



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:15 pm BST

PDB ID : 3KYM
Title : Crystal structure of Li33 IgG2 di-Fab
Authors : Silvian, L.F.; Pepinsky, R.B.; Walus, L.
Deposited on : 2009-12-06
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

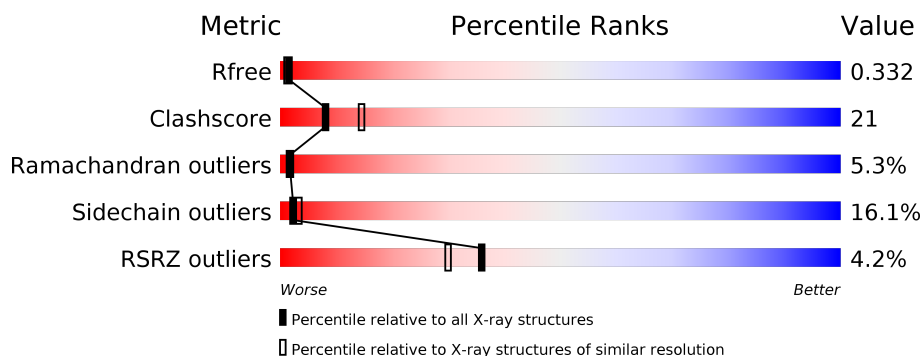
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	<div> <div></div> <div> <div></div> <div>62%</div> <div>33%</div> <div>5%</div> </div> </div>
1	C	214	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> </div> </div>
1	E	214	<div> <div></div> <div> <div></div> <div>60%</div> <div>31%</div> <div>8%</div> </div> </div>
1	G	214	<div> <div></div> <div> <div></div> <div>67%</div> <div>28%</div> <div>.</div> </div> </div>
1	I	214	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>.</div> </div> </div>
1	K	214	<div> <div>10%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>14%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	214	
1	O	214	
2	B	227	
2	D	227	
2	F	227	
2	H	227	
2	J	227	
2	L	227	
2	N	227	
2	P	227	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26358 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Light Chain Li33 IgG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			
1	C	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			
1	E	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			
1	G	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			
1	I	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			
1	K	209	Total	C	N	O	S	0	0	0
			1605	1001	273	326	5			
1	M	208	Total	C	N	O	S	0	0	0
			1597	1000	268	324	5			
1	O	213	Total	C	N	O	S	0	0	0
			1640	1026	277	332	5			

- Molecule 2 is a protein called Heavy Chain Li33 IgG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1672	1057	283	325	7			
2	D	220	Total	C	N	O	S	0	0	0
			1672	1057	283	325	7			
2	F	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			
2	H	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			
2	J	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			
2	L	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			

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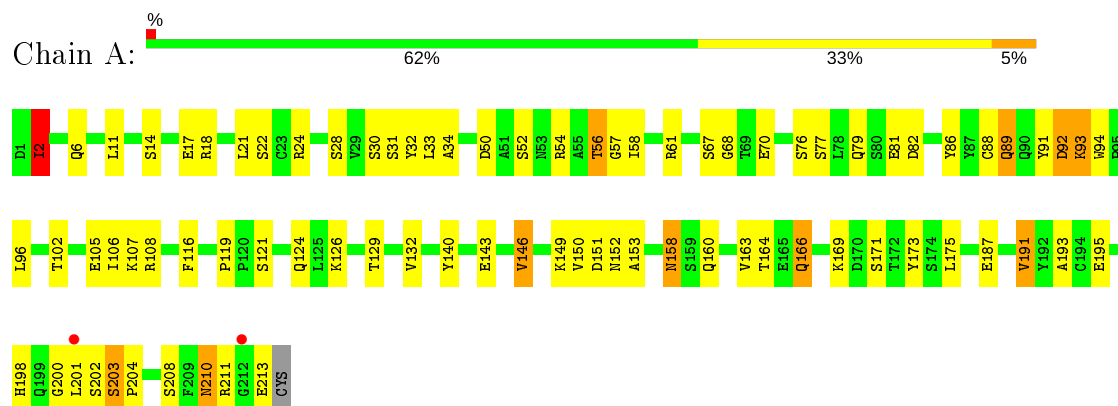
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			
2	P	219	Total	C	N	O	S	0	0	0
			1657	1048	278	324	7			

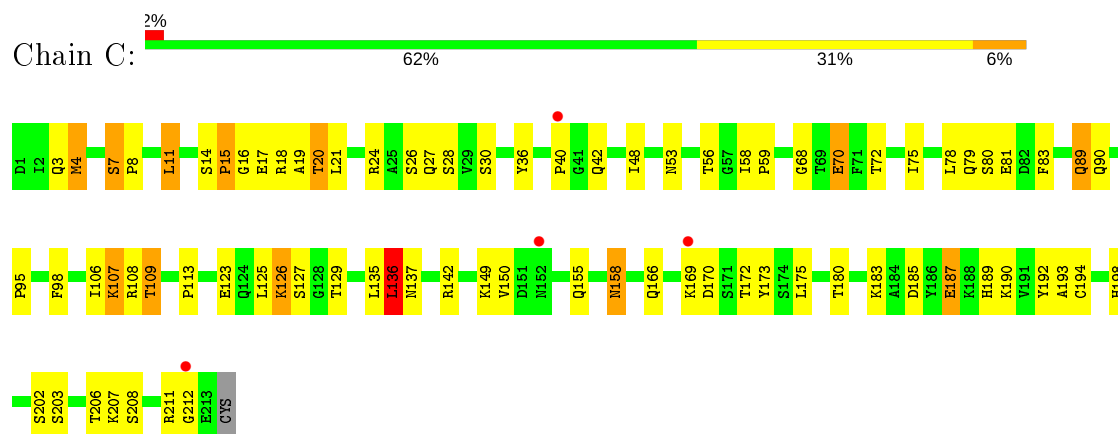
3 Residue-property plots [i](#)

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

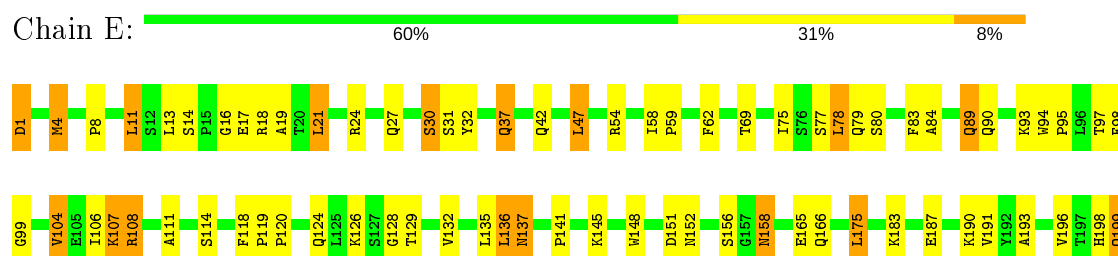
• Molecule 1: Light Chain Li33 IgG2



• Molecule 1: Light Chain Li33 IgG2



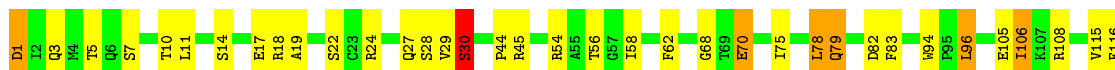
• Molecule 1: Light Chain Li33 IgG2





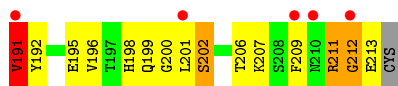
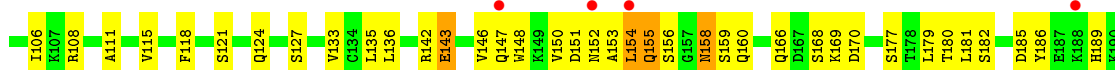
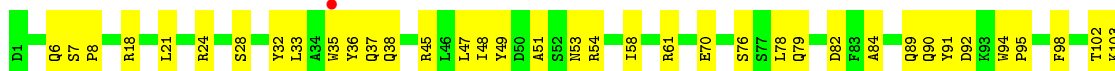
• Molecule 1: Light Chain Li33 IgG2

Chain G: 67% 28% .



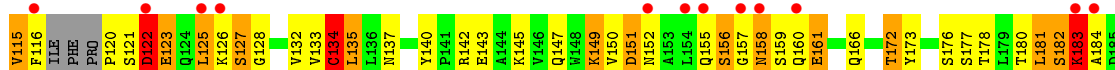
• Molecule 1: Light Chain Li33 IgG2

Chain I: 5% 57% 38% .



• Molecule 1: Light Chain Li33 IgG2

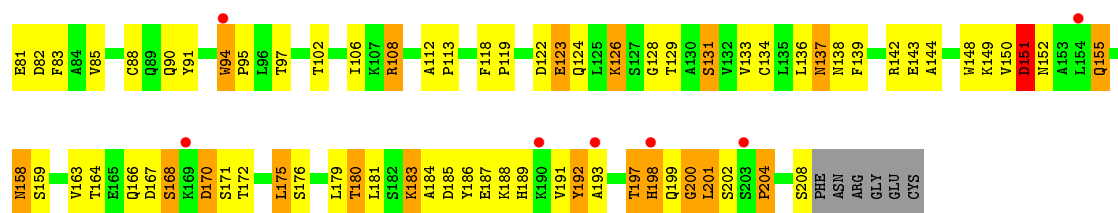
Chain K: 10% 52% 29% 14% . .



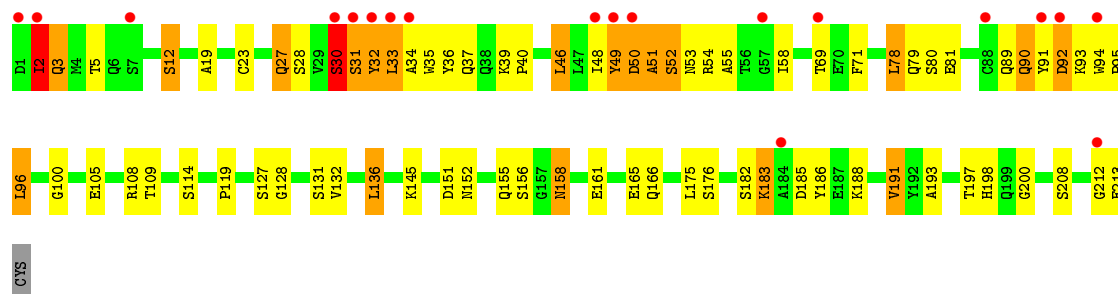
• Molecule 1: Light Chain Li33 IgG2

Chain M: 4% 47% 36% 14% .

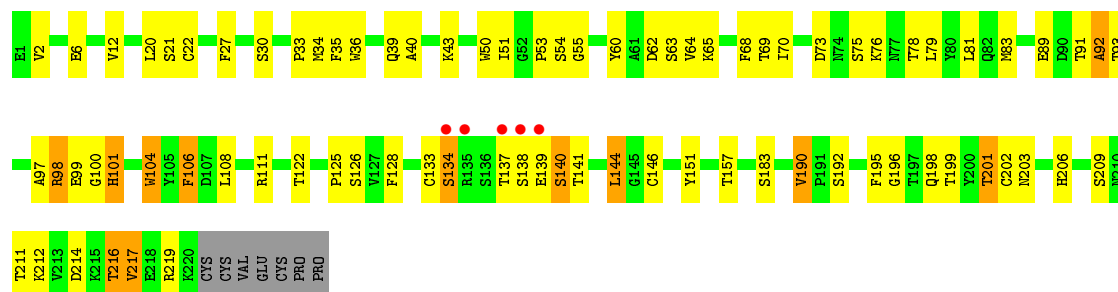




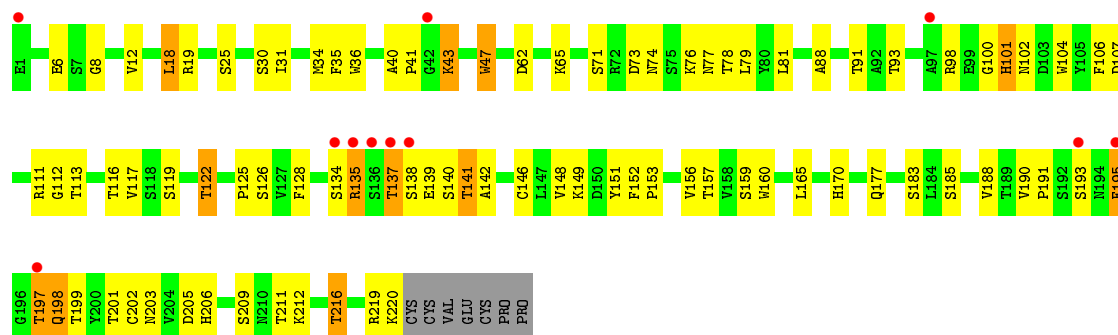
• Molecule 1: Light Chain Li33 IgG2



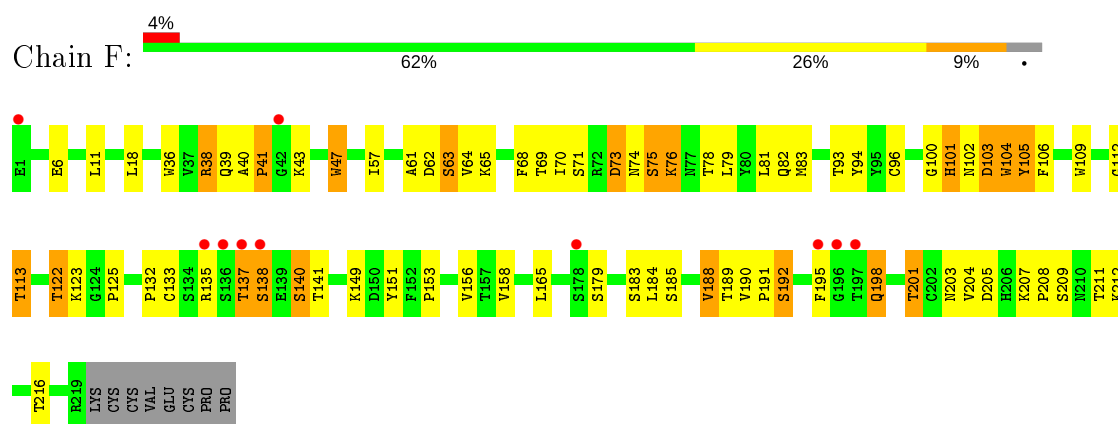
• Molecule 2: Heavy Chain Li33 IgG2



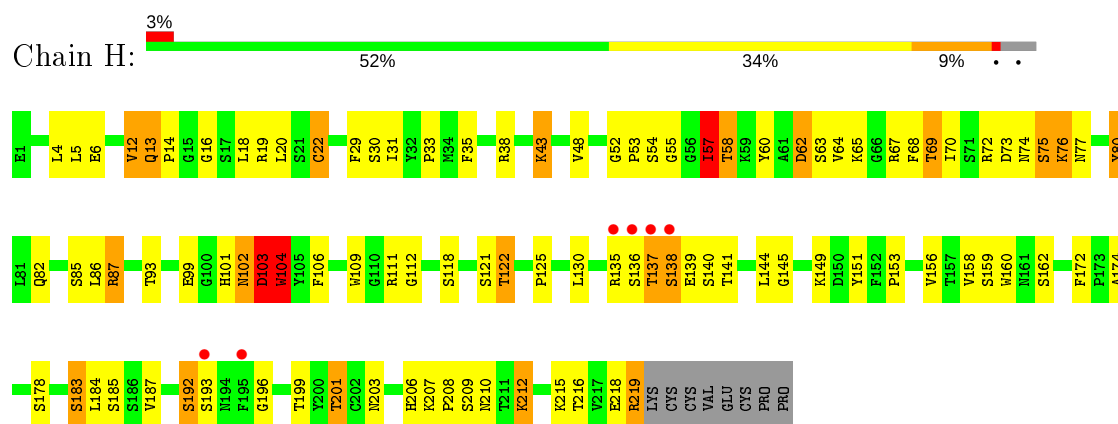
• Molecule 2: Heavy Chain Li33 IgG2



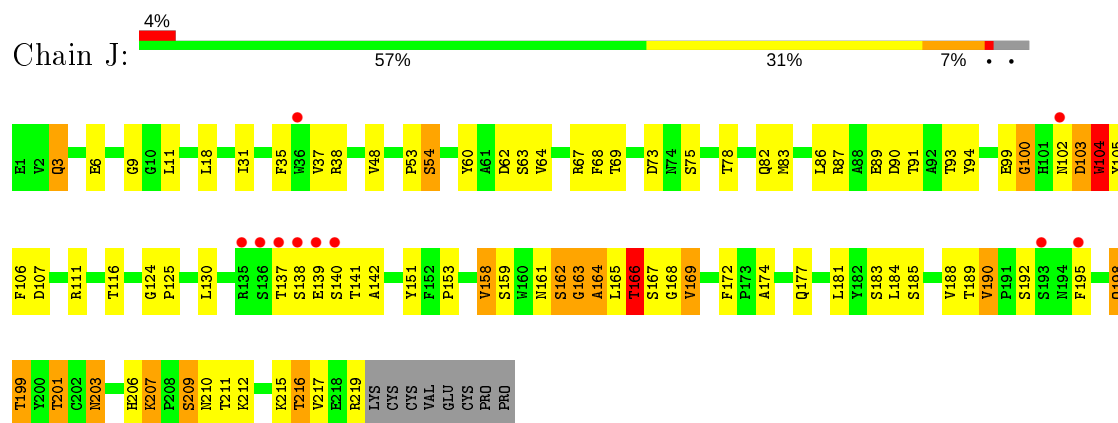
• Molecule 2: Heavy Chain Li33 IgG2



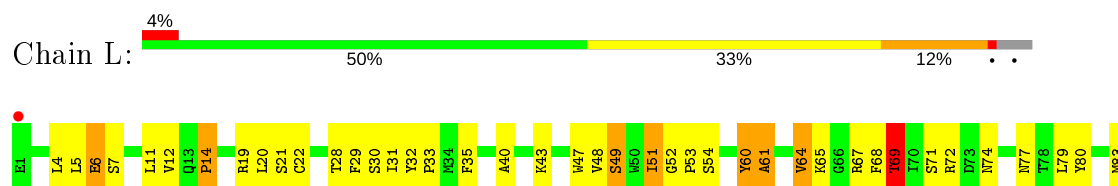
• Molecule 2: Heavy Chain Li33 IgG2

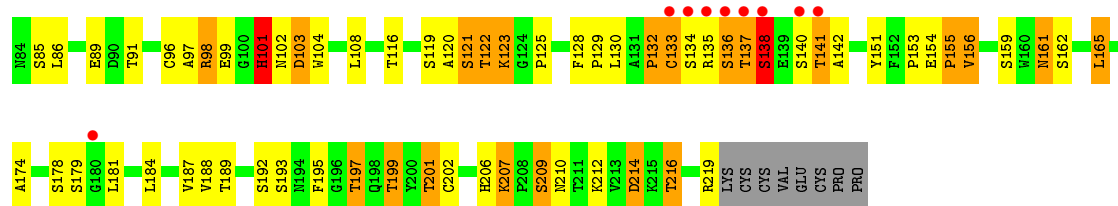


• Molecule 2: Heavy Chain Li33 IgG2

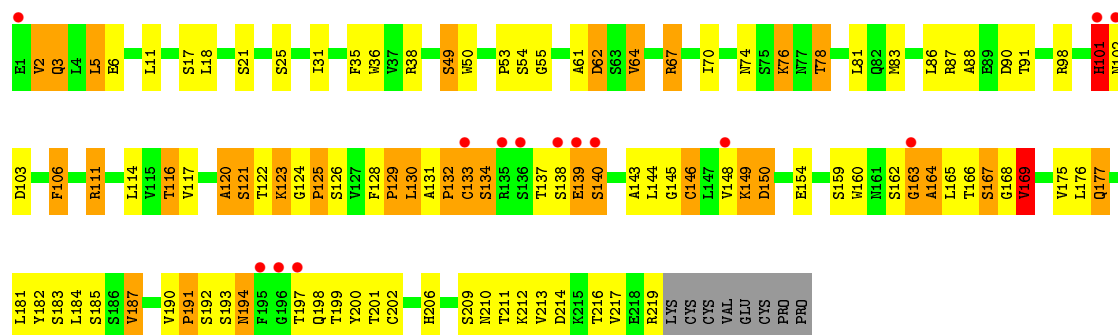


• Molecule 2: Heavy Chain Li33 IgG2

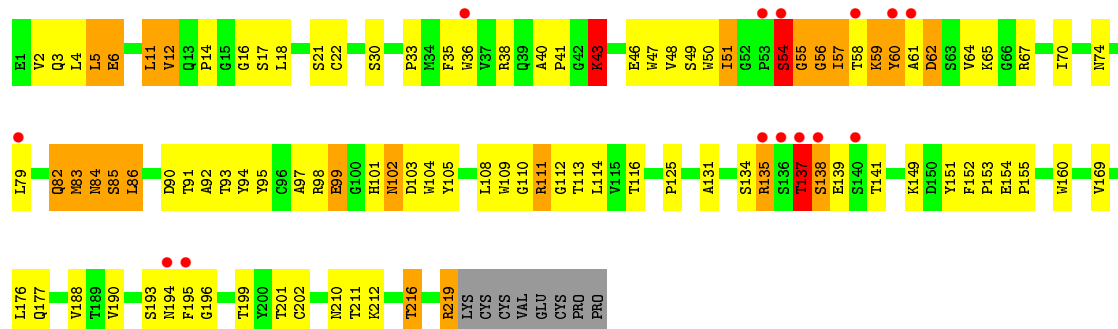




● Molecule 2: Heavy Chain Li33 IgG2



● Molecule 2: Heavy Chain Li33 IgG2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.67Å 109.55Å 118.43Å 61.46° 79.29° 87.59°	Depositor
Resolution (Å)	19.96 – 2.62 19.95 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.96-2.62) 97.0 (19.95-2.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.63Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.259 , 0.339 0.256 , 0.332	Depositor DCC
R_{free} test set	5749 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26358	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.57	0/1676	0.74	0/2275
1	C	0.56	0/1676	0.69	1/2275 (0.0%)
1	E	0.63	0/1676	0.76	1/2275 (0.0%)
1	G	0.67	0/1676	0.76	0/2275
1	I	0.64	0/1676	0.79	0/2275
1	K	0.66	0/1638	0.87	0/2220
1	M	0.58	0/1632	0.77	1/2217 (0.0%)
1	O	0.63	0/1676	0.75	0/2275
2	B	0.61	0/1716	0.76	0/2338
2	D	0.59	1/1716 (0.1%)	0.72	0/2338
2	F	0.64	0/1707	0.76	1/2327 (0.0%)
2	H	0.64	0/1707	0.79	0/2327
2	J	0.63	0/1707	0.77	0/2327
2	L	0.62	0/1707	0.76	0/2327
2	N	0.59	0/1707	0.78	1/2327 (0.0%)
2	P	0.61	0/1701	0.77	0/2320
All	All	0.62	1/26994 (0.0%)	0.77	5/36718 (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
1	G	0	1
1	K	0	2
2	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	202	CYS	CB-SG	-6.20	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	CA-CB-CG	6.63	130.54	115.30
1	E	47	LEU	CA-CB-CG	5.61	128.21	115.30
2	N	114	LEU	CA-CB-CG	5.22	127.31	115.30
1	M	78	LEU	CA-CB-CG	5.12	127.08	115.30
2	F	38	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	7	SER	Peptide
2	H	103	ASP	Peptide
1	K	109	THR	Peptide
1	K	114	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1640	0	1589	47	0
1	C	1640	0	1589	56	0
1	E	1640	0	1589	67	0
1	G	1640	0	1589	46	0
1	I	1640	0	1589	73	0
1	K	1605	0	1556	115	0
1	M	1597	0	1552	114	0
1	O	1640	0	1589	71	0
2	B	1672	0	1622	57	0
2	D	1672	0	1622	57	0
2	F	1663	0	1609	61	0
2	H	1663	0	1609	81	0
2	J	1663	0	1609	74	0
2	L	1663	0	1609	84	0
2	N	1663	0	1609	109	0
2	P	1657	0	1598	100	0
All	All	26358	0	25529	1105	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 21.

All (1105) 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:H:76:LYS:HE2	1:M:32:TYR:CE2	1.45	1.48
2:N:102:ASN:N	2:N:103:ASP:HB2	1.16	1.43
2:N:102:ASN:H	2:N:103:ASP:CB	1.45	1.28
2:H:76:LYS:HE2	1:M:32:TYR:CZ	1.74	1.23
2:P:56:GLY:CA	2:P:57:ILE:HG12	1.76	1.15
1:G:187:GLU:HA	1:G:211:ARG:NH1	1.59	1.15
2:N:130:LEU:CD1	2:N:160:TRP:HH2	1.59	1.14
2:L:102:ASN:HA	2:L:103:ASP:HB3	1.21	1.13
2:H:137:THR:HA	2:H:138:SER:HB3	1.16	1.13
2:P:85:SER:HA	2:P:86:LEU:HB2	1.29	1.13
2:H:76:LYS:CE	1:M:32:TYR:CE2	2.32	1.12
1:K:120:PRO:HA	1:K:121:SER:HB2	1.29	1.12
1:K:189:HIS:HA	1:K:190:LYS:HB2	1.22	1.11
1:M:112:ALA:HB2	1:M:201:LEU:HD13	1.33	1.11
2:N:130:LEU:HD21	2:N:144:LEU:HB3	1.14	1.11
1:O:31:SER:O	1:O:51:ALA:HA	1.50	1.10
1:M:122:ASP:O	1:M:123:GLU:HB2	1.53	1.08
1:O:105:GLU:HG2	1:O:166:GLN:HE22	1.13	1.08
2:J:158:VAL:HG13	2:J:159:SER:H	0.94	1.07
2:H:57:ILE:HG23	2:H:58:THR:H	1.14	1.07
2:H:19:ARG:HH12	2:N:102:ASN:HB2	1.20	1.07
1:O:33:LEU:HD22	1:O:34:ALA:H	1.14	1.06
1:C:108:ARG:NH2	1:C:170:ASP:O	1.88	1.05
1:K:113:PRO:HD2	1:K:137:ASN:O	1.57	1.05
2:H:76:LYS:CE	1:M:32:TYR:HE2	1.68	1.04
2:N:102:ASN:N	2:N:103:ASP:CB	2.11	1.03
2:P:56:GLY:HA2	2:P:57:ILE:CG1	1.89	1.03
2:F:201:THR:HB	2:F:216:THR:HG22	1.38	1.02
1:K:108:ARG:HG2	1:K:108:ARG:HH21	1.25	1.02
2:N:130:LEU:HD13	2:N:160:TRP:HH2	1.20	1.02
2:H:75:SER:HB2	2:H:76:LYS:HE3	1.40	1.01
2:N:176:LEU:HA	2:N:177:GLN:HB2	1.06	1.01
2:N:130:LEU:HD21	2:N:144:LEU:CB	1.92	1.00
1:G:187:GLU:HA	1:G:211:ARG:HH12	0.85	1.00
2:N:130:LEU:HD22	2:N:217:VAL:HG11	1.40	0.99
1:G:187:GLU:CA	1:G:211:ARG:HH12	1.75	0.99
2:L:30:SER:HA	2:L:74:ASN:ND2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:SER:HA	2:L:74:ASN:HD21	1.20	0.99
2:P:56:GLY:HA2	2:P:57:ILE:HG12	1.00	0.99
2:L:101:HIS:CD2	2:L:102:ASN:H	1.80	0.98
2:J:158:VAL:HG13	2:J:159:SER:N	1.73	0.98
1:A:158:ASN:HD22	1:A:158:ASN:H	1.09	0.98
2:L:102:ASN:HA	2:L:103:ASP:CB	1.94	0.97
1:E:19:ALA:HB2	1:E:78:LEU:HD21	1.41	0.97
1:K:108:ARG:HG3	1:K:109:THR:HA	1.47	0.97
1:K:189:HIS:CA	1:K:190:LYS:HB2	1.93	0.97
2:B:137:THR:HA	2:B:138:SER:HB2	1.47	0.97
2:N:176:LEU:HA	2:N:177:GLN:CB	1.94	0.97
2:N:176:LEU:CA	2:N:177:GLN:HB2	1.95	0.96
2:J:163:GLY:O	2:J:165:LEU:HD13	1.64	0.96
1:K:106:ILE:HG22	1:K:107:LYS:H	1.29	0.96
2:N:175:VAL:HG12	2:N:176:LEU:H	1.32	0.95
2:J:158:VAL:CG1	2:J:159:SER:H	1.78	0.95
1:E:106:ILE:H	1:E:166:GLN:HE22	1.07	0.94
2:H:57:ILE:CG2	2:H:58:THR:H	1.78	0.94
2:H:137:THR:HA	2:H:138:SER:CB	1.96	0.94
2:L:161:ASN:H	2:L:161:ASN:HD22	1.08	0.94
2:N:130:LEU:CD1	2:N:160:TRP:CH2	2.49	0.93
2:D:137:THR:HB	2:D:139:GLU:HB2	1.50	0.93
1:M:118:PHE:HB3	2:N:131:ALA:HB3	1.49	0.93
1:K:189:HIS:HA	1:K:190:LYS:CB	1.98	0.93
2:H:57:ILE:HG23	2:H:58:THR:N	1.81	0.92
2:P:48:VAL:O	2:P:61:ALA:HB1	1.69	0.92
2:P:83:MET:N	2:P:84:ASN:HB2	1.84	0.92
1:K:145:LYS:HB2	1:K:198:HIS:CE1	2.05	0.91
2:N:130:LEU:HD13	2:N:160:TRP:CH2	2.06	0.90
2:L:137:THR:HA	2:L:138:SER:HB2	1.53	0.90
1:K:24:ARG:HH22	1:K:70:GLU:HG2	1.36	0.89
2:D:201:THR:HG22	2:D:216:THR:HB	1.54	0.89
1:O:93:LYS:HA	2:P:104:TRP:HD1	1.35	0.89
1:I:136:LEU:HD21	1:I:196:VAL:HG21	1.54	0.89
1:K:120:PRO:HA	1:K:121:SER:CB	1.95	0.89
1:K:187:GLU:O	1:K:188:LYS:HD2	1.73	0.89
2:D:198:GLN:NE2	1:M:61:ARG:HH11	1.69	0.89
2:H:16:GLY:O	2:H:86:LEU:HD13	1.73	0.89
2:D:206:HIS:HB3	2:D:211:THR:HB	1.55	0.87
1:O:33:LEU:HD23	1:O:90:GLN:H	1.38	0.87
2:P:125:PRO:HB3	2:P:151:TYR:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:VAL:O	1:I:155:GLN:NE2	2.07	0.87
2:H:137:THR:CA	2:H:138:SER:HB3	2.03	0.87
1:M:124:GLN:HG3	2:N:128:PHE:CD1	2.09	0.87
2:B:201:THR:HG22	2:B:216:THR:HB	1.55	0.87
2:B:35:PHE:HE2	2:B:99:GLU:HB3	1.37	0.87
2:F:190:VAL:HG23	2:F:195:PHE:HE2	1.39	0.87
2:H:76:LYS:NZ	1:M:32:TYR:OH	2.08	0.86
2:P:49:SER:HA	2:P:61:ALA:HB2	1.54	0.86
1:G:96:LEU:HD21	2:H:104:TRP:CD1	2.10	0.86
2:N:130:LEU:HG	2:N:145:GLY:N	1.91	0.85
1:A:151:ASP:HA	1:A:191:VAL:HG13	1.57	0.85
2:P:83:MET:H	2:P:84:ASN:HB2	1.37	0.85
1:O:2:ILE:HD11	1:O:95:PRO:HD2	1.58	0.85
1:K:161:GLU:HB3	1:K:177:SER:HA	1.57	0.85
2:D:91:THR:HG23	2:D:116:THR:HA	1.59	0.85
2:H:76:LYS:HE2	1:M:32:TYR:OH	1.77	0.85
1:C:19:ALA:HB2	1:C:78:LEU:HD21	1.59	0.84
2:J:137:THR:HA	2:J:138:SER:HB3	1.57	0.84
1:M:24:ARG:HG3	1:M:24:ARG:HH21	1.41	0.84
1:O:33:LEU:HD22	1:O:34:ALA:N	1.91	0.84
1:O:33:LEU:CD2	1:O:90:GLN:H	1.91	0.84
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.60	0.84
2:L:161:ASN:H	2:L:161:ASN:ND2	1.75	0.84
1:O:48:ILE:HA	1:O:53:ASN:O	1.79	0.83
1:I:38:GLN:O	1:I:84:ALA:HB1	1.79	0.83
1:I:150:VAL:HB	1:I:155:GLN:OE1	1.78	0.82
1:G:106:ILE:H	1:G:166:GLN:HE22	1.26	0.82
2:H:76:LYS:HE2	1:M:32:TYR:HE2	1.03	0.82
1:O:93:LYS:HA	2:P:104:TRP:CD1	2.13	0.82
2:L:35:PHE:HE2	2:L:99:GLU:HB3	1.44	0.82
2:H:19:ARG:NH1	2:N:102:ASN:HB2	1.95	0.81
2:D:100:GLY:O	2:D:101:HIS:HB3	1.78	0.81
1:E:119:PRO:HG3	2:F:133:CYS:HB3	1.63	0.81
2:H:76:LYS:CE	1:M:32:TYR:OH	2.29	0.81
2:N:53:PRO:O	2:N:54:SER:HB3	1.80	0.81
2:D:122:THR:HG21	2:P:74:ASN:HB3	1.63	0.80
2:N:154:GLU:HG2	2:N:182:TYR:CE1	2.16	0.80
1:I:195:GLU:OE2	1:I:206:THR:HA	1.80	0.80
1:A:158:ASN:HD22	1:A:158:ASN:N	1.78	0.80
1:M:163:VAL:HG22	1:M:175:LEU:HG	1.63	0.80
1:K:115:VAL:O	1:K:115:VAL:HG12	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:LYS:HA	1:K:186:TYR:CD2	2.16	0.79
1:I:49:TYR:O	1:I:53:ASN:HB2	1.82	0.79
1:M:108:ARG:NH2	1:M:170:ASP:O	2.16	0.78
2:B:97:ALA:O	2:B:98:ARG:HB3	1.83	0.78
2:L:137:THR:HA	2:L:138:SER:CB	2.13	0.78
2:P:64:VAL:HG11	2:P:67:ARG:HH21	1.45	0.78
2:D:198:GLN:HE22	1:M:61:ARG:HH11	1.28	0.78
2:B:139:GLU:O	2:B:140:SER:HB3	1.83	0.78
2:D:122:THR:HG21	2:P:74:ASN:CB	2.14	0.77
1:M:197:THR:HG23	1:M:204:PRO:HB3	1.67	0.77
1:K:150:VAL:HG21	1:K:155:GLN:HB3	1.66	0.77
2:P:6:GLU:OE2	2:P:112:GLY:HA2	1.82	0.77
1:K:159:SER:HA	1:K:160:GLN:HB2	1.64	0.77
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.67	0.77
1:K:135:LEU:HD22	2:L:187:VAL:HG21	1.65	0.76
2:P:35:PHE:HB2	2:P:97:ALA:HB3	1.66	0.76
1:C:36:TYR:HH	2:D:106:PHE:HD2	1.32	0.76
1:I:98:PHE:HZ	2:J:106:PHE:HE2	1.33	0.76
2:J:64:VAL:HG22	2:J:68:PHE:CD1	2.20	0.76
2:P:85:SER:CA	2:P:86:LEU:HB2	2.14	0.76
2:H:207:LYS:HD2	2:N:55:GLY:O	1.85	0.76
2:P:154:GLU:HB2	2:P:155:PRO:HA	1.68	0.76
1:I:94:TRP:NE1	2:J:104:TRP:NE1	2.33	0.76
1:I:136:LEU:CD2	1:I:196:VAL:HG21	2.15	0.75
1:M:144:ALA:HA	1:M:198:HIS:HB2	1.68	0.75
2:H:76:LYS:CE	1:M:32:TYR:CZ	2.63	0.75
1:M:24:ARG:HA	1:M:69:THR:O	1.86	0.75
1:O:91:TYR:HE1	2:P:104:TRP:H	1.35	0.75
2:P:22:CYS:HB3	2:P:79:LEU:HB3	1.69	0.75
2:B:35:PHE:CE2	2:B:99:GLU:HB3	2.21	0.75
2:N:130:LEU:HD11	2:N:160:TRP:HH2	1.48	0.75
1:E:199:GLN:O	1:E:199:GLN:HG2	1.87	0.75
2:J:104:TRP:H	2:J:104:TRP:HE3	1.34	0.75
2:L:161:ASN:N	2:L:161:ASN:HD22	1.85	0.74
2:P:83:MET:CA	2:P:84:ASN:HB2	2.17	0.74
2:H:20:LEU:O	2:H:80:TYR:HB3	1.87	0.74
1:K:109:THR:HB	1:K:140:TYR:CD2	2.22	0.74
1:O:2:ILE:O	1:O:3:GLN:HB2	1.87	0.74
2:P:48:VAL:O	2:P:61:ALA:CB	2.36	0.73
1:E:1:ASP:HB3	1:E:95:PRO:HD2	1.68	0.73
1:O:105:GLU:HG2	1:O:166:GLN:NE2	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:163:GLY:O	2:J:165:LEU:CD1	2.35	0.73
1:K:105:GLU:HG3	1:K:173:TYR:OH	1.88	0.73
2:B:36:TRP:HD1	2:B:70:ILE:HD12	1.53	0.73
1:K:181:LEU:O	1:K:182:SER:HB3	1.87	0.73
1:O:105:GLU:CG	1:O:166:GLN:HE22	1.96	0.73
2:L:97:ALA:O	2:L:108:LEU:O	2.07	0.73
2:F:190:VAL:HG23	2:F:195:PHE:CE2	2.22	0.73
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.70	0.73
2:J:166:THR:OG1	2:J:167:SER:N	2.22	0.73
2:L:137:THR:CA	2:L:138:SER:HB2	2.19	0.72
2:P:64:VAL:HG11	2:P:67:ARG:NH2	2.04	0.72
1:K:108:ARG:CG	1:K:108:ARG:HH21	2.00	0.72
1:O:158:ASN:H	1:O:158:ASN:HD22	1.35	0.72
1:G:158:ASN:HD22	1:G:158:ASN:H	1.36	0.72
1:K:181:LEU:HG	1:K:182:SER:H	1.54	0.72
2:P:5:LEU:O	2:P:5:LEU:HG	1.87	0.72
2:B:97:ALA:O	2:B:108:LEU:O	2.07	0.72
2:N:177:GLN:HG3	2:N:181:LEU:O	1.88	0.72
2:F:137:THR:HA	2:F:138:SER:CB	2.19	0.72
2:H:19:ARG:HH12	2:N:102:ASN:CB	2.00	0.72
1:C:8:PRO:HD2	1:C:11:LEU:HD21	1.72	0.71
1:K:145:LYS:HB2	1:K:198:HIS:ND1	2.06	0.71
1:I:91:TYR:HB2	2:J:104:TRP:HB2	1.71	0.71
1:E:135:LEU:HD11	1:E:137:ASN:HD22	1.54	0.71
1:M:61:ARG:NH2	1:M:82:ASP:OD1	2.23	0.71
1:K:120:PRO:CA	1:K:121:SER:CB	2.67	0.70
1:M:150:VAL:O	1:M:150:VAL:HG13	1.91	0.70
2:D:199:THR:OG1	1:K:125:LEU:HB2	1.91	0.70
1:C:158:ASN:H	1:C:158:ASN:HD22	1.39	0.70
2:F:198:GLN:HA	2:F:198:GLN:NE2	2.06	0.70
1:K:120:PRO:CA	1:K:121:SER:HB2	2.15	0.70
1:E:83:PHE:HA	1:E:104:VAL:CG1	2.21	0.70
2:F:73:ASP:O	2:F:76:LYS:HG2	1.91	0.70
1:E:84:ALA:H	1:E:104:VAL:HG12	1.56	0.70
2:H:67:ARG:NH1	2:H:87:ARG:HD2	2.06	0.70
1:I:94:TRP:CE2	2:J:104:TRP:NE1	2.60	0.70
1:I:150:VAL:HB	1:I:155:GLN:CD	2.12	0.70
1:C:19:ALA:CB	1:C:78:LEU:HD21	2.22	0.69
1:E:158:ASN:N	1:E:158:ASN:HD22	1.89	0.69
2:H:13:GLN:HA	2:H:118:SER:O	1.91	0.69
1:M:106:ILE:H	1:M:166:GLN:HE22	1.37	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:122:ASP:O	1:M:123:GLU:CB	2.34	0.69
1:C:113:PRO:HD3	1:C:198:HIS:CD2	2.27	0.69
1:M:128:GLY:HA2	1:M:183:LYS:HB3	1.75	0.69
2:L:125:PRO:HB3	2:L:151:TYR:HB3	1.72	0.69
1:G:125:LEU:O	1:G:127:SER:N	2.26	0.69
2:J:189:THR:O	2:J:190:VAL:HG13	1.93	0.69
2:J:103:ASP:O	2:J:105:TYR:N	2.23	0.69
1:G:62:PHE:CE1	1:G:75:ILE:HG12	2.27	0.69
1:K:109:THR:HB	1:K:140:TYR:HD2	1.56	0.69
2:N:133:CYS:SG	2:N:134:SER:N	2.66	0.69
1:G:193:ALA:HB2	1:G:208:SER:HB3	1.74	0.68
2:L:122:THR:O	2:L:123:LYS:HB2	1.93	0.68
2:J:48:VAL:HG13	2:J:64:VAL:HG21	1.73	0.68
2:P:137:THR:HB	2:P:139:GLU:HG3	1.74	0.68
2:P:51:ILE:HD13	2:P:59:LYS:HB2	1.76	0.68
2:F:73:ASP:CG	2:F:76:LYS:HG3	2.14	0.68
1:I:7:SER:HA	1:I:8:PRO:C	2.13	0.68
1:K:186:TYR:CE1	1:K:187:GLU:HG2	2.29	0.68
1:M:124:GLN:NE2	1:M:124:GLN:HA	2.09	0.68
1:M:119:PRO:HD3	2:N:133:CYS:HB2	1.74	0.68
2:B:33:PRO:HB2	2:B:99:GLU:HG2	1.76	0.68
2:L:30:SER:CA	2:L:74:ASN:HD21	2.04	0.68
1:E:21:LEU:HD12	1:E:21:LEU:N	2.08	0.68
2:L:35:PHE:CE2	2:L:99:GLU:HB3	2.28	0.68
1:G:211:ARG:HD2	1:G:211:ARG:O	1.93	0.68
2:P:91:THR:HG23	2:P:116:THR:HA	1.76	0.68
2:F:62:ASP:O	2:F:64:VAL:N	2.27	0.67
2:H:80:TYR:HE2	2:N:102:ASN:CG	1.98	0.67
2:L:103:ASP:O	2:L:104:TRP:HB2	1.93	0.67
2:L:97:ALA:O	2:L:98:ARG:HB3	1.94	0.67
2:P:33:PRO:O	2:P:99:GLU:OE2	2.12	0.67
2:H:149:LYS:HA	2:H:183:SER:HB2	1.76	0.67
1:I:21:LEU:HD23	1:I:102:THR:HB	1.75	0.67
2:L:14:PRO:CD	2:L:119:SER:HB3	2.24	0.67
1:M:179:LEU:H	1:M:179:LEU:HD23	1.59	0.67
2:N:130:LEU:HD11	2:N:160:TRP:CH2	2.25	0.67
1:O:198:HIS:CD2	1:O:200:GLY:H	2.11	0.67
2:P:17:SER:HA	2:P:84:ASN:H	1.58	0.67
1:C:126:LYS:HD2	2:L:201:THR:HG21	1.77	0.67
1:I:91:TYR:CB	2:J:104:TRP:HB2	2.24	0.67
1:K:106:ILE:HG22	1:K:107:LYS:N	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:GLN:HA	1:M:155:GLN:HE21	1.60	0.67
2:N:130:LEU:HB2	2:N:146:CYS:SG	2.35	0.67
2:P:33:PRO:HG2	2:P:104:TRP:HH2	1.59	0.67
1:E:106:ILE:H	1:E:166:GLN:NE2	1.87	0.67
1:K:195:GLU:HA	1:K:204:PRO:HB3	1.77	0.67
1:M:151:ASP:OD1	1:M:192:TYR:HA	1.95	0.67
2:J:137:THR:HA	2:J:138:SER:CB	2.24	0.67
2:D:78:THR:HG21	1:O:93:LYS:NZ	2.10	0.67
2:F:11:LEU:HD23	2:F:122:THR:HG22	1.77	0.67
1:O:158:ASN:N	1:O:158:ASN:HD22	1.92	0.67
1:C:36:TYR:HE1	1:C:89:GLN:HE21	1.43	0.66
2:N:209:SER:O	2:N:211:THR:N	2.22	0.66
2:L:161:ASN:ND2	2:L:161:ASN:N	2.39	0.66
1:A:198:HIS:CD2	1:A:200:GLY:H	2.13	0.66
1:A:79:GLN:NE2	1:O:81:GLU:HG2	2.10	0.66
2:F:73:ASP:C	2:F:76:LYS:HG2	2.16	0.66
1:M:94:TRP:CD1	1:M:95:PRO:HA	2.31	0.66
1:C:126:LYS:HG3	2:L:199:THR:HG21	1.78	0.66
1:E:120:PRO:HD3	1:E:132:VAL:HG22	1.77	0.66
1:O:33:LEU:HD23	1:O:90:GLN:N	2.11	0.66
2:N:125:PRO:O	2:N:126:SER:OG	2.10	0.66
1:K:128:GLY:O	1:K:183:LYS:HB3	1.95	0.66
2:J:64:VAL:HG22	2:J:68:PHE:CE1	2.31	0.66
1:O:91:TYR:HE1	2:P:104:TRP:N	1.93	0.65
2:L:30:SER:CA	2:L:74:ASN:ND2	2.56	0.65
2:J:153:PRO:O	2:J:206:HIS:HE1	1.79	0.65
2:F:198:GLN:HA	2:F:198:GLN:HE21	1.62	0.65
1:K:183:LYS:HA	1:K:186:TYR:HD2	1.61	0.65
1:O:37:GLN:OE1	1:O:39:LYS:HE3	1.96	0.65
2:P:99:GLU:CD	2:P:99:GLU:N	2.50	0.65
1:C:8:PRO:HD2	1:C:11:LEU:CD2	2.25	0.65
1:K:120:PRO:HG2	1:K:132:VAL:HA	1.78	0.65
1:E:128:GLY:HA2	1:E:183:LYS:HB2	1.77	0.65
1:C:166:GLN:HG3	1:C:173:TYR:CE2	2.32	0.65
2:J:87:ARG:O	2:J:90:ASP:N	2.27	0.65
1:K:151:ASP:OD2	1:K:189:HIS:ND1	2.30	0.65
2:P:57:ILE:O	2:P:59:LYS:HE3	1.97	0.65
2:J:142:ALA:HB3	2:J:195:PHE:HE2	1.62	0.65
1:C:17:GLU:O	1:C:78:LEU:HD23	1.97	0.64
1:I:124:GLN:O	1:I:127:SER:HB3	1.97	0.64
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:120:PRO:HD3	1:K:133:VAL:O	1.97	0.64
1:K:120:PRO:CD	1:K:133:VAL:O	2.45	0.64
1:K:64:GLY:HA2	1:K:72:THR:O	1.98	0.64
2:D:198:GLN:HE22	1:M:59:PRO:HB3	1.62	0.64
1:G:198:HIS:CD2	1:G:200:GLY:H	2.14	0.64
1:A:119:PRO:HG3	2:B:133:CYS:HB3	1.80	0.64
2:L:161:ASN:HB3	2:L:201:THR:HG23	1.79	0.64
1:C:158:ASN:H	1:C:158:ASN:ND2	1.95	0.63
1:G:29:VAL:O	1:G:30:SER:HB2	1.95	0.63
2:H:75:SER:HB2	2:H:76:LYS:CE	2.24	0.63
1:I:147:GLN:HB3	1:I:195:GLU:HB3	1.81	0.63
2:H:76:LYS:CD	1:M:32:TYR:CE2	2.80	0.63
2:N:101:HIS:C	2:N:103:ASP:HB2	2.11	0.63
1:I:150:VAL:HG13	1:I:192:TYR:HA	1.80	0.63
1:M:143:GLU:OE1	1:M:198:HIS:HB3	1.99	0.63
1:E:106:ILE:N	1:E:166:GLN:HE22	1.90	0.63
1:I:195:GLU:OE2	1:I:206:THR:CA	2.45	0.63
2:L:51:ILE:CG2	2:L:72:ARG:HH21	2.12	0.63
2:P:33:PRO:HG2	2:P:104:TRP:CH2	2.34	0.63
2:L:122:THR:OG1	2:L:123:LYS:N	2.30	0.63
2:D:76:LYS:O	2:D:77:ASN:HB2	1.98	0.62
2:J:60:TYR:CE1	2:J:68:PHE:O	2.53	0.62
2:N:91:THR:HG23	2:N:116:THR:HA	1.80	0.62
2:J:3:GLN:HA	2:J:3:GLN:HE21	1.64	0.62
2:L:123:LYS:O	2:L:151:TYR:HA	2.00	0.62
2:L:31:ILE:O	2:L:53:PRO:HB3	1.99	0.62
2:P:56:GLY:N	2:P:57:ILE:HG12	2.14	0.62
1:K:122:ASP:OD2	2:L:129:PRO:HG2	2.00	0.62
2:L:83:MET:HB3	2:L:86:LEU:HD21	1.82	0.62
2:N:143:ALA:O	2:N:144:LEU:HD12	2.00	0.62
2:F:137:THR:HA	2:F:138:SER:HB3	1.79	0.62
1:K:150:VAL:O	1:K:151:ASP:HB2	1.98	0.62
2:N:102:ASN:CA	2:N:103:ASP:HB2	2.26	0.62
1:A:107:LYS:HA	1:A:140:TYR:OH	1.99	0.62
1:E:8:PRO:HG2	1:E:11:LEU:HD13	1.81	0.62
1:E:132:VAL:HG12	1:E:148:TRP:CH2	2.35	0.62
1:O:165:GLU:HA	1:O:165:GLU:OE1	1.99	0.62
2:J:60:TYR:HE1	2:J:68:PHE:O	1.84	0.61
1:M:155:GLN:CA	1:M:155:GLN:HE21	2.12	0.61
2:D:206:HIS:HD2	2:D:209:SER:OG	1.83	0.61
2:J:201:THR:HG22	2:J:216:THR:HB	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:LYS:O	1:K:208:SER:HB2	2.00	0.61
2:L:101:HIS:CG	2:L:102:ASN:H	2.17	0.61
1:M:119:PRO:CD	2:N:133:CYS:HB2	2.30	0.61
1:O:145:LYS:HB3	1:O:197:THR:OG1	2.00	0.61
1:C:166:GLN:HG3	1:C:173:TYR:CZ	2.35	0.61
1:E:104:VAL:O	1:E:104:VAL:CG1	2.48	0.61
1:K:161:GLU:HB3	1:K:176:SER:O	2.00	0.61
2:N:128:PHE:O	2:N:130:LEU:N	2.33	0.61
2:H:29:PHE:CD1	2:H:77:ASN:HA	2.35	0.61
2:H:80:TYR:CE2	2:N:102:ASN:CG	2.74	0.61
1:E:183:LYS:HG2	1:E:187:GLU:OE2	2.00	0.61
2:L:155:PRO:O	2:L:156:VAL:HB	2.00	0.61
1:M:79:GLN:HE21	1:M:79:GLN:N	1.99	0.61
1:K:120:PRO:CD	1:K:133:VAL:H	2.14	0.61
1:O:49:TYR:O	1:O:50:ASP:CB	2.48	0.61
2:H:69:THR:HG22	2:H:82:GLN:HB3	1.81	0.61
1:O:23:CYS:HB2	1:O:35:TRP:CH2	2.36	0.61
1:K:1:ASP:HB3	1:K:95:PRO:HD2	1.83	0.60
2:L:97:ALA:O	2:L:98:ARG:CB	2.49	0.60
1:M:79:GLN:HE21	1:M:79:GLN:CA	2.15	0.60
2:H:122:THR:HG21	2:N:74:ASN:HB2	1.83	0.60
1:K:115:VAL:O	1:K:115:VAL:CG1	2.49	0.60
2:L:135:ARG:O	2:L:136:SER:HB3	2.01	0.60
2:B:137:THR:CA	2:B:138:SER:HB2	2.25	0.60
1:I:94:TRP:HE1	2:J:104:TRP:HE1	1.49	0.60
1:K:149:LYS:NZ	1:K:152:ASN:HA	2.16	0.60
2:N:17:SER:HA	2:N:83:MET:O	2.02	0.60
2:D:201:THR:CG2	2:D:216:THR:HB	2.31	0.60
2:L:153:PRO:O	2:L:206:HIS:HE1	1.84	0.60
1:K:210:ASN:N	1:K:210:ASN:HD22	1.97	0.60
2:L:101:HIS:CD2	2:L:102:ASN:N	2.62	0.60
1:M:124:GLN:NE2	2:N:128:PHE:CE2	2.70	0.60
1:O:96:LEU:HD11	2:P:104:TRP:HB3	1.84	0.59
2:H:62:ASP:HA	2:H:65:LYS:HG2	1.83	0.59
2:J:206:HIS:CD2	2:J:209:SER:HB2	2.38	0.59
2:H:12:VAL:HG11	2:H:18:LEU:HG	1.85	0.59
2:P:40:ALA:HB3	2:P:43:LYS:HB2	1.84	0.59
1:I:143:GLU:HG3	1:I:143:GLU:O	2.02	0.59
1:K:155:GLN:HG2	1:K:156:SER:N	2.17	0.59
2:L:102:ASN:CA	2:L:103:ASP:CB	2.75	0.59
1:E:203:SER:HB2	1:E:204:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:GLU:OE2	2:H:103:ASP:HB3	2.03	0.59
1:K:187:GLU:OE1	1:K:187:GLU:HA	2.03	0.59
2:D:78:THR:HG21	1:O:93:LYS:HZ3	1.67	0.59
1:G:62:PHE:CD1	1:G:75:ILE:HG12	2.38	0.59
1:A:79:GLN:NE2	1:O:81:GLU:H	2.01	0.59
2:B:202:CYS:O	2:B:214:ASP:HA	2.02	0.59
1:M:158:ASN:HD22	1:M:179:LEU:HB3	1.67	0.59
2:N:125:PRO:O	2:N:149:LYS:O	2.20	0.59
1:C:187:GLU:HG2	1:C:211:ARG:NH1	2.18	0.58
2:F:106:PHE:HD2	2:F:109:TRP:CZ2	2.21	0.58
2:F:11:LEU:CD2	2:F:122:THR:HG22	2.32	0.58
1:E:104:VAL:O	1:E:104:VAL:HG13	2.01	0.58
1:E:93:LYS:HB2	1:E:93:LYS:NZ	2.18	0.58
2:F:75:SER:C	2:F:76:LYS:HD3	2.23	0.58
2:N:130:LEU:HD22	2:N:217:VAL:CG1	2.25	0.58
1:O:49:TYR:HB2	1:O:54:ARG:C	2.24	0.58
2:B:73:ASP:OD2	2:B:76:LYS:N	2.35	0.58
1:C:137:ASN:HD21	2:D:170:HIS:CD2	2.21	0.58
2:H:137:THR:HB	2:H:139:GLU:OE2	2.03	0.58
1:M:198:HIS:O	1:M:200:GLY:N	2.37	0.58
1:M:192:TYR:O	1:M:208:SER:HA	2.03	0.58
2:B:137:THR:HB	2:B:139:GLU:N	2.18	0.58
2:D:141:THR:HA	2:D:191:PRO:HA	1.85	0.58
2:B:144:LEU:CD1	2:B:217:VAL:HG21	2.34	0.58
2:B:190:VAL:HG23	2:B:195:PHE:CZ	2.38	0.58
2:F:192:SER:O	2:F:195:PHE:HB2	2.03	0.58
2:H:64:VAL:HG13	2:H:68:PHE:HB2	1.84	0.58
1:M:192:TYR:N	1:M:192:TYR:HD1	2.02	0.58
1:A:158:ASN:ND2	1:A:158:ASN:N	2.52	0.58
2:D:88:ALA:HA	2:D:117:VAL:HB	1.85	0.58
2:L:101:HIS:CG	2:L:102:ASN:N	2.72	0.58
2:N:175:VAL:O	2:N:182:TYR:HD2	1.87	0.58
1:O:182:SER:OG	1:O:185:ASP:HB2	2.04	0.58
2:B:36:TRP:CD1	2:B:70:ILE:HD12	2.38	0.58
2:D:201:THR:HG22	2:D:216:THR:CB	2.32	0.58
1:G:54:ARG:HD3	1:G:58:ILE:HG22	1.85	0.58
1:K:161:GLU:CB	1:K:176:SER:O	2.52	0.58
1:A:166:GLN:OE1	1:A:173:TYR:CZ	2.57	0.57
1:E:21:LEU:HD12	1:E:21:LEU:H	1.67	0.57
2:H:103:ASP:N	2:H:103:ASP:OD2	2.36	0.57
2:N:64:VAL:O	2:N:67:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:83:MET:HA	2:P:84:ASN:HB2	1.85	0.57
2:D:160:TRP:CE3	2:D:201:THR:O	2.57	0.57
2:D:19:ARG:HD3	2:P:102:ASN:CG	2.25	0.57
1:C:15:PRO:HB2	2:N:164:ALA:HB2	1.87	0.57
2:H:130:LEU:HD11	2:H:185:SER:OG	2.04	0.57
1:I:94:TRP:CZ2	2:J:104:TRP:CD1	2.92	0.57
2:J:207:LYS:NZ	2:J:207:LYS:H	2.02	0.57
1:G:28:SER:HA	1:G:68:GLY:O	2.03	0.57
2:L:61:ALA:HB3	2:L:64:VAL:HG12	1.87	0.57
2:N:111:ARG:HG3	2:N:111:ARG:HH11	1.67	0.57
2:N:61:ALA:O	2:N:64:VAL:N	2.33	0.57
2:P:50:TRP:CZ3	2:P:59:LYS:HG2	2.39	0.57
2:B:64:VAL:HG13	2:B:68:PHE:HB2	1.85	0.57
2:F:62:ASP:C	2:F:64:VAL:H	2.08	0.57
1:I:94:TRP:CE2	2:J:104:TRP:CD1	2.92	0.57
2:N:67:ARG:NH2	2:N:90:ASP:OD2	2.37	0.57
2:B:139:GLU:O	2:B:140:SER:CB	2.52	0.57
2:F:122:THR:HB	2:F:153:PRO:HD3	1.87	0.57
2:F:141:THR:HA	2:F:191:PRO:HA	1.86	0.57
1:M:131:SER:HA	1:M:180:THR:H	1.69	0.57
2:N:130:LEU:HD12	2:N:146:CYS:N	2.20	0.57
1:M:148:TRP:O	1:M:155:GLN:HB2	2.05	0.57
2:N:111:ARG:HG3	2:N:111:ARG:NH1	2.19	0.57
2:N:137:THR:HB	2:N:138:SER:HB2	1.85	0.57
1:O:91:TYR:CE1	2:P:104:TRP:N	2.72	0.57
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.84	0.57
1:C:14:SER:CA	1:C:107:LYS:HB3	2.35	0.57
2:J:100:GLY:HA2	2:J:107:ASP:HB3	1.86	0.57
2:J:153:PRO:O	2:J:206:HIS:CE1	2.57	0.57
1:A:89:GLN:HE21	1:A:91:TYR:HB3	1.70	0.56
2:F:165:LEU:HD21	2:F:188:VAL:HG21	1.87	0.56
1:K:108:ARG:NH2	1:K:108:ARG:HG2	2.05	0.56
2:L:179:SER:HB3	2:L:181:LEU:HD12	1.86	0.56
1:I:35:TRP:HB2	1:I:48:ILE:HB	1.86	0.56
1:C:3:GLN:HB2	1:C:26:SER:HB3	1.87	0.56
1:K:108:ARG:HG3	1:K:109:THR:CA	2.30	0.56
2:P:57:ILE:HG13	2:P:59:LYS:CE	2.35	0.56
2:D:137:THR:HA	2:D:138:SER:HB3	1.87	0.56
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.87	0.56
2:D:149:LYS:HE2	2:D:177:GLN:HE22	1.71	0.56
1:G:158:ASN:H	1:G:158:ASN:ND2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:PHE:HZ	2:H:104:TRP:NE1	2.03	0.56
2:J:158:VAL:O	2:J:203:ASN:O	2.23	0.56
2:P:64:VAL:O	2:P:64:VAL:HG12	2.06	0.56
1:E:158:ASN:HD22	1:E:158:ASN:H	1.50	0.56
2:D:137:THR:HA	2:D:138:SER:CB	2.35	0.56
2:D:98:ARG:HH21	2:D:107:ASP:CG	2.09	0.56
2:L:51:ILE:HG21	2:L:72:ARG:HD2	1.88	0.56
2:B:97:ALA:HB1	2:B:106:PHE:HB3	1.87	0.56
1:O:2:ILE:O	1:O:3:GLN:CB	2.54	0.56
1:M:175:LEU:HD23	1:M:176:SER:H	1.70	0.55
1:C:14:SER:HA	1:C:107:LYS:HB3	1.88	0.55
2:H:35:PHE:CD2	2:H:106:PHE:HE1	2.24	0.55
2:F:189:THR:O	2:F:190:VAL:HG13	2.06	0.55
2:J:83:MET:HB3	2:J:86:LEU:HD21	1.88	0.55
2:N:132:PRO:HD2	2:N:133:CYS:H	1.71	0.55
2:N:130:LEU:CD2	2:N:144:LEU:HB3	2.09	0.55
2:N:213:VAL:HG22	2:N:214:ASP:H	1.72	0.55
2:P:11:LEU:O	2:P:12:VAL:HG13	2.07	0.55
2:P:57:ILE:HG13	2:P:59:LYS:HE3	1.88	0.55
1:M:175:LEU:HD23	1:M:176:SER:N	2.21	0.55
1:M:200:GLY:O	1:M:201:LEU:HD12	2.07	0.55
1:A:14:SER:HB2	1:A:17:GLU:HG3	1.88	0.55
1:C:192:TYR:O	1:C:208:SER:HA	2.06	0.55
1:M:192:TYR:CD1	1:M:192:TYR:N	2.74	0.55
1:M:28:SER:HA	1:M:68:GLY:HA2	1.89	0.55
1:M:32:TYR:O	1:M:90:GLN:HA	2.06	0.55
1:A:106:ILE:H	1:A:166:GLN:NE2	2.04	0.55
1:A:79:GLN:HE22	1:O:81:GLU:H	1.55	0.55
2:F:74:ASN:C	2:F:76:LYS:H	2.09	0.55
1:I:150:VAL:HG13	1:I:191:VAL:O	2.04	0.55
1:K:181:LEU:HG	1:K:182:SER:N	2.21	0.55
2:P:201:THR:HB	2:P:216:THR:HB	1.88	0.55
2:D:19:ARG:HD3	2:P:102:ASN:ND2	2.21	0.55
2:B:2:VAL:HG13	2:B:27:PHE:HD1	1.72	0.55
1:I:98:PHE:CZ	2:J:106:PHE:HE2	2.20	0.55
2:F:103:ASP:N	2:F:103:ASP:OD2	2.41	0.54
1:G:115:VAL:CG1	1:G:207:LYS:HG2	2.37	0.54
1:G:125:LEU:C	1:G:127:SER:H	2.10	0.54
2:N:206:HIS:O	2:N:209:SER:O	2.25	0.54
1:C:28:SER:HA	1:C:68:GLY:O	2.08	0.54
1:K:54:ARG:HD2	1:K:58:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:SER:HA	1:O:105:GLU:O	2.08	0.54
1:I:182:SER:OG	1:I:185:ASP:HB2	2.08	0.54
2:P:30:SER:O	2:P:54:SER:HB2	2.07	0.54
2:D:137:THR:CB	2:D:139:GLU:HB2	2.32	0.54
1:K:186:TYR:CD1	1:K:187:GLU:HG2	2.41	0.54
2:L:206:HIS:CD2	2:L:209:SER:HB2	2.43	0.54
2:L:30:SER:CB	2:L:74:ASN:ND2	2.70	0.54
2:P:110:GLY:O	2:P:111:ARG:HG3	2.07	0.54
2:J:53:PRO:O	2:J:54:SER:HB3	2.08	0.54
2:P:18:LEU:N	2:P:83:MET:O	2.27	0.54
1:A:163:VAL:HG12	1:A:164:THR:O	2.06	0.54
1:I:148:TRP:CE3	1:I:179:LEU:HD22	2.42	0.54
1:I:61:ARG:NH2	1:I:82:ASP:OD1	2.35	0.54
2:J:124:GLY:CA	2:J:209:SER:OG	2.55	0.54
2:L:174:ALA:HB2	2:L:184:LEU:HD23	1.90	0.54
1:K:126:LYS:O	1:K:127:SER:CB	2.56	0.54
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.88	0.54
1:O:128:GLY:HA2	1:O:183:LYS:HB2	1.90	0.54
1:K:126:LYS:O	1:K:127:SER:HB2	2.06	0.54
2:N:175:VAL:HG12	2:N:176:LEU:N	2.14	0.54
1:E:83:PHE:CD2	1:E:106:ILE:HG12	2.44	0.53
2:H:80:TYR:HE2	2:N:102:ASN:OD1	1.92	0.53
2:L:14:PRO:CG	2:L:119:SER:HB3	2.38	0.53
1:M:24:ARG:HG3	1:M:24:ARG:NH2	2.15	0.53
1:M:25:ALA:O	1:M:69:THR:HG22	2.08	0.53
1:O:185:ASP:O	1:O:188:LYS:HB2	2.08	0.53
2:P:54:SER:O	2:P:55:GLY:C	2.47	0.53
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.48	0.53
2:L:51:ILE:HG23	2:L:52:GLY:O	2.08	0.53
2:B:62:ASP:C	2:B:64:VAL:H	2.11	0.53
2:F:76:LYS:HD2	1:I:32:TYR:OH	2.08	0.53
2:P:5:LEU:HD12	2:P:111:ARG:NH2	2.23	0.53
2:P:82:GLN:HA	2:P:83:MET:HB3	1.90	0.53
1:I:180:THR:O	1:I:181:LEU:HD23	2.09	0.53
1:K:157:GLY:O	1:K:159:SER:N	2.41	0.53
2:F:64:VAL:HG13	2:F:68:PHE:HB2	1.90	0.53
1:K:6:GLN:HG2	1:K:23:CYS:SG	2.49	0.53
1:E:83:PHE:HA	1:E:104:VAL:HG13	1.91	0.53
1:K:186:TYR:HE1	1:K:187:GLU:HG2	1.72	0.53
1:C:125:LEU:HD22	1:C:183:LYS:HG3	1.89	0.53
1:M:48:ILE:HG23	1:M:53:ASN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:GLU:HA	1:G:176:SER:O	2.09	0.53
2:J:209:SER:HB3	2:J:211:THR:HG23	1.91	0.53
1:K:33:LEU:HD11	1:K:88:CYS:HB2	1.91	0.53
2:L:165:LEU:HD12	2:L:188:VAL:HG21	1.90	0.53
2:D:122:THR:CG2	2:P:74:ASN:HB3	2.37	0.53
1:E:198:HIS:HD2	1:E:200:GLY:H	1.55	0.53
2:J:35:PHE:CE2	2:J:99:GLU:HG3	2.44	0.53
2:L:6:GLU:HA	2:L:21:SER:O	2.08	0.53
2:N:111:ARG:CG	2:N:111:ARG:HH11	2.22	0.53
2:N:169:VAL:O	2:N:169:VAL:CG1	2.56	0.53
1:C:194:CYS:O	1:C:206:THR:HA	2.09	0.53
1:G:10:THR:CG2	1:G:11:LEU:N	2.72	0.53
2:J:158:VAL:CG1	2:J:159:SER:N	2.48	0.53
1:K:120:PRO:HD2	1:K:133:VAL:H	1.72	0.53
2:H:76:LYS:HD2	1:M:32:TYR:CE2	2.44	0.53
1:E:196:VAL:O	1:E:204:PRO:HA	2.09	0.52
1:M:155:GLN:NE2	1:M:155:GLN:HA	2.23	0.52
1:M:47:LEU:HA	1:M:58:ILE:HG13	1.90	0.52
1:A:124:GLN:HG3	2:B:128:PHE:CE2	2.43	0.52
1:G:19:ALA:HB2	1:G:78:LEU:HD21	1.91	0.52
1:K:106:ILE:H	1:K:166:GLN:HE22	1.57	0.52
1:M:124:GLN:NE2	2:N:128:PHE:CZ	2.77	0.52
1:E:84:ALA:N	1:E:104:VAL:HG12	2.24	0.52
1:E:108:ARG:NH1	1:E:111:ALA:HB2	2.24	0.52
1:E:95:PRO:HB3	2:F:47:TRP:CZ3	2.43	0.52
1:G:186:TYR:HA	1:G:192:TYR:OH	2.09	0.52
2:H:206:HIS:HD2	2:H:209:SER:OG	1.93	0.52
1:K:120:PRO:HD2	1:K:133:VAL:O	2.09	0.52
1:M:137:ASN:ND2	1:M:138:ASN:OD1	2.42	0.52
2:P:85:SER:HA	2:P:86:LEU:CB	2.18	0.52
1:E:132:VAL:HG12	1:E:148:TRP:HH2	1.74	0.52
2:F:6:GLU:OE1	2:F:112:GLY:HA2	2.09	0.52
1:G:14:SER:O	1:G:17:GLU:HB2	2.08	0.52
1:K:116:PHE:HD2	2:L:141:THR:HG23	1.75	0.52
1:M:150:VAL:O	1:M:150:VAL:CG1	2.56	0.52
2:D:198:GLN:NE2	1:M:59:PRO:HB3	2.24	0.52
2:J:201:THR:HA	2:J:216:THR:HA	1.91	0.52
1:K:77:SER:O	1:K:79:GLN:OE1	2.27	0.52
2:L:120:ALA:O	2:L:121:SER:C	2.47	0.52
2:L:49:SER:OG	2:L:60:TYR:HB3	2.09	0.52
1:M:24:ARG:HG2	1:M:69:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:103:ASP:HB2	2:P:105:TYR:CE2	2.45	0.52
2:H:62:ASP:C	2:H:64:VAL:H	2.12	0.52
2:N:49:SER:HB3	2:N:70:ILE:HD12	1.92	0.52
1:C:108:ARG:HG2	1:C:109:THR:N	2.25	0.52
2:L:161:ASN:CB	2:L:201:THR:HG23	2.40	0.52
2:N:209:SER:C	2:N:211:THR:H	2.10	0.52
2:B:33:PRO:HG3	2:B:53:PRO:HD3	1.92	0.52
1:M:85:VAL:HA	1:M:102:THR:O	2.10	0.52
1:O:36:TYR:HE1	1:O:89:GLN:HB2	1.75	0.52
1:E:95:PRO:CB	2:F:47:TRP:CZ3	2.93	0.51
1:K:155:GLN:HG2	1:K:156:SER:H	1.75	0.51
2:N:83:MET:HB3	2:N:86:LEU:HD21	1.92	0.51
1:A:198:HIS:HD2	1:A:200:GLY:H	1.58	0.51
2:D:73:ASP:OD2	2:D:76:LYS:HG2	2.10	0.51
1:E:4:MET:HB3	1:E:99:GLY:HA2	1.92	0.51
2:B:144:LEU:HD12	2:B:217:VAL:HG21	1.92	0.51
2:B:40:ALA:HB3	2:B:43:LYS:HD2	1.91	0.51
1:I:61:ARG:HH21	1:I:82:ASP:CG	2.12	0.51
2:P:4:LEU:CD1	2:P:108:LEU:O	2.58	0.51
1:C:4:MET:HE2	1:C:90:GLN:HB3	1.92	0.51
2:B:60:TYR:CE1	2:B:69:THR:HA	2.45	0.51
1:M:124:GLN:CD	2:N:128:PHE:CG	2.84	0.51
2:N:130:LEU:HG	2:N:145:GLY:CA	2.40	0.51
2:P:219:ARG:NE	2:P:219:ARG:O	2.37	0.51
2:L:132:PRO:O	2:L:133:CYS:HB2	2.11	0.51
2:L:174:ALA:HA	2:L:184:LEU:HB3	1.93	0.51
1:A:28:SER:HA	1:A:68:GLY:O	2.11	0.51
1:A:6:GLN:NE2	1:A:86:TYR:O	2.41	0.51
1:E:201:LEU:HD22	1:E:205:VAL:HG23	1.93	0.51
2:J:91:THR:HG23	2:J:116:THR:HA	1.93	0.51
1:M:34:ALA:HA	1:M:48:ILE:O	2.11	0.51
2:N:177:GLN:CG	2:N:181:LEU:O	2.58	0.51
2:N:194:ASN:CG	2:N:197:THR:HB	2.31	0.51
2:B:140:SER:OG	2:B:141:THR:N	2.43	0.51
2:B:206:HIS:HD2	2:B:209:SER:OG	1.94	0.51
2:D:6:GLU:OE2	2:D:112:GLY:N	2.44	0.51
2:J:142:ALA:HB3	2:J:195:PHE:CE2	2.44	0.51
1:O:108:ARG:HG2	1:O:109:THR:N	2.26	0.51
1:O:49:TYR:CD2	1:O:55:ALA:HA	2.46	0.51
2:F:201:THR:HA	2:F:216:THR:HA	1.93	0.51
1:G:115:VAL:HG12	1:G:207:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:HIS:CB	1:K:190:LYS:HB2	2.39	0.51
1:O:155:GLN:HB3	1:O:158:ASN:HD21	1.75	0.51
2:J:68:PHE:HD2	2:J:83:MET:HG2	1.76	0.50
1:K:196:VAL:HG13	1:K:198:HIS:CE1	2.46	0.50
2:H:210:ASN:OD1	2:H:212:LYS:HE2	2.11	0.50
1:I:191:VAL:HG13	1:I:191:VAL:O	2.11	0.50
1:M:50:ASP:OD1	1:M:91:TYR:OH	2.21	0.50
2:B:91:THR:O	2:B:92:ALA:HB2	2.11	0.50
2:F:36:TRP:CD1	2:F:81:LEU:HD13	2.47	0.50
1:K:120:PRO:N	1:K:121:SER:HG	2.09	0.50
2:L:20:LEU:O	2:L:80:TYR:HA	2.12	0.50
2:P:194:ASN:C	2:P:196:GLY:H	2.15	0.50
2:F:18:LEU:O	2:F:83:MET:N	2.37	0.50
2:J:35:PHE:HE2	2:J:99:GLU:HG3	1.76	0.50
2:N:3:GLN:HE21	2:N:5:LEU:HD12	1.76	0.50
1:C:79:GLN:HG3	1:C:80:SER:H	1.76	0.50
2:D:122:THR:HG21	2:P:74:ASN:HB2	1.91	0.50
1:E:190:LYS:HE2	1:E:213:GLU:H	1.77	0.50
2:J:64:VAL:HG13	2:J:68:PHE:HB2	1.92	0.50
2:N:102:ASN:ND2	2:N:102:ASN:O	2.44	0.50
1:A:210:ASN:ND2	1:A:210:ASN:H	2.09	0.50
2:F:104:TRP:O	2:F:105:TYR:O	2.30	0.50
1:I:21:LEU:HD23	1:I:102:THR:CB	2.40	0.50
1:M:11:LEU:HD12	1:M:12:SER:N	2.26	0.50
2:B:51:ILE:HD11	2:B:55:GLY:HA2	1.93	0.50
1:E:24:ARG:HA	1:E:69:THR:O	2.12	0.50
1:G:5:THR:HB	1:G:24:ARG:HB3	1.94	0.50
1:O:89:GLN:HE22	2:P:105:TYR:HA	1.77	0.50
1:E:62:PHE:CE1	1:E:75:ILE:HG12	2.47	0.50
1:E:118:PHE:HE2	2:F:132:PRO:HD3	1.77	0.50
1:K:145:LYS:HB2	1:K:198:HIS:HE1	1.72	0.50
2:P:54:SER:OG	2:P:74:ASN:ND2	2.45	0.50
1:G:24:ARG:HH11	1:G:70:GLU:HG2	1.77	0.49
1:O:32:TYR:HA	1:O:50:ASP:OD1	2.12	0.49
1:O:19:ALA:HB2	1:O:78:LEU:HD21	1.94	0.49
1:O:90:GLN:HG2	1:O:91:TYR:N	2.27	0.49
1:G:125:LEU:HD23	1:G:130:ALA:HB2	1.93	0.49
2:D:195:PHE:HB2	1:K:211:ARG:HG3	1.94	0.49
2:L:30:SER:CB	2:L:74:ASN:HD22	2.24	0.49
2:N:6:GLU:HA	2:N:21:SER:O	2.12	0.49
2:P:137:THR:O	2:P:138:SER:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ASN:HD22	1:G:158:ASN:N	2.01	0.49
2:H:158:VAL:HA	2:H:203:ASN:O	2.12	0.49
1:K:191:VAL:HA	1:K:208:SER:CB	2.41	0.49
1:M:158:ASN:HD22	1:M:179:LEU:CB	2.26	0.49
2:B:190:VAL:O	2:B:195:PHE:CZ	2.66	0.49
1:E:209:PHE:HB2	2:F:133:CYS:SG	2.52	0.49
1:G:125:LEU:C	1:G:127:SER:N	2.65	0.49
2:P:169:VAL:HG22	2:P:188:VAL:HB	1.94	0.49
2:B:6:GLU:HA	2:B:21:SER:O	2.12	0.49
1:C:108:ARG:HG2	1:C:109:THR:H	1.77	0.49
1:I:98:PHE:HZ	2:J:106:PHE:CE2	2.23	0.49
1:K:159:SER:HB3	1:K:178:THR:O	2.13	0.49
1:A:32:TYR:CD2	1:A:92:ASP:HB2	2.47	0.49
2:B:2:VAL:HG12	2:B:108:LEU:HD21	1.95	0.49
1:I:115:VAL:HG13	1:I:136:LEU:HD23	1.93	0.49
2:P:18:LEU:O	2:P:83:MET:O	2.30	0.49
2:L:14:PRO:HG2	2:L:119:SER:HB3	1.95	0.49
2:L:29:PHE:CD1	2:L:77:ASN:HA	2.48	0.49
1:M:7:SER:O	1:M:22:SER:HB2	2.11	0.49
1:C:125:LEU:O	1:C:127:SER:N	2.46	0.49
1:C:24:ARG:CG	1:C:70:GLU:HG2	2.42	0.49
2:H:153:PRO:O	2:H:206:HIS:HE1	1.95	0.49
1:I:186:TYR:O	1:I:192:TYR:OH	2.30	0.49
1:K:121:SER:O	1:K:122:ASP:O	2.31	0.49
2:P:6:GLU:OE2	2:P:112:GLY:CA	2.55	0.49
1:I:151:ASP:O	1:I:153:ALA:N	2.33	0.49
2:N:76:LYS:HB2	2:N:78:THR:CG2	2.43	0.49
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.48	0.48
1:E:47:LEU:HA	1:E:58:ILE:HG13	1.95	0.48
2:H:60:TYR:OH	2:H:69:THR:HA	2.12	0.48
1:M:124:GLN:CD	2:N:128:PHE:CD2	2.87	0.48
2:P:16:GLY:O	2:P:85:SER:N	2.46	0.48
2:D:35:PHE:HZ	2:D:104:TRP:HD1	1.60	0.48
1:G:105:GLU:HG2	1:G:166:GLN:NE2	2.27	0.48
1:I:136:LEU:HD21	1:I:196:VAL:CG2	2.34	0.48
1:A:175:LEU:HD23	1:A:175:LEU:C	2.33	0.48
1:A:32:TYR:HB3	1:A:91:TYR:CD1	2.49	0.48
1:G:105:GLU:HG2	1:G:106:ILE:N	2.29	0.48
1:K:108:ARG:HD3	1:K:108:ARG:C	2.33	0.48
1:K:182:SER:O	1:K:186:TYR:HB3	2.12	0.48
2:P:210:ASN:OD1	2:P:212:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:O	1:E:107:LYS:N	2.45	0.48
2:J:137:THR:CA	2:J:138:SER:HB3	2.34	0.48
2:J:198:GLN:O	2:J:199:THR:C	2.51	0.48
1:K:209:PHE:HD1	1:K:209:PHE:O	1.96	0.48
1:M:137:ASN:HD22	1:M:138:ASN:N	2.12	0.48
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.95	0.48
1:G:83:PHE:CD2	1:G:106:ILE:HG12	2.49	0.48
1:M:198:HIS:C	1:M:200:GLY:H	2.17	0.48
2:N:36:TRP:CD1	2:N:81:LEU:HD13	2.48	0.48
1:O:49:TYR:O	1:O:50:ASP:HB2	2.14	0.48
1:K:145:LYS:HD2	1:K:198:HIS:ND1	2.29	0.48
1:K:2:ILE:HD12	1:K:2:ILE:H	1.79	0.48
2:N:123:LYS:HD2	2:N:124:GLY:H	1.79	0.48
2:J:68:PHE:CD2	2:J:83:MET:HG2	2.48	0.48
2:P:176:LEU:HD23	2:P:177:GLN:O	2.13	0.48
2:P:54:SER:O	2:P:56:GLY:N	2.47	0.48
1:A:146:VAL:HA	1:A:195:GLU:O	2.14	0.48
1:A:34:ALA:O	1:A:88:CYS:HA	2.14	0.48
2:L:48:VAL:HG12	2:L:49:SER:HB2	1.95	0.48
2:P:38:ARG:HH12	2:P:90:ASP:HA	1.79	0.48
1:C:21:LEU:O	1:C:72:THR:HA	2.14	0.48
1:K:181:LEU:CG	1:K:182:SER:H	2.25	0.48
1:O:49:TYR:H	1:O:53:ASN:C	2.18	0.48
2:B:100:GLY:O	2:B:101:HIS:O	2.32	0.48
1:E:158:ASN:N	1:E:158:ASN:ND2	2.59	0.48
1:I:108:ARG:HH11	1:I:111:ALA:HB2	1.77	0.48
2:P:41:PRO:HD3	2:P:92:ALA:HA	1.96	0.48
1:G:116:PHE:HZ	2:H:141:THR:HG23	1.79	0.47
1:K:108:ARG:HH22	1:K:172:THR:HG23	1.79	0.47
1:M:4:MET:CE	1:M:90:GLN:HB3	2.43	0.47
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.95	0.47
1:A:203:SER:HB2	1:A:204:PRO:CD	2.44	0.47
2:D:101:HIS:HA	2:D:102:ASN:HA	1.63	0.47
2:J:174:ALA:HA	2:J:184:LEU:HB3	1.95	0.47
1:K:210:ASN:HD22	1:K:210:ASN:H	1.59	0.47
1:O:27:GLN:HG3	1:O:28:SER:N	2.30	0.47
2:H:172:PHE:HD1	2:H:185:SER:O	1.97	0.47
2:J:172:PHE:O	2:J:184:LEU:HD22	2.14	0.47
2:L:68:PHE:O	2:L:69:THR:HB	2.15	0.47
2:N:217:VAL:O	2:N:219:ARG:N	2.40	0.47
1:O:48:ILE:HG23	1:O:53:ASN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ALA:HB2	1:E:208:SER:CB	2.45	0.47
2:F:209:SER:HA	2:J:73:ASP:HA	1.96	0.47
1:G:44:PRO:HG2	2:H:109:TRP:CE3	2.50	0.47
1:I:201:LEU:O	1:I:202:SER:CB	2.63	0.47
1:I:94:TRP:HA	1:I:95:PRO:O	2.14	0.47
2:J:69:THR:HB	2:J:82:GLN:HB3	1.96	0.47
1:M:151:ASP:HB2	1:M:189:HIS:HB3	1.96	0.47
2:D:165:LEU:HD21	2:D:188:VAL:HG21	1.95	0.47
1:K:108:ARG:NH2	1:K:108:ARG:CG	2.68	0.47
1:C:193:ALA:HB2	1:C:208:SER:HB3	1.97	0.47
1:G:133:VAL:HG22	1:G:178:THR:OG1	2.14	0.47
1:K:111:ALA:O	1:K:112:ALA:HB3	2.15	0.47
1:M:33:LEU:CD1	1:M:88:CYS:HB2	2.45	0.47
1:A:56:THR:HG23	1:A:57:GLY:N	2.29	0.47
1:C:150:VAL:HB	1:C:155:GLN:NE2	2.29	0.47
2:H:184:LEU:C	2:H:184:LEU:HD12	2.34	0.47
1:O:39:LYS:O	1:O:40:PRO:C	2.52	0.47
2:H:207:LYS:N	2:H:208:PRO:CD	2.78	0.47
2:J:163:GLY:O	2:J:164:ALA:C	2.53	0.47
1:K:105:GLU:HG2	1:K:166:GLN:HE22	1.79	0.47
2:N:190:VAL:HG21	2:N:200:TYR:OH	2.14	0.47
1:A:116:PHE:HZ	2:B:141:THR:HG23	1.79	0.47
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.18	0.47
1:E:4:MET:CE	1:E:90:GLN:HB3	2.45	0.47
2:F:73:ASP:CB	2:F:76:LYS:HG3	2.45	0.47
2:P:56:GLY:CA	2:P:57:ILE:CG1	2.69	0.47
2:P:67:ARG:HH11	2:P:86:LEU:N	2.12	0.47
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.96	0.47
1:C:123:GLU:HG2	2:D:128:PHE:CD1	2.50	0.47
1:C:40:PRO:C	1:C:42:GLN:H	2.18	0.47
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.96	0.47
1:I:90:GLN:OE1	1:I:92:ASP:N	2.27	0.47
2:J:37:VAL:HG12	2:J:38:ARG:N	2.30	0.47
1:M:186:TYR:C	1:M:188:LYS:H	2.18	0.47
2:B:190:VAL:O	2:B:195:PHE:HZ	1.98	0.46
2:B:97:ALA:O	2:B:98:ARG:CB	2.50	0.46
1:E:193:ALA:CB	1:E:208:SER:HB3	2.45	0.46
2:H:13:GLN:O	2:H:14:PRO:C	2.51	0.46
2:F:76:LYS:HB3	1:I:32:TYR:CE2	2.50	0.46
1:K:115:VAL:HG22	1:K:134:CYS:HA	1.96	0.46
2:P:104:TRP:HA	2:P:104:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:4:LEU:HD11	2:P:108:LEU:O	2.16	0.46
1:C:83:PHE:CD2	1:C:106:ILE:HG12	2.51	0.46
1:C:79:GLN:C	1:C:81:GLU:H	2.19	0.46
2:F:207:LYS:N	2:F:208:PRO:CD	2.78	0.46
1:G:142:ARG:HD3	1:G:163:VAL:HG11	1.97	0.46
2:H:35:PHE:CD2	2:H:106:PHE:CE1	3.04	0.46
1:M:128:GLY:O	1:M:183:LYS:N	2.48	0.46
2:N:124:GLY:O	2:N:150:ASP:O	2.33	0.46
1:O:50:ASP:O	1:O:52:SER:N	2.49	0.46
1:E:21:LEU:CD1	1:E:21:LEU:N	2.78	0.46
2:F:140:SER:O	2:F:192:SER:OG	2.33	0.46
2:L:32:TYR:HA	2:L:33:PRO:HD3	1.78	0.46
1:M:152:ASN:CG	1:M:152:ASN:O	2.54	0.46
1:I:159:SER:O	1:I:160:GLN:HG3	2.15	0.46
2:J:163:GLY:O	2:J:165:LEU:N	2.48	0.46
2:J:38:ARG:HD3	2:J:94:TYR:CE2	2.50	0.46
2:J:53:PRO:O	2:J:54:SER:CB	2.63	0.46
1:M:186:TYR:O	1:M:188:LYS:N	2.41	0.46
2:N:159:SER:HB3	2:N:163:GLY:HA2	1.98	0.46
1:O:182:SER:OG	1:O:185:ASP:CB	2.63	0.46
1:A:54:ARG:HG2	1:A:58:ILE:HB	1.98	0.46
1:E:193:ALA:HB2	1:E:208:SER:HB3	1.97	0.46
2:N:120:ALA:O	2:N:121:SER:CB	2.64	0.46
1:O:175:LEU:HD23	1:O:176:SER:N	2.30	0.46
2:H:218:GLU:O	2:H:219:ARG:C	2.54	0.46
1:M:17:GLU:O	1:M:77:SER:HA	2.14	0.46
2:N:146:CYS:O	2:N:185:SER:HA	2.14	0.46
1:C:136:LEU:HG	1:C:175:LEU:HD22	1.97	0.46
1:K:2:ILE:N	1:K:2:ILE:HD12	2.31	0.46
2:P:125:PRO:CB	2:P:151:TYR:HB3	2.37	0.46
2:D:193:SER:C	2:D:195:PHE:H	2.19	0.46
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.30	0.46
1:M:32:TYR:HD1	1:M:91:TYR:CE2	2.34	0.46
1:O:92:ASP:HB3	1:O:93:LYS:H	1.60	0.46
1:A:21:LEU:HD23	1:A:102:THR:HB	1.97	0.46
1:A:24:ARG:HG2	1:A:70:GLU:HA	1.98	0.46
2:H:145:GLY:HA2	2:H:160:TRP:CZ2	2.50	0.46
2:J:161:ASN:HB2	2:J:165:LEU:HB2	1.98	0.46
1:K:110:VAL:HG23	1:K:111:ALA:N	2.31	0.46
2:H:101:HIS:O	2:H:102:ASN:C	2.54	0.46
2:L:65:LYS:C	2:L:67:ARG:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:163:GLY:O	2:N:164:ALA:HB2	2.16	0.46
2:H:158:VAL:HG12	2:H:159:SER:N	2.30	0.45
2:H:201:THR:HB	2:H:216:THR:HA	1.97	0.45
2:H:60:TYR:OH	2:H:70:ILE:N	2.36	0.45
2:J:169:VAL:H	2:J:188:VAL:HA	1.81	0.45
1:O:31:SER:C	1:O:33:LEU:H	2.19	0.45
1:O:30:SER:HB3	1:O:31:SER:H	1.44	0.45
1:C:158:ASN:N	1:C:158:ASN:HD22	2.01	0.45
1:C:48:ILE:HG23	1:C:53:ASN:O	2.16	0.45
2:F:76:LYS:CD	1:I:32:TYR:OH	2.64	0.45
2:F:38:ARG:HD3	2:F:94:TYR:CE2	2.51	0.45
2:L:103:ASP:O	2:L:104:TRP:CB	2.64	0.45
1:M:118:PHE:HB2	1:M:133:VAL:HB	1.97	0.45
2:P:36:TRP:HD1	2:P:70:ILE:HD12	1.81	0.45
1:A:151:ASP:O	1:A:152:ASN:HB2	2.16	0.45
2:F:93:THR:HA	2:F:113:THR:O	2.16	0.45
2:H:52:GLY:O	2:H:55:GLY:N	2.43	0.45
2:L:91:THR:HG23	2:L:116:THR:HA	1.98	0.45
1:I:115:VAL:HG13	1:I:136:LEU:CD2	2.46	0.45
1:M:179:LEU:HA	1:M:180:THR:HB	1.99	0.45
2:D:152:PHE:HA	2:D:153:PRO:HA	1.73	0.45
2:D:19:ARG:NH1	2:P:102:ASN:OD1	2.50	0.45
1:K:183:LYS:CA	1:K:186:TYR:CD2	2.94	0.45
2:P:160:TRP:CH2	2:P:202:CYS:HB3	2.52	0.45
1:A:210:ASN:ND2	1:A:210:ASN:N	2.64	0.45
2:B:106:PHE:N	2:B:106:PHE:CD1	2.85	0.45
1:I:48:ILE:HA	1:I:53:ASN:O	2.16	0.45
1:I:47:LEU:HD23	1:I:58:ILE:HD12	1.99	0.45
1:K:105:GLU:HG2	1:K:106:ILE:N	2.32	0.45
1:K:210:ASN:HB2	1:K:211:ARG:NH2	2.31	0.45
2:P:104:TRP:HE3	2:P:104:TRP:HA	1.81	0.45
1:K:159:SER:HB2	1:K:160:GLN:C	2.36	0.45
1:M:83:PHE:CZ	1:M:106:ILE:HG12	2.52	0.45
2:N:130:LEU:HD23	2:N:217:VAL:HG21	1.97	0.45
1:E:198:HIS:CD2	1:E:200:GLY:H	2.34	0.45
1:G:136:LEU:HD23	1:G:136:LEU:N	2.32	0.45
1:O:119:PRO:HD2	2:P:131:ALA:O	2.17	0.45
1:C:4:MET:CE	1:C:90:GLN:HB3	2.47	0.45
2:D:148:VAL:HG11	2:D:156:VAL:HG11	1.98	0.45
2:J:125:PRO:HB3	2:J:151:TYR:HB3	1.98	0.45
1:K:108:ARG:H	1:K:109:THR:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:126:SER:HB2	2:N:128:PHE:HE2	1.82	0.45
2:N:184:LEU:HD12	2:N:184:LEU:C	2.37	0.45
1:O:136:LEU:N	1:O:136:LEU:HD23	2.32	0.45
1:O:36:TYR:OH	1:O:89:GLN:NE2	2.50	0.45
1:C:108:ARG:NH2	1:C:172:THR:HG23	2.33	0.44
2:D:30:SER:HB3	2:D:74:ASN:HB3	1.99	0.44
2:L:121:SER:OG	2:L:122:THR:N	2.51	0.44
2:N:120:ALA:O	2:N:121:SER:HB2	2.16	0.44
2:D:142:ALA:N	2:D:190:VAL:O	2.41	0.44
2:D:206:HIS:CD2	2:D:209:SER:OG	2.67	0.44
2:H:33:PRO:HG2	2:H:99:GLU:HB3	2.00	0.44
1:I:108:ARG:NH1	1:I:111:ALA:HB2	2.32	0.44
1:I:36:TYR:HA	1:I:45:ARG:O	2.17	0.44
1:M:150:VAL:O	1:M:151:ASP:C	2.56	0.44
1:O:89:GLN:O	1:O:90:GLN:HB3	2.17	0.44
1:E:135:LEU:HD11	1:E:137:ASN:ND2	2.28	0.44
1:I:191:VAL:HA	1:I:209:PHE:O	2.17	0.44
2:J:177:GLN:HB2	2:J:181:LEU:O	2.18	0.44
2:N:137:THR:HA	2:N:138:SER:HA	1.74	0.44
2:P:59:LYS:C	2:P:60:TYR:HD2	2.20	0.44
1:A:18:ARG:HE	1:A:18:ARG:HB2	1.56	0.44
2:B:34:MET:SD	2:B:98:ARG:HA	2.57	0.44
1:C:193:ALA:HA	1:C:207:LYS:O	2.17	0.44
2:H:43:LYS:N	2:H:43:LYS:HD3	2.33	0.44
2:N:35:PHE:CE1	2:N:50:TRP:HD1	2.36	0.44
2:P:36:TRP:HA	2:P:95:TYR:O	2.17	0.44
1:C:15:PRO:C	1:C:17:GLU:H	2.21	0.44
2:F:70:ILE:HD11	2:F:79:LEU:HD11	1.99	0.44
2:H:174:ALA:HA	2:H:184:LEU:HB3	1.99	0.44
2:H:53:PRO:O	2:H:72:ARG:HD3	2.17	0.44
1:I:18:ARG:HA	1:I:76:SER:O	2.17	0.44
2:L:154:GLU:HG2	2:L:155:PRO:HA	1.99	0.44
1:M:139:PHE:HE1	1:M:142:ARG:O	2.00	0.44
1:O:151:ASP:HA	1:O:191:VAL:HG12	2.00	0.44
1:O:54:ARG:HB3	1:O:58:ILE:HB	2.00	0.44
1:K:159:SER:HA	1:K:160:GLN:CB	2.40	0.44
1:K:48:ILE:HA	1:K:53:ASN:O	2.18	0.44
1:O:46:LEU:HD23	1:O:55:ALA:HB2	1.99	0.44
2:H:35:PHE:CZ	2:H:104:TRP:NE1	2.84	0.44
2:D:198:GLN:NE2	1:M:61:ARG:HD3	2.32	0.44
2:N:191:PRO:O	2:N:193:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:SER:HB2	1:E:204:PRO:CD	2.48	0.44
1:E:95:PRO:HB3	2:F:47:TRP:HZ3	1.83	0.44
2:H:72:ARG:NE	2:H:74:ASN:OD1	2.44	0.44
1:I:212:GLY:O	1:I:213:GLU:HG2	2.18	0.44
1:M:149:LYS:HB2	1:M:193:ALA:HB3	2.00	0.44
1:M:37:GLN:O	1:M:44:PRO:HA	2.18	0.44
1:G:135:LEU:C	1:G:136:LEU:HD23	2.39	0.43
1:K:108:ARG:NH2	1:K:172:THR:HG23	2.33	0.43
2:L:142:ALA:HB3	2:L:195:PHE:CE2	2.53	0.43
1:M:94:TRP:CD1	1:M:95:PRO:CA	3.01	0.43
2:N:130:LEU:HB2	2:N:146:CYS:HA	2.00	0.43
2:N:199:THR:HG22	2:N:200:TYR:N	2.32	0.43
2:P:6:GLU:OE2	2:P:94:TYR:O	2.36	0.43
1:A:50:ASP:OD1	1:A:91:TYR:OH	2.31	0.43
2:D:8:GLY:O	2:D:18:LEU:HD21	2.18	0.43
1:O:33:LEU:HD21	1:O:90:GLN:H	1.76	0.43
2:P:137:THR:O	2:P:138:SER:HB3	2.17	0.43
2:B:144:LEU:HD13	2:B:217:VAL:HG21	2.00	0.43
1:C:7:SER:HA	1:C:8:PRO:HA	1.85	0.43
1:E:124:GLN:HG2	1:E:129:THR:O	2.17	0.43
1:E:165:GLU:OE2	1:E:165:GLU:HA	2.18	0.43
2:P:137:THR:OG1	2:P:138:SER:N	2.50	0.43
1:I:115:VAL:HB	1:I:207:LYS:HG3	2.00	0.43
1:I:198:HIS:O	1:I:200:GLY:N	2.51	0.43
1:I:147:GLN:HE21	1:I:154:LEU:HD11	1.83	0.43
1:I:195:GLU:OE2	1:I:206:THR:N	2.52	0.43
2:F:76:LYS:HD2	1:I:32:TYR:CE2	2.53	0.43
1:O:193:ALA:CB	1:O:208:SER:HB3	2.48	0.43
2:B:20:LEU:HG	2:B:83:MET:CE	2.49	0.43
2:B:89:GLU:O	2:B:89:GLU:HG2	2.18	0.43
2:H:52:GLY:H	2:H:57:ILE:HG22	1.84	0.43
1:K:210:ASN:ND2	1:K:210:ASN:N	2.67	0.43
1:O:91:TYR:CE1	2:P:103:ASP:HB3	2.54	0.43
2:P:38:ARG:NH1	2:P:90:ASP:HA	2.34	0.43
1:C:79:GLN:O	1:C:83:PHE:CE1	2.71	0.43
1:G:117:ILE:HG23	1:G:117:ILE:O	2.19	0.43
1:G:1:ASP:OD1	1:G:1:ASP:C	2.57	0.43
1:E:141:PRO:O	1:E:198:HIS:HE1	2.00	0.43
2:H:63:SER:O	2:H:67:ARG:NH2	2.50	0.43
2:J:124:GLY:HA2	2:J:125:PRO:HD3	1.72	0.43
1:K:147:GLN:O	1:K:195:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:ILE:HG21	2:L:72:ARG:HH21	1.83	0.43
1:M:175:LEU:CD2	1:M:176:SER:N	2.81	0.43
1:M:4:MET:HE1	1:M:90:GLN:HB3	1.99	0.43
2:B:50:TRP:CG	2:B:51:ILE:N	2.87	0.43
2:J:106:PHE:CD1	2:J:106:PHE:N	2.85	0.43
1:K:106:ILE:CG2	1:K:107:LYS:N	2.80	0.43
2:L:4:LEU:HB3	2:L:22:CYS:SG	2.59	0.43
2:N:88:ALA:HA	2:N:117:VAL:HB	2.00	0.43
2:P:134:SER:HB2	2:P:137:THR:HG21	2.00	0.43
1:A:166:GLN:HG3	1:A:171:SER:O	2.19	0.43
1:E:95:PRO:CB	2:F:47:TRP:HZ3	2.32	0.43
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.84	0.43
1:K:81:GLU:H	1:K:81:GLU:CD	2.22	0.43
1:K:126:LYS:HE3	2:L:128:PHE:HE1	1.84	0.43
2:N:129:PRO:O	2:N:130:LEU:C	2.56	0.43
2:N:154:GLU:CG	2:N:182:TYR:CE1	2.96	0.43
2:P:6:GLU:OE2	2:P:95:TYR:HA	2.19	0.43
1:A:150:VAL:O	1:A:151:ASP:HB2	2.19	0.42
1:C:125:LEU:HD23	1:C:125:LEU:HA	1.76	0.42
1:I:108:ARG:HD2	1:I:170:ASP:O	2.19	0.42
2:J:125:PRO:CB	2:J:151:TYR:HB3	2.48	0.42
1:K:159:SER:HB2	1:K:160:GLN:O	2.19	0.42
2:N:144:LEU:O	2:N:187:VAL:HA	2.19	0.42
2:P:47:TRP:HH2	2:P:62:ASP:H	1.65	0.42
1:A:2:ILE:HD11	1:A:93:LYS:HB3	2.00	0.42
2:F:68:PHE:HA	2:F:82:GLN:O	2.19	0.42
1:M:124:GLN:CG	2:N:128:PHE:CG	3.02	0.42
1:O:183:LYS:O	1:O:186:TYR:N	2.52	0.42
2:P:102:ASN:HD22	2:P:102:ASN:HA	1.64	0.42
2:P:50:TRP:CZ3	2:P:59:LYS:CG	3.01	0.42
2:P:6:GLU:H	2:P:6:GLU:HG2	1.47	0.42
2:P:86:LEU:HA	2:P:86:LEU:HD23	1.76	0.42
2:D:159:SER:OG	2:D:203:ASN:HB2	2.19	0.42
1:E:95:PRO:HB2	2:F:47:TRP:CZ3	2.53	0.42
2:H:38:ARG:HD3	2:H:48:VAL:HG22	2.01	0.42
2:L:219:ARG:O	2:L:219:ARG:HG3	2.19	0.42
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.55	0.42
1:M:124:GLN:CG	2:N:128:PHE:CD1	2.91	0.42
2:N:133:CYS:O	2:N:134:SER:HB2	2.19	0.42
1:O:27:GLN:CG	1:O:28:SER:N	2.83	0.42
1:A:106:ILE:H	1:A:166:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:CYS:HB3	2:L:79:LEU:HB3	2.00	0.42
1:M:124:GLN:HG3	2:N:128:PHE:CG	2.54	0.42
1:M:50:ASP:O	1:M:51:ALA:HB3	2.19	0.42
2:B:35:PHE:CZ	2:B:104:TRP:CD1	3.08	0.42
1:C:125:LEU:C	1:C:127:SER:H	2.21	0.42
2:H:52:GLY:H	2:H:57:ILE:CG2	2.32	0.42
2:J:99:GLU:OE2	2:J:102:ASN:O	2.36	0.42
1:K:24:ARG:NH2	1:K:70:GLU:HG2	2.18	0.42
2:N:31:ILE:O	2:N:53:PRO:HG3	2.19	0.42
2:P:152:PHE:HA	2:P:153:PRO:HA	1.86	0.42
2:P:194:ASN:O	2:P:196:GLY:N	2.51	0.42
2:B:195:PHE:O	2:B:196:GLY:C	2.58	0.42
1:K:203:SER:HA	1:K:204:PRO:HD3	1.85	0.42
2:L:201:THR:HA	2:L:216:THR:HA	2.01	0.42
1:M:126:LYS:C	1:M:126:LYS:HE2	2.40	0.42
1:M:151:ASP:O	1:M:189:HIS:ND1	2.53	0.42
1:M:155:GLN:NE2	1:M:155:GLN:CA	2.82	0.42
1:C:58:ILE:HA	1:C:59:PRO:HD3	1.92	0.42
2:F:100:GLY:O	2:F:101:HIS:O	2.37	0.42
2:F:62:ASP:C	2:F:64:VAL:N	2.70	0.42
1:G:10:THR:HG22	1:G:11:LEU:N	2.34	0.42
2:H:19:ARG:HH22	2:N:102:ASN:HB3	1.84	0.42
1:K:120:PRO:HG3	2:L:130:LEU:HD22	2.02	0.42
2:N:213:VAL:HG22	2:N:214:ASP:N	2.35	0.42
1:A:149:LYS:HA	1:A:153:ALA:O	2.20	0.42
2:B:39:GLN:O	2:B:92:ALA:HB1	2.20	0.42
2:B:54:SER:HA	1:E:32:TYR:CZ	2.55	0.42
2:H:6:GLU:OE1	2:H:112:GLY:HA2	2.20	0.42
1:K:189:HIS:O	1:K:209:PHE:HE1	2.02	0.42
2:P:93:THR:HG22	2:P:114:LEU:HD13	2.02	0.42
2:D:40:ALA:O	2:D:43:LYS:HB2	2.20	0.42
2:F:158:VAL:HG22	2:F:204:VAL:HG22	2.02	0.42
1:I:106:ILE:H	1:I:166:GLN:HE22	1.68	0.42
2:J:139:GLU:HB3	2:J:140:SER:H	1.41	0.42
2:L:207:LYS:HE2	2:L:207:LYS:HA	2.01	0.42
1:O:161:GLU:HA	1:O:176:SER:O	2.19	0.42
2:D:93:THR:HA	2:D:113:THR:O	2.19	0.41
2:L:47:TRP:CG	2:L:48:VAL:N	2.88	0.41
1:O:93:LYS:O	1:O:94:TRP:CD1	2.73	0.41
1:C:135:LEU:HD11	1:C:137:ASN:HD22	1.84	0.41
1:K:120:PRO:HG3	1:K:133:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:SER:O	1:M:170:ASP:N	2.48	0.41
1:M:197:THR:HB	1:M:198:HIS:H	1.40	0.41
2:N:61:ALA:O	2:N:62:ASP:C	2.59	0.41
1:C:189:HIS:O	1:C:211:ARG:HD3	2.20	0.41
1:E:136:LEU:HD11	1:E:196:VAL:CG1	2.49	0.41
1:E:30:SER:HB3	1:E:31:SER:H	1.73	0.41
2:F:74:ASN:O	2:F:76:LYS:N	2.49	0.41
2:F:76:LYS:HD2	1:I:32:TYR:CZ	2.55	0.41
1:I:94:TRP:CZ2	2:J:104:TRP:NE1	2.88	0.41
1:K:120:PRO:HG2	1:K:132:VAL:CA	2.49	0.41
1:K:120:PRO:CG	1:K:133:VAL:H	2.32	0.41
1:M:158:ASN:ND2	1:M:159:SER:H	2.18	0.41
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.02	0.41
2:B:20:LEU:HB2	2:B:81:LEU:HB3	2.03	0.41
1:I:115:VAL:HA	1:I:135:LEU:O	2.20	0.41
1:K:196:VAL:HG22	1:K:197:THR:H	1.86	0.41
1:M:183:LYS:HG2	1:M:184:ALA:N	2.36	0.41
1:E:37:GLN:CB	1:E:47:LEU:HD21	2.50	0.41
2:J:87:ARG:O	2:J:90:ASP:HB2	2.20	0.41
1:M:163:VAL:CG2	1:M:175:LEU:HG	2.43	0.41
1:M:36:TYR:OH	2:N:106:PHE:HD1	2.03	0.41
1:G:198:HIS:HD2	1:G:200:GLY:H	1.66	0.41
2:H:75:SER:CB	2:H:76:LYS:HZ1	2.33	0.41
1:I:118:PHE:HD1	1:I:133:VAL:HG12	1.85	0.41
2:F:73:ASP:OD2	2:F:76:LYS:HG3	2.20	0.41
1:I:191:VAL:O	1:I:191:VAL:CG1	2.68	0.41
2:J:124:GLY:HA2	2:J:209:SER:OG	2.20	0.41
2:L:132:PRO:O	2:L:133:CYS:CB	2.68	0.41
2:N:123:LYS:HE2	2:N:181:LEU:HD13	2.03	0.41
1:G:79:GLN:O	1:G:82:ASP:HB2	2.21	0.41
1:I:195:GLU:OE2	1:I:206:THR:CG2	2.68	0.41
2:J:161:ASN:CB	2:J:165:LEU:HD22	2.50	0.41
2:B:60:TYR:CZ	2:B:69:THR:HA	2.56	0.41
1:E:16:GLY:O	1:E:77:SER:OG	2.32	0.41
1:E:203:SER:O	1:E:204:PRO:C	2.58	0.41
1:I:211:ARG:O	1:I:213:GLU:N	2.53	0.41
1:M:54:ARG:HD3	1:M:59:PRO:O	2.21	0.41
2:N:102:ASN:H	2:N:103:ASP:CG	2.13	0.41
1:A:210:ASN:HD22	1:A:210:ASN:H	1.68	0.41
1:A:96:LEU:HD11	2:B:104:TRP:HB3	2.02	0.41
1:K:122:ASP:OD1	1:K:123:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:158:ASN:ND2	1:M:179:LEU:CB	2.84	0.41
2:N:2:VAL:HA	2:N:25:SER:O	2.21	0.41
2:B:195:PHE:HD2	2:B:195:PHE:H	1.69	0.41
2:F:61:ALA:O	2:F:64:VAL:HB	2.20	0.41
1:G:105:GLU:HG2	1:G:106:ILE:H	1.85	0.41
1:I:189:HIS:O	1:I:211:ARG:HD3	2.21	0.41
2:L:206:HIS:HD2	2:L:209:SER:HB2	1.84	0.41
1:M:158:ASN:ND2	1:M:179:LEU:HB3	2.32	0.41
2:N:148:VAL:O	2:N:183:SER:HA	2.21	0.41
1:C:89:GLN:HB2	1:C:98:PHE:CD2	2.56	0.40
1:C:95:PRO:HB2	2:D:47:TRP:CZ3	2.56	0.40
1:I:158:ASN:N	1:I:158:ASN:HD22	2.20	0.40
1:M:46:LEU:HA	1:M:46:LEU:HD12	1.94	0.40
1:O:105:GLU:CG	1:O:166:GLN:NE2	2.73	0.40
1:A:56:THR:HG23	1:A:57:GLY:H	1.86	0.40
1:C:123:GLU:HG2	2:D:128:PHE:HD1	1.86	0.40
2:F:6:GLU:OE2	2:F:96:CYS:SG	2.80	0.40
1:G:135:LEU:HD22	2:H:187:VAL:HG11	2.03	0.40
2:H:30:SER:O	2:H:53:PRO:HB3	2.21	0.40
1:I:94:TRP:HA	1:I:95:PRO:C	2.41	0.40
1:K:191:VAL:HA	1:K:208:SER:HB3	2.03	0.40
2:L:51:ILE:HG22	2:L:72:ARG:HH21	1.86	0.40
1:M:134:CYS:HB2	1:M:148:TRP:CH2	2.57	0.40
1:A:193:ALA:CB	1:A:208:SER:HB3	2.50	0.40
1:G:158:ASN:N	1:G:158:ASN:ND2	2.65	0.40
1:K:113:PRO:HG2	1:K:137:ASN:HB3	2.04	0.40
2:L:68:PHE:O	2:L:69:THR:CB	2.69	0.40
2:B:20:LEU:HG	2:B:83:MET:HE2	2.02	0.40
1:E:17:GLU:HG2	1:E:18:ARG:H	1.87	0.40
2:F:39:GLN:NE2	2:F:43:LYS:O	2.31	0.40
1:I:90:GLN:C	1:I:90:GLN:CD	2.79	0.40
2:L:30:SER:HB2	2:L:74:ASN:ND2	2.36	0.40
1:M:167:ASP:O	1:M:171:SER:HA	2.21	0.40
1:M:27:GLN:O	1:M:28:SER:C	2.59	0.40
1:C:20:THR:HG22	1:C:72:THR:HG21	2.03	0.40
1:E:175:LEU:C	1:E:175:LEU:HD23	2.42	0.40
1:E:37:GLN:HB3	1:E:47:LEU:HD21	2.02	0.40
1:E:54:ARG:HD3	1:E:59:PRO:O	2.21	0.40
1:E:89:GLN:HG3	1:E:98:PHE:CE2	2.55	0.40
2:F:40:ALA:HA	2:F:41:PRO:HD2	1.79	0.40
2:J:162:SER:HA	2:J:203:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:SER:O	1:K:210:ASN:ND2	2.55	0.40
2:P:109:TRP:N	2:P:109:TRP:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/214 (99%)	190 (90%)	17 (8%)	4 (2%)	8	14
1	C	211/214 (99%)	183 (87%)	24 (11%)	4 (2%)	8	14
1	E	211/214 (99%)	195 (92%)	14 (7%)	2 (1%)	17	33
1	G	211/214 (99%)	190 (90%)	19 (9%)	2 (1%)	17	33
1	I	211/214 (99%)	183 (87%)	19 (9%)	9 (4%)	2	3
1	K	205/214 (96%)	151 (74%)	33 (16%)	21 (10%)	0	0
1	M	206/214 (96%)	173 (84%)	20 (10%)	13 (6%)	1	1
1	O	211/214 (99%)	178 (84%)	17 (8%)	16 (8%)	1	1
2	B	218/227 (96%)	185 (85%)	26 (12%)	7 (3%)	4	5
2	D	218/227 (96%)	187 (86%)	23 (11%)	8 (4%)	3	4
2	F	217/227 (96%)	191 (88%)	18 (8%)	8 (4%)	3	4
2	H	217/227 (96%)	184 (85%)	22 (10%)	11 (5%)	2	2
2	J	217/227 (96%)	178 (82%)	24 (11%)	15 (7%)	1	1
2	L	217/227 (96%)	175 (81%)	22 (10%)	20 (9%)	1	0
2	N	217/227 (96%)	169 (78%)	24 (11%)	24 (11%)	0	0
2	P	217/227 (96%)	170 (78%)	29 (13%)	18 (8%)	1	0
All	All	3415/3528 (97%)	2882 (84%)	351 (10%)	182 (5%)	2	2

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	SER
2	B	101	HIS
2	B	134	SER
2	B	140	SER
2	D	135	ARG
2	D	195	PHE
1	E	126	LYS
2	F	63	SER
2	F	101	HIS
2	F	104	TRP
2	F	105	TYR
1	G	126	LYS
2	H	102	ASN
2	H	104	TRP
2	H	137	THR
2	H	162	SER
2	H	192	SER
1	I	51	ALA
1	I	202	SER
2	J	54	SER
2	J	104	TRP
2	J	164	ALA
2	J	166	THR
2	J	198	GLN
1	K	111	ALA
1	K	112	ALA
1	K	122	ASP
1	K	127	SER
1	K	134	CYS
1	K	158	ASN
1	K	182	SER
1	K	196	VAL
2	L	60	TYR
2	L	69	THR
2	L	123	LYS
2	L	132	PRO
2	L	133	CYS
2	L	134	SER
2	L	136	SER
2	L	138	SER
1	M	151	ASP
1	M	198	HIS

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Mol	Chain	Res	Type
1	M	199	GLN
1	M	202	SER
2	N	101	HIS
2	N	120	ALA
2	N	132	PRO
2	N	150	ASP
2	N	163	GLY
2	N	164	ALA
2	N	177	GLN
2	N	192	SER
2	N	210	ASN
1	O	2	ILE
1	O	3	GLN
1	O	30	SER
1	O	100	GLY
2	P	57	ILE
2	P	84	ASN
2	P	85	SER
2	P	86	LEU
2	P	135	ARG
2	P	138	SER
2	P	195	PHE
1	A	2	ILE
2	B	63	SER
1	C	126	LYS
2	D	137	THR
1	E	211	ARG
2	F	75	SER
1	G	30	SER
2	H	136	SER
1	I	152	ASN
1	I	168	SER
1	I	191	VAL
1	I	212	GLY
2	J	89	GLU
2	J	163	GLY
2	J	168	GLY
2	J	199	THR
1	K	151	ASP
1	K	183	LYS
1	K	184	ALA
1	K	190	LYS

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Mol	Chain	Res	Type
2	L	101	HIS
2	L	103	ASP
2	L	140	SER
2	L	156	VAL
2	L	197	THR
2	L	214	ASP
1	M	59	PRO
1	M	123	GLU
1	M	180	THR
1	M	200	GLY
2	N	129	PRO
2	N	130	LEU
2	N	133	CYS
2	N	134	SER
2	N	167	SER
1	O	50	ASP
1	O	51	ALA
1	O	92	ASP
1	O	96	LEU
1	O	183	LYS
1	O	212	GLY
2	P	43	LYS
2	P	56	GLY
1	A	30	SER
2	B	92	ALA
2	B	104	TRP
1	C	16	GLY
1	C	212	GLY
2	D	41	PRO
2	D	140	SER
2	F	41	PRO
2	H	57	ILE
2	H	196	GLY
2	J	100	GLY
2	J	162	SER
1	K	110	VAL
1	K	156	SER
1	K	181	LEU
2	L	14	PRO
2	L	61	ALA
2	L	121	SER
1	M	30	SER

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Mol	Chain	Res	Type
1	M	158	ASN
1	M	187	GLU
2	N	125	PRO
2	N	162	SER
2	N	165	LEU
2	N	194	ASN
1	O	127	SER
2	P	98	ARG
2	P	137	THR
1	A	211	ARG
2	D	101	HIS
2	D	134	SER
2	F	137	THR
2	F	140	SER
2	H	58	THR
2	H	138	SER
2	H	140	SER
1	I	28	SER
1	I	154	LEU
1	I	199	GLN
1	K	198	HIS
1	K	210	ASN
2	L	98	ARG
2	L	137	THR
2	L	155	PRO
1	M	28	SER
2	N	62	ASP
2	N	139	GLU
2	P	54	SER
2	P	58	THR
2	P	83	MET
2	B	98	ARG
2	D	197	THR
2	J	169	VAL
2	J	192	SER
2	N	140	SER
1	O	31	SER
1	O	90	GLN
1	O	152	ASN
2	P	2	VAL
2	J	158	VAL
1	K	204	PRO

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Mol	Chain	Res	Type
1	M	204	PRO
2	N	169	VAL
2	N	191	PRO
1	O	32	TYR
1	O	52	SER
2	P	14	PRO
2	P	101	HIS
1	C	15	PRO
2	J	9	GLY
1	K	106	ILE
1	K	68	GLY
2	P	55	GLY
1	K	115	VAL
2	N	168	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/185 (100%)	151 (82%)	33 (18%)	2	2
1	C	184/185 (100%)	159 (86%)	25 (14%)	3	5
1	E	184/185 (100%)	154 (84%)	30 (16%)	2	3
1	G	184/185 (100%)	157 (85%)	27 (15%)	3	4
1	I	184/185 (100%)	164 (89%)	20 (11%)	6	11
1	K	180/185 (97%)	144 (80%)	36 (20%)	1	2
1	M	180/185 (97%)	145 (81%)	35 (19%)	1	2
1	O	184/185 (100%)	163 (89%)	21 (11%)	5	9
2	B	186/193 (96%)	160 (86%)	26 (14%)	3	5
2	D	186/193 (96%)	160 (86%)	26 (14%)	3	5
2	F	185/193 (96%)	155 (84%)	30 (16%)	2	3
2	H	185/193 (96%)	151 (82%)	34 (18%)	1	2
2	J	185/193 (96%)	155 (84%)	30 (16%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	185/193 (96%)	147 (80%)	38 (20%)	1	1
2	N	185/193 (96%)	152 (82%)	33 (18%)	2	2
2	P	184/193 (95%)	155 (84%)	29 (16%)	2	3
All	All	2945/3024 (97%)	2472 (84%)	473 (16%)	2	3

All (473) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	11	LEU
1	A	22	SER
1	A	31	SER
1	A	33	LEU
1	A	52	SER
1	A	56	THR
1	A	67	SER
1	A	76	SER
1	A	77	SER
1	A	81	GLU
1	A	89	GLN
1	A	92	ASP
1	A	93	LYS
1	A	94	TRP
1	A	105	GLU
1	A	108	ARG
1	A	121	SER
1	A	126	LYS
1	A	129	THR
1	A	132	VAL
1	A	143	GLU
1	A	146	VAL
1	A	158	ASN
1	A	160	GLN
1	A	166	GLN
1	A	169	LYS
1	A	187	GLU
1	A	191	VAL
1	A	201	LEU
1	A	203	SER
1	A	210	ASN
1	A	213	GLU

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Mol	Chain	Res	Type
2	B	12	VAL
2	B	30	SER
2	B	65	LYS
2	B	75	SER
2	B	78	THR
2	B	93	THR
2	B	106	PHE
2	B	111	ARG
2	B	122	THR
2	B	126	SER
2	B	134	SER
2	B	144	LEU
2	B	146	CYS
2	B	157	THR
2	B	183	SER
2	B	190	VAL
2	B	192	SER
2	B	198	GLN
2	B	199	THR
2	B	201	THR
2	B	203	ASN
2	B	211	THR
2	B	212	LYS
2	B	216	THR
2	B	217	VAL
2	B	219	ARG
1	C	4	MET
1	C	7	SER
1	C	11	LEU
1	C	18	ARG
1	C	20	THR
1	C	27	GLN
1	C	30	SER
1	C	56	THR
1	C	70	GLU
1	C	75	ILE
1	C	89	GLN
1	C	107	LYS
1	C	109	THR
1	C	129	THR
1	C	136	LEU
1	C	142	ARG

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Mol	Chain	Res	Type
1	C	149	LYS
1	C	158	ASN
1	C	169	LYS
1	C	180	THR
1	C	185	ASP
1	C	187	GLU
1	C	190	LYS
1	C	202	SER
1	C	203	SER
2	D	12	VAL
2	D	18	LEU
2	D	25	SER
2	D	31	ILE
2	D	43	LYS
2	D	47	TRP
2	D	62	ASP
2	D	65	LYS
2	D	71	SER
2	D	111	ARG
2	D	119	SER
2	D	122	THR
2	D	126	SER
2	D	135	ARG
2	D	141	THR
2	D	146	CYS
2	D	157	THR
2	D	183	SER
2	D	185	SER
2	D	197	THR
2	D	198	GLN
2	D	205	ASP
2	D	212	LYS
2	D	216	THR
2	D	219	ARG
2	D	220	LYS
1	E	1	ASP
1	E	4	MET
1	E	11	LEU
1	E	14	SER
1	E	21	LEU
1	E	27	GLN
1	E	30	SER

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Mol	Chain	Res	Type
1	E	37	GLN
1	E	42	GLN
1	E	78	LEU
1	E	79	GLN
1	E	80	SER
1	E	89	GLN
1	E	94	TRP
1	E	97	THR
1	E	104	VAL
1	E	107	LYS
1	E	108	ARG
1	E	114	SER
1	E	136	LEU
1	E	137	ASN
1	E	145	LYS
1	E	151	ASP
1	E	152	ASN
1	E	156	SER
1	E	158	ASN
1	E	175	LEU
1	E	191	VAL
1	E	199	GLN
1	E	202	SER
2	F	47	TRP
2	F	57	ILE
2	F	63	SER
2	F	65	LYS
2	F	69	THR
2	F	71	SER
2	F	73	ASP
2	F	76	LYS
2	F	78	THR
2	F	102	ASN
2	F	103	ASP
2	F	113	THR
2	F	122	THR
2	F	123	LYS
2	F	135	ARG
2	F	138	SER
2	F	149	LYS
2	F	156	VAL
2	F	179	SER

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Mol	Chain	Res	Type
2	F	183	SER
2	F	184	LEU
2	F	185	SER
2	F	188	VAL
2	F	192	SER
2	F	198	GLN
2	F	201	THR
2	F	203	ASN
2	F	205	ASP
2	F	211	THR
2	F	212	LYS
1	G	1	ASP
1	G	3	GLN
1	G	18	ARG
1	G	22	SER
1	G	27	GLN
1	G	30	SER
1	G	45	ARG
1	G	56	THR
1	G	70	GLU
1	G	78	LEU
1	G	79	GLN
1	G	94	TRP
1	G	96	LEU
1	G	106	ILE
1	G	108	ARG
1	G	146	VAL
1	G	147	GLN
1	G	149	LYS
1	G	158	ASN
1	G	162	SER
1	G	163	VAL
1	G	181	LEU
1	G	188	LYS
1	G	197	THR
1	G	199	GLN
1	G	203	SER
1	G	208	SER
2	H	5	LEU
2	H	12	VAL
2	H	13	GLN
2	H	22	CYS

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Mol	Chain	Res	Type
2	H	31	ILE
2	H	43	LYS
2	H	54	SER
2	H	57	ILE
2	H	62	ASP
2	H	69	THR
2	H	73	ASP
2	H	75	SER
2	H	76	LYS
2	H	80	TYR
2	H	85	SER
2	H	87	ARG
2	H	93	THR
2	H	103	ASP
2	H	104	TRP
2	H	111	ARG
2	H	121	SER
2	H	122	THR
2	H	135	ARG
2	H	144	LEU
2	H	156	VAL
2	H	178	SER
2	H	183	SER
2	H	192	SER
2	H	193	SER
2	H	199	THR
2	H	201	THR
2	H	212	LYS
2	H	215	LYS
2	H	219	ARG
1	I	6	GLN
1	I	24	ARG
1	I	33	LEU
1	I	54	ARG
1	I	70	GLU
1	I	78	LEU
1	I	79	GLN
1	I	89	GLN
1	I	103	LYS
1	I	121	SER
1	I	142	ARG
1	I	143	GLU

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Mol	Chain	Res	Type
1	I	146	VAL
1	I	155	GLN
1	I	156	SER
1	I	158	ASN
1	I	169	LYS
1	I	177	SER
1	I	191	VAL
1	I	211	ARG
2	J	3	GLN
2	J	6	GLU
2	J	11	LEU
2	J	18	LEU
2	J	31	ILE
2	J	62	ASP
2	J	63	SER
2	J	67	ARG
2	J	75	SER
2	J	78	THR
2	J	93	THR
2	J	103	ASP
2	J	104	TRP
2	J	111	ARG
2	J	130	LEU
2	J	141	THR
2	J	166	THR
2	J	183	SER
2	J	185	SER
2	J	190	VAL
2	J	201	THR
2	J	203	ASN
2	J	207	LYS
2	J	209	SER
2	J	210	ASN
2	J	212	LYS
2	J	215	LYS
2	J	216	THR
2	J	217	VAL
2	J	219	ARG
1	K	3	GLN
1	K	5	THR
1	K	11	LEU
1	K	14	SER

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Mol	Chain	Res	Type
1	K	21	LEU
1	K	23	CYS
1	K	24	ARG
1	K	27	GLN
1	K	33	LEU
1	K	50	ASP
1	K	67	SER
1	K	78	LEU
1	K	93	LYS
1	K	105	GLU
1	K	108	ARG
1	K	109	THR
1	K	122	ASP
1	K	123	GLU
1	K	125	LEU
1	K	134	CYS
1	K	135	LEU
1	K	142	ARG
1	K	143	GLU
1	K	149	LYS
1	K	158	ASN
1	K	161	GLU
1	K	172	THR
1	K	180	THR
1	K	183	LYS
1	K	186	TYR
1	K	187	GLU
1	K	188	LYS
1	K	196	VAL
1	K	209	PHE
1	K	210	ASN
1	K	211	ARG
2	L	5	LEU
2	L	6	GLU
2	L	7	SER
2	L	11	LEU
2	L	12	VAL
2	L	19	ARG
2	L	28	THR
2	L	49	SER
2	L	51	ILE
2	L	54	SER

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Mol	Chain	Res	Type
2	L	64	VAL
2	L	69	THR
2	L	71	SER
2	L	85	SER
2	L	89	GLU
2	L	96	CYS
2	L	101	HIS
2	L	122	THR
2	L	138	SER
2	L	141	THR
2	L	159	SER
2	L	161	ASN
2	L	162	SER
2	L	165	LEU
2	L	178	SER
2	L	189	THR
2	L	192	SER
2	L	193	SER
2	L	197	THR
2	L	199	THR
2	L	201	THR
2	L	202	CYS
2	L	207	LYS
2	L	209	SER
2	L	210	ASN
2	L	212	LYS
2	L	214	ASP
2	L	216	THR
1	M	11	LEU
1	M	17	GLU
1	M	20	THR
1	M	27	GLN
1	M	30	SER
1	M	33	LEU
1	M	48	ILE
1	M	52	SER
1	M	56	THR
1	M	69	THR
1	M	74	THR
1	M	79	GLN
1	M	81	GLU
1	M	94	TRP

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Mol	Chain	Res	Type
1	M	97	THR
1	M	108	ARG
1	M	126	LYS
1	M	129	THR
1	M	131	SER
1	M	136	LEU
1	M	137	ASN
1	M	151	ASP
1	M	155	GLN
1	M	164	THR
1	M	168	SER
1	M	170	ASP
1	M	172	THR
1	M	175	LEU
1	M	181	LEU
1	M	183	LYS
1	M	185	ASP
1	M	191	VAL
1	M	192	TYR
1	M	197	THR
1	M	201	LEU
2	N	2	VAL
2	N	3	GLN
2	N	5	LEU
2	N	11	LEU
2	N	18	LEU
2	N	38	ARG
2	N	49	SER
2	N	64	VAL
2	N	67	ARG
2	N	76	LYS
2	N	78	THR
2	N	87	ARG
2	N	98	ARG
2	N	101	HIS
2	N	106	PHE
2	N	111	ARG
2	N	116	THR
2	N	121	SER
2	N	122	THR
2	N	123	LYS
2	N	139	GLU

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Mol	Chain	Res	Type
2	N	140	SER
2	N	146	CYS
2	N	149	LYS
2	N	166	THR
2	N	167	SER
2	N	169	VAL
2	N	187	VAL
2	N	198	GLN
2	N	201	THR
2	N	202	CYS
2	N	212	LYS
2	N	216	THR
1	O	2	ILE
1	O	5	THR
1	O	12	SER
1	O	27	GLN
1	O	30	SER
1	O	33	LEU
1	O	46	LEU
1	O	49	TYR
1	O	69	THR
1	O	71	PHE
1	O	78	LEU
1	O	79	GLN
1	O	80	SER
1	O	114	SER
1	O	131	SER
1	O	132	VAL
1	O	136	LEU
1	O	156	SER
1	O	158	ASN
1	O	191	VAL
1	O	213	GLU
2	P	3	GLN
2	P	5	LEU
2	P	6	GLU
2	P	11	LEU
2	P	12	VAL
2	P	21	SER
2	P	43	LYS
2	P	46	GLU
2	P	51	ILE

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Mol	Chain	Res	Type
2	P	54	SER
2	P	59	LYS
2	P	60	TYR
2	P	62	ASP
2	P	65	LYS
2	P	82	GLN
2	P	99	GLU
2	P	102	ASN
2	P	111	ARG
2	P	113	THR
2	P	135	ARG
2	P	137	THR
2	P	141	THR
2	P	149	LYS
2	P	190	VAL
2	P	193	SER
2	P	199	THR
2	P	211	THR
2	P	216	THR
2	P	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	89	GLN
1	A	137	ASN
1	A	158	ASN
1	A	198	HIS
1	A	210	ASN
2	B	74	ASN
2	B	177	GLN
2	B	206	HIS
1	C	37	GLN
1	C	89	GLN
1	C	137	ASN
1	C	147	GLN
1	C	158	ASN
1	C	198	HIS
2	D	177	GLN
2	D	194	ASN
2	D	198	GLN

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Mol	Chain	Res	Type
2	D	206	HIS
1	E	42	GLN
1	E	89	GLN
1	E	137	ASN
1	E	158	ASN
1	E	166	GLN
1	E	198	HIS
2	F	177	GLN
2	F	194	ASN
2	F	198	GLN
2	F	206	HIS
1	G	27	GLN
1	G	158	ASN
1	G	166	GLN
1	G	198	HIS
2	H	77	ASN
2	H	177	GLN
2	H	206	HIS
1	I	42	GLN
1	I	89	GLN
1	I	152	ASN
1	I	158	ASN
1	I	166	GLN
1	I	198	HIS
1	I	210	ASN
2	J	3	GLN
2	J	206	HIS
1	K	3	GLN
1	K	27	GLN
1	K	137	ASN
1	K	147	GLN
1	K	152	ASN
1	K	158	ASN
1	K	160	GLN
1	K	166	GLN
1	K	210	ASN
2	L	74	ASN
2	L	101	HIS
2	L	161	ASN
2	L	177	GLN
2	L	198	GLN
2	L	206	HIS

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Mol	Chain	Res	Type
2	L	210	ASN
1	M	42	GLN
1	M	79	GLN
1	M	124	GLN
1	M	137	ASN
1	M	138	ASN
1	M	155	GLN
1	M	158	ASN
1	M	166	GLN
2	N	3	GLN
2	N	82	GLN
2	N	102	ASN
2	N	170	HIS
1	O	42	GLN
1	O	89	GLN
1	O	137	ASN
1	O	158	ASN
1	O	166	GLN
1	O	198	HIS
2	P	3	GLN
2	P	206	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/214 (99%)	-0.13	2 (0%) 84 82	27, 47, 64, 73	0
1	C	213/214 (99%)	0.17	4 (1%) 66 62	40, 57, 68, 75	0
1	E	213/214 (99%)	-0.26	0 100 100	25, 39, 53, 64	0
1	G	213/214 (99%)	-0.34	1 (0%) 91 89	18, 35, 49, 66	0
1	I	213/214 (99%)	0.10	10 (4%) 31 25	18, 41, 74, 83	0
1	K	209/214 (97%)	0.37	21 (10%) 7 4	26, 49, 89, 100	0
1	M	208/214 (97%)	0.22	8 (3%) 40 34	33, 55, 73, 78	0
1	O	213/214 (99%)	0.20	19 (8%) 9 6	27, 46, 73, 83	0
2	B	220/227 (96%)	-0.05	5 (2%) 60 55	29, 47, 67, 76	0
2	D	220/227 (96%)	0.09	11 (5%) 28 23	37, 47, 70, 81	0
2	F	219/227 (96%)	0.08	10 (4%) 32 26	25, 42, 61, 73	0
2	H	219/227 (96%)	-0.05	6 (2%) 54 49	28, 38, 65, 72	0
2	J	219/227 (96%)	0.08	10 (4%) 32 26	26, 44, 67, 77	0
2	L	219/227 (96%)	0.21	10 (4%) 32 26	31, 50, 71, 85	0
2	N	219/227 (96%)	0.42	14 (6%) 19 15	32, 56, 80, 86	0
2	P	219/227 (96%)	0.31	14 (6%) 19 15	35, 51, 74, 78	0
All	All	3449/3528 (97%)	0.09	145 (4%) 36 30	18, 47, 72, 100	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	SER	8.9
2	F	136	SER	7.8
2	F	137	THR	7.5
2	N	195	PHE	6.8
2	N	136	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	O	32	TYR	6.0
2	L	140	SER	5.9
2	L	137	THR	5.7
2	L	136	SER	5.5
2	J	137	THR	5.3
2	F	196	GLY	5.3
2	F	135	ARG	5.3
2	P	137	THR	5.2
2	N	139	GLU	5.2
2	P	136	SER	5.2
1	K	184	ALA	5.1
1	M	198	HIS	5.0
2	H	137	THR	4.9
1	I	201	LEU	4.8
1	O	49	TYR	4.7
2	J	136	SER	4.6
2	N	138	SER	4.5
2	J	138	SER	4.4
1	O	92	ASP	4.3
2	P	58	THR	4.3
2	H	136	SER	4.3
2	L	138	SER	4.3
2	P	138	SER	4.2
1	K	209	PHE	4.1
1	O	212	GLY	4.1
1	O	57	GLY	4.0
2	H	193	SER	4.0
2	D	137	THR	3.8
2	L	133	CYS	3.8
2	F	42	GLY	3.8
2	N	163	GLY	3.7
2	B	137	THR	3.6
1	M	190	LYS	3.6
2	F	197	THR	3.6
2	L	134	SER	3.6
2	D	197	THR	3.6
1	K	157	GLY	3.6
1	O	94	TRP	3.5
1	K	195	GLU	3.5
1	M	94	TRP	3.5
1	I	209	PHE	3.4
1	O	50	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	P	194	ASN	3.3
1	O	30	SER	3.2
2	D	134	SER	3.2
2	N	135	ARG	3.2
2	D	195	PHE	3.1
2	D	135	ARG	3.1
1	O	1	ASP	3.1
2	P	140	SER	3.1
1	K	160	GLN	3.1
1	K	197	THR	3.0
1	I	212	GLY	3.0
1	O	91	TYR	3.0
2	F	1	GLU	3.0
1	K	158	ASN	3.0
1	K	109	THR	3.0
1	C	169	LYS	2.9
2	N	101	HIS	2.9
1	M	203	SER	2.9
2	B	135	ARG	2.9
2	J	135	ARG	2.9
1	M	169	LYS	2.8
2	J	102	ASN	2.8
2	J	140	SER	2.8
2	D	138	SER	2.8
2	F	195	PHE	2.8
2	J	139	GLU	2.8
1	K	189	HIS	2.8
2	L	1	GLU	2.8
1	O	33	LEU	2.8
2	L	135	ARG	2.7
1	K	203	SER	2.7
2	N	133	CYS	2.7
1	K	122	ASP	2.7
2	J	193	SER	2.7
2	H	195	PHE	2.7
2	J	195	PHE	2.7
2	P	135	ARG	2.7
1	O	48	ILE	2.6
2	D	193	SER	2.6
1	I	152	ASN	2.6
1	O	2	ILE	2.6
2	N	102	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	60	TYR	2.6
1	K	126	LYS	2.5
2	H	138	SER	2.5
1	K	125	LEU	2.5
1	O	184	ALA	2.5
2	L	141	THR	2.5
1	K	196	VAL	2.5
1	I	210	ASN	2.5
2	F	138	SER	2.4
1	G	212	GLY	2.4
2	N	196	GLY	2.4
1	M	154	LEU	2.4
1	I	147	GLN	2.4
2	J	36	TRP	2.4
1	M	41	GLY	2.4
1	I	35	TRP	2.4
2	P	36	TRP	2.4
1	K	152	ASN	2.3
2	N	197	THR	2.3
1	K	211	ARG	2.3
1	K	154	LEU	2.3
2	N	140	SER	2.3
1	K	116	PHE	2.3
2	N	1	GLU	2.3
1	C	212	GLY	2.2
1	O	88	CYS	2.2
2	B	134	SER	2.2
1	O	34	ALA	2.2
2	D	42	GLY	2.2
1	A	201	LEU	2.2
1	I	188	LYS	2.2
1	A	212	GLY	2.2
2	B	138	SER	2.2
2	D	1	GLU	2.2
1	O	69	THR	2.1
1	O	7	SER	2.1
1	I	191	VAL	2.1
2	L	180	GLY	2.1
2	P	79	LEU	2.1
1	M	193	ALA	2.1
2	P	61	ALA	2.1
1	K	155	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	31	SER	2.1
1	I	154	LEU	2.1
2	B	139	GLU	2.1
1	C	152	ASN	2.1
1	K	94	TRP	2.1
2	P	195	PHE	2.1
1	C	40	PRO	2.1
1	K	183	LYS	2.1
2	H	135	ARG	2.1
2	P	54	SER	2.0
2	P	53	PRO	2.0
2	D	97	ALA	2.0
2	F	178	SER	2.0
2	N	148	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.