN
3	L	137	ASN
1	M	126	HIS
1	N	126	HIS
3	O	90	GLN
3	O	137	ASN
3	P	90	GLN
3	P	137	ASN
2	F	31	ASN
2	F	59	ASN
2	G	31	ASN
2	G	59	ASN
2	K	31	ASN
2	K	59	ASN
2	Q	31	ASN
2	Q	59	ASN
2	R	31	ASN
2	R	59	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	142:ASP	C	143:THR	N	5.10
1	F	142:ASP	C	143:THR	N	5.10
1	G	142:ASP	C	143:THR	N	5.10
1	K	142:ASP	C	143:THR	N	5.10
1	Q	142:ASP	C	143:THR	N	5.10
1	R	142:ASP	C	143:THR	N	5.10
1	D	139:VAL	C	140:CYS	N	4.96
1	F	139:VAL	C	140:CYS	N	4.96
1	G	139:VAL	C	140:CYS	N	4.96
1	K	139:VAL	C	140:CYS	N	4.96
1	Q	139:VAL	C	140:CYS	N	4.96
1	R	139:VAL	C	140:CYS	N	4.96
1	D	123:VAL	C	124:SER	N	3.58
1	F	123:VAL	C	124:SER	N	3.58
1	G	123:VAL	C	124:SER	N	3.58
1	K	123:VAL	C	124:SER	N	3.58
1	Q	123:VAL	C	124:SER	N	3.58
1	R	123:VAL	C	124:SER	N	3.58
1	E	107:LYS	C	108:ARG	N	2.25
1	H	107:LYS	C	108:ARG	N	2.25
1	I	107:LYS	C	108:ARG	N	2.25
1	L	107:LYS	C	108:ARG	N	2.25
1	O	107:LYS	C	108:ARG	N	2.25
1	P	107:LYS	C	108:ARG	N	2.25

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23293. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

This section was not generated.