



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 AM UTC

PDB ID : 3KYM / pdb_00003kym
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

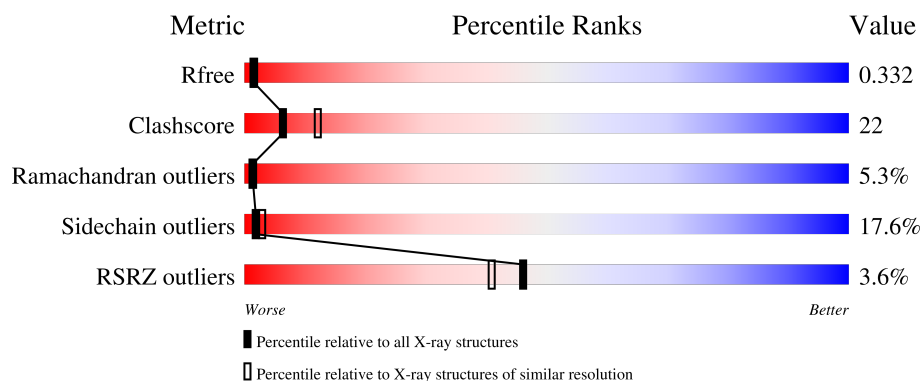
1 Overall quality at a glance

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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 59% 34% 6%
1	C	214	 60% 32% 7%
1	E	214	 58% 33% 8%
1	G	214	 64% 30% 5% •
1	I	214	 4% 54% 41% 5%

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Mol	Chain	Length	Quality of chain
1	K	214	
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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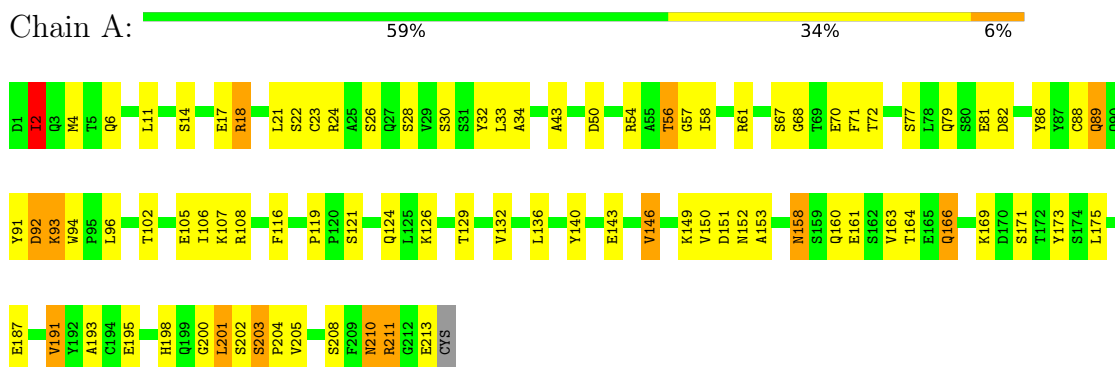
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	219	Total	C	N	O	S	0	0	0
			1663	1051	281	324	7			
2	P	219	Total	C	N	O	S	0	0	0
			1657	1048	278	324	7			

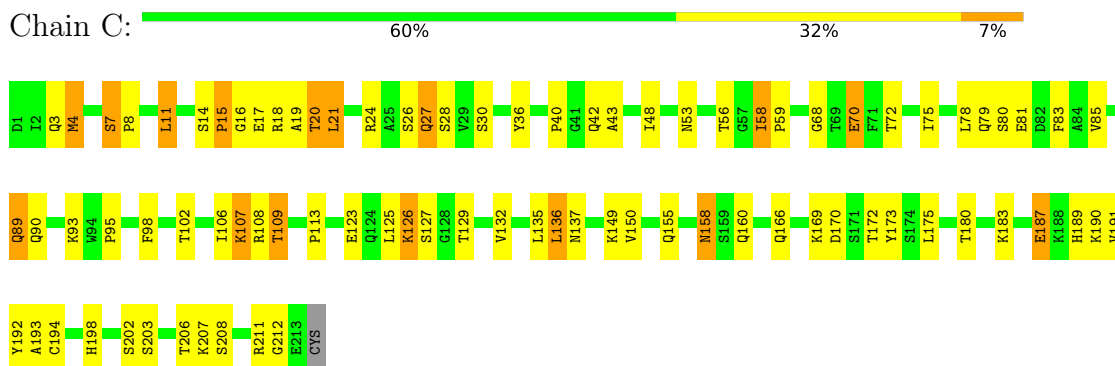
3 Residue-property plots [i](#)

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

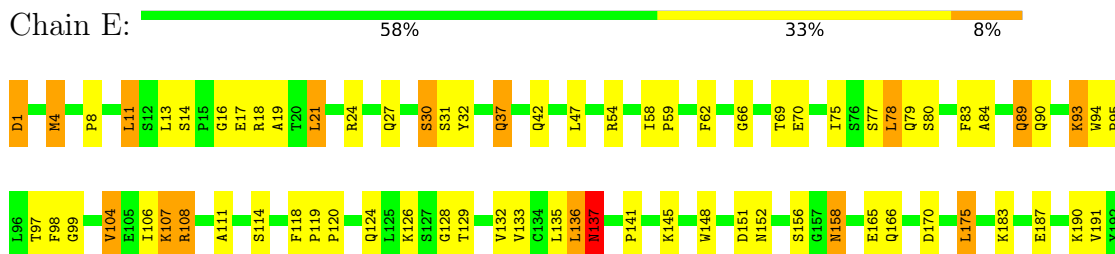
• Molecule 1: Light Chain Li33 IgG2



• Molecule 1: Light Chain Li33 IgG2



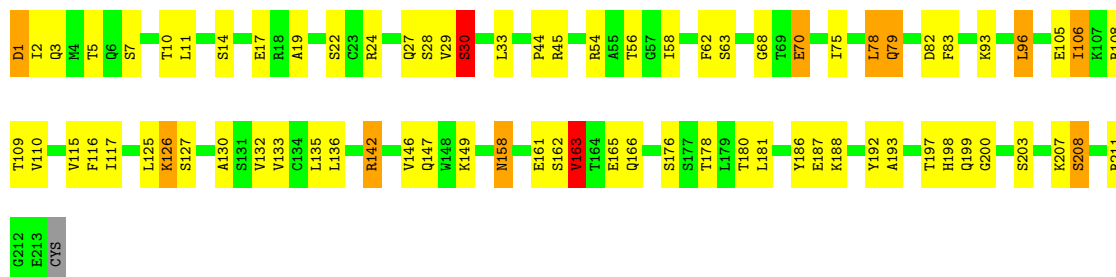
• Molecule 1: Light Chain Li33 IgG2





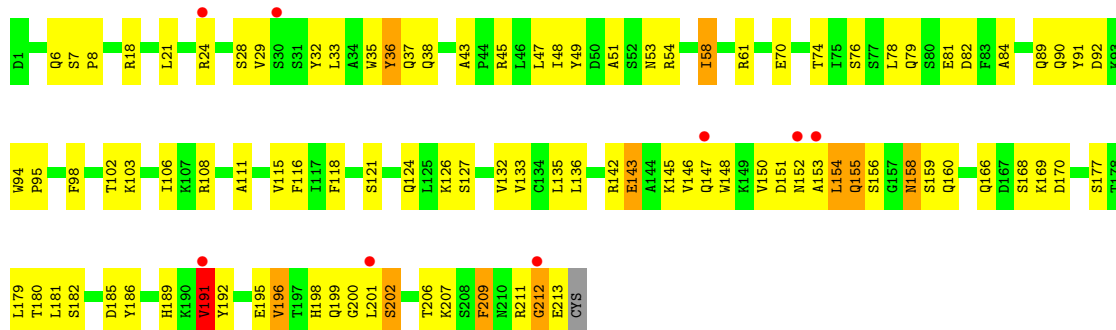
• Molecule 1: Light Chain Li33 IgG2

Chain G: 64% 30% 5% •



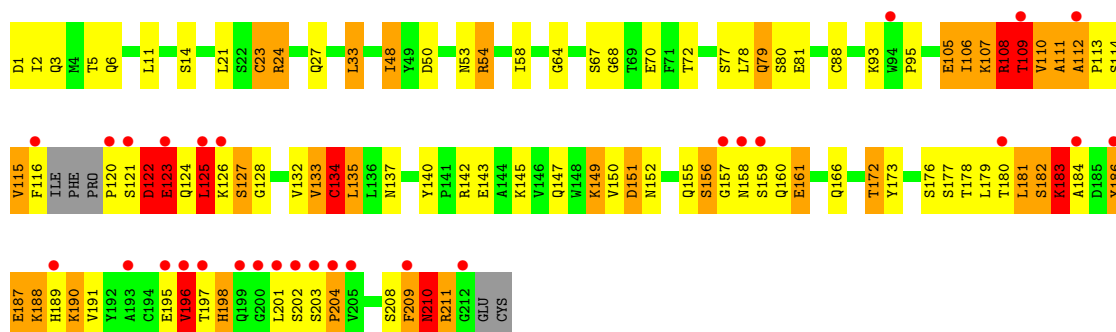
• Molecule 1: Light Chain Li33 IgG2

Chain I: 4% 54% 41% 5%



• Molecule 1: Light Chain Li33 IgG2

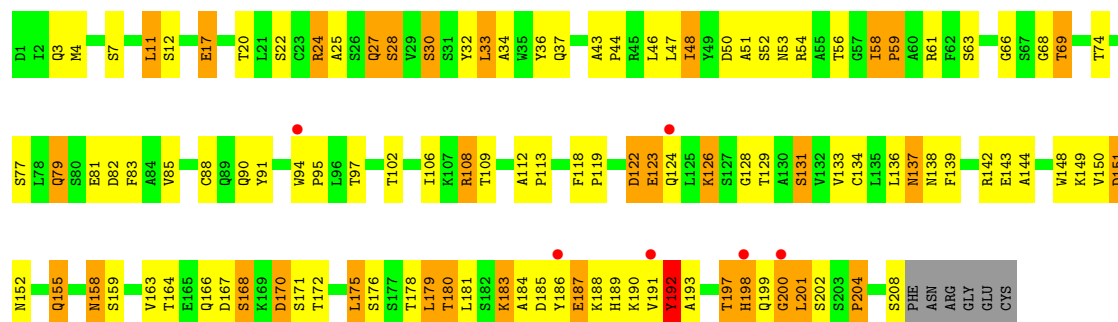
Chain K: 14% 50% 29% 14% • •



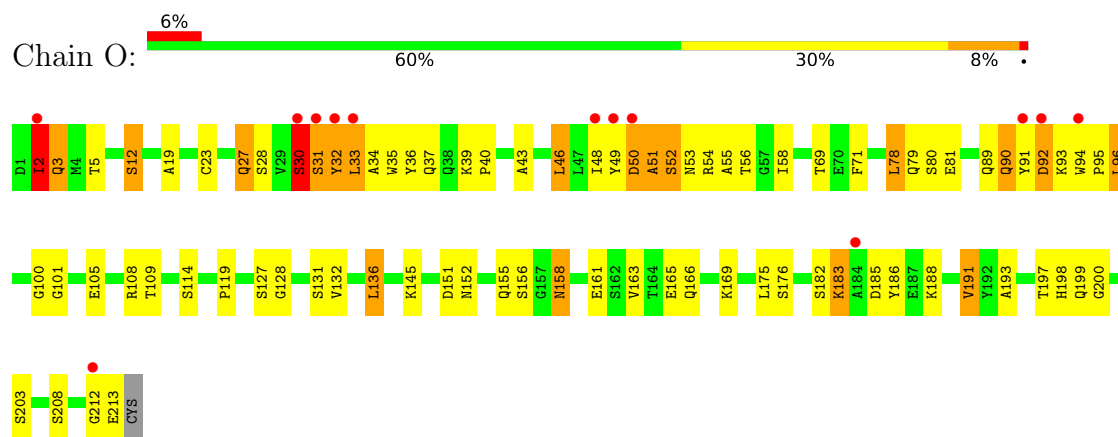
• Molecule 1: Light Chain Li33 IgG2

Chain M: 3% 44% 37% 15% •

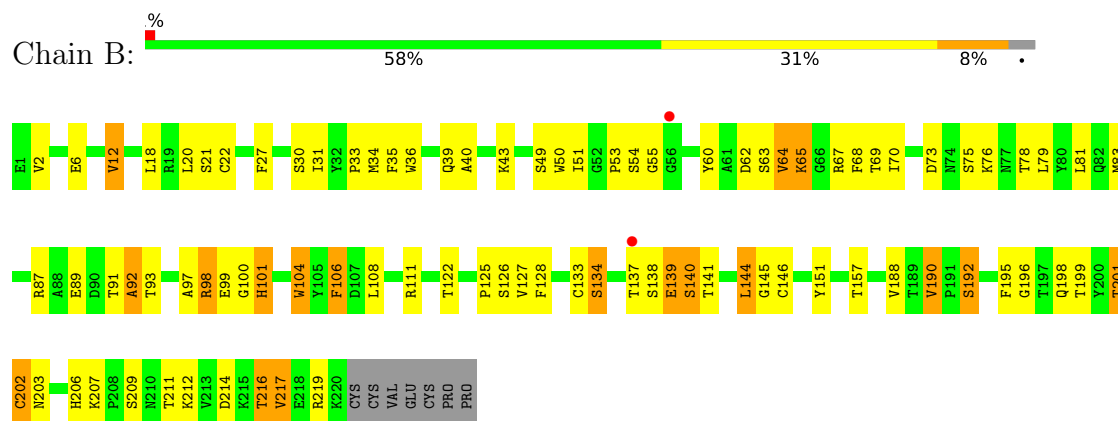




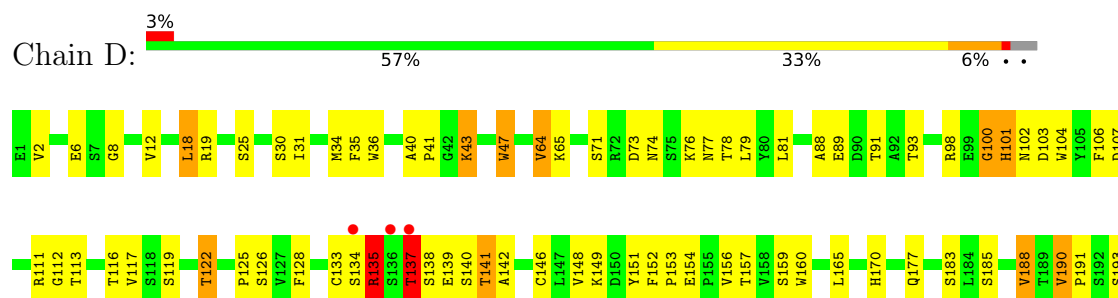
• Molecule 1: Light Chain Li33 IgG2



• Molecule 2: Heavy Chain Li33 IgG2

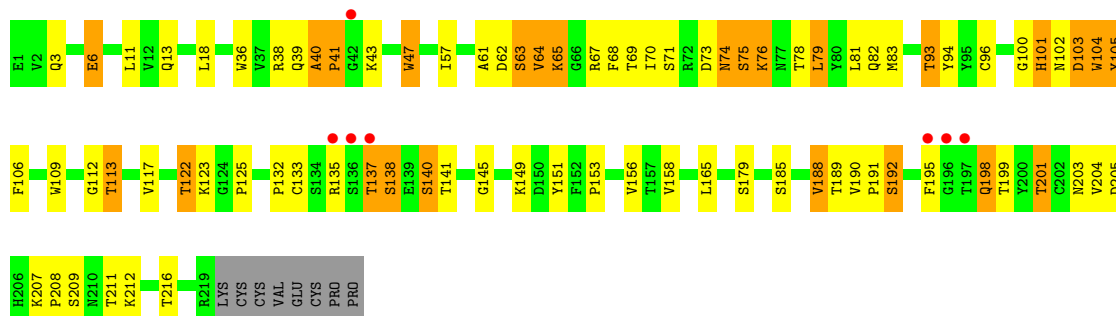


• Molecule 2: Heavy Chain Li33 IgG2

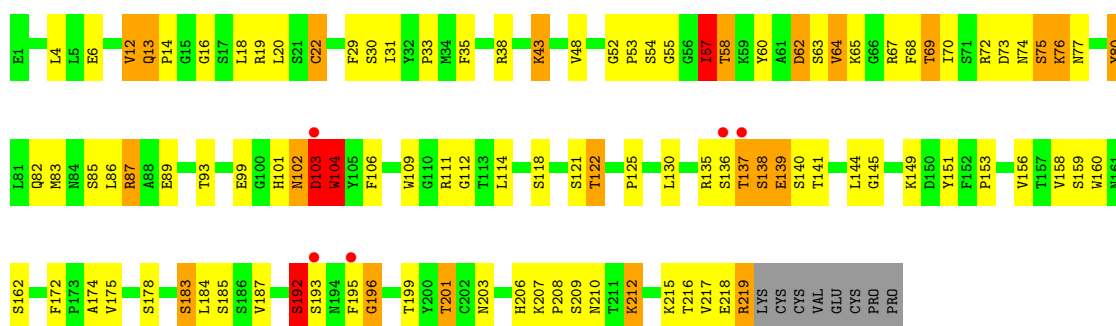




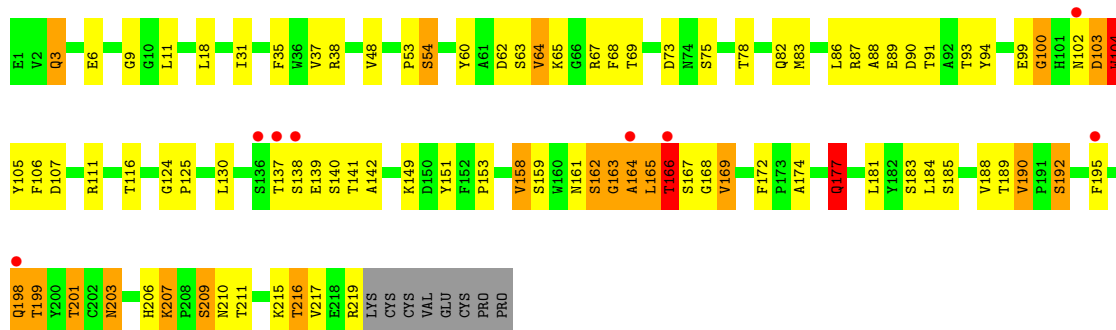
• Molecule 2: Heavy Chain Li33 IgG2



• Molecule 2: Heavy Chain Li33 IgG2

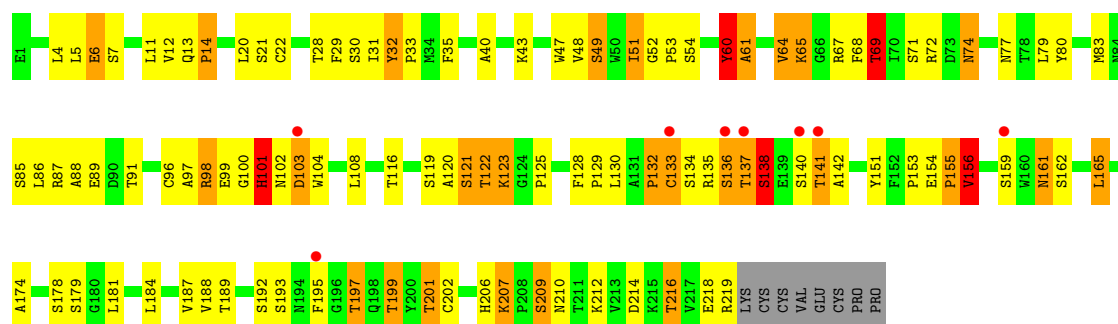


• Molecule 2: Heavy Chain Li33 IgG2

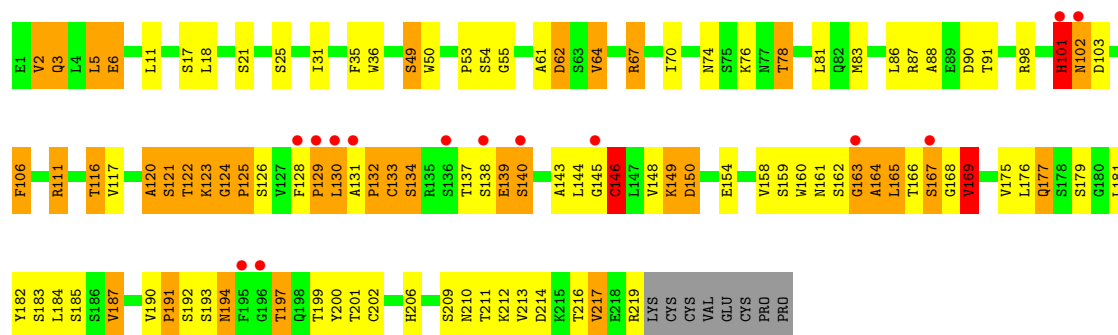


• Molecule 2: Heavy Chain Li33 IgG2

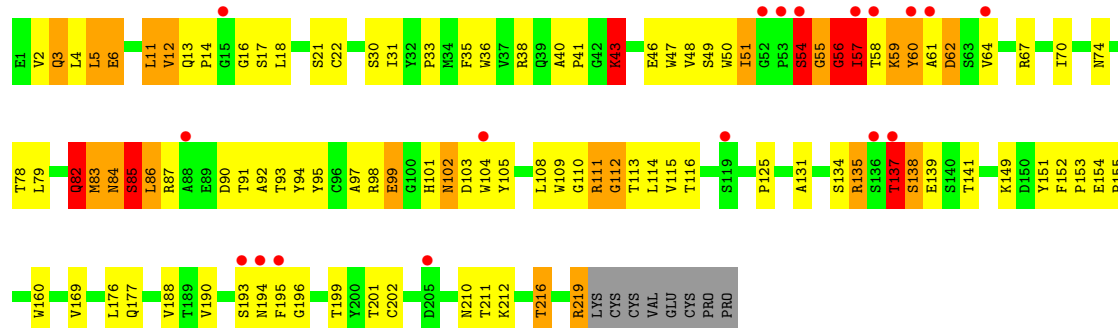




● Molecule 2: Heavy Chain Li33 IgG2



● 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 19.96 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.96-2.62) 96.8 (19.96-2.62)	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)	0.31 , 46.8	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	0.74	0/1676	1.07	6/2275 (0.3%)
1	C	0.69	0/1676	1.00	5/2275 (0.2%)
1	E	0.77	0/1676	1.03	3/2275 (0.1%)
1	G	0.81	0/1676	1.04	4/2275 (0.2%)
1	I	0.78	0/1676	1.09	7/2275 (0.3%)
1	K	0.84	2/1638 (0.1%)	1.17	10/2220 (0.5%)
1	M	0.74	0/1632	1.10	12/2217 (0.5%)
1	O	0.75	0/1676	1.05	3/2275 (0.1%)
2	B	0.75	0/1716	1.09	8/2338 (0.3%)
2	D	0.73	0/1716	1.00	5/2338 (0.2%)
2	F	0.78	0/1707	1.08	8/2327 (0.3%)
2	H	0.80	0/1707	1.08	3/2327 (0.1%)
2	J	0.80	0/1707	1.02	2/2327 (0.1%)
2	L	0.76	0/1707	1.09	7/2327 (0.3%)
2	N	0.75	2/1707 (0.1%)	1.09	5/2327 (0.2%)
2	P	0.81	0/1701	1.08	12/2320 (0.5%)
All	All	0.77	4/26994 (0.0%)	1.07	100/36718 (0.3%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	101	HIS	CA-C	6.10	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	108	ARG	CA-C	5.48	1.60	1.52
1	K	107	LYS	N-CA	5.31	1.52	1.45
2	N	122	THR	CA-CB	5.06	1.61	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	13	GLN	CA-C-N	8.83	130.88	119.84
2	P	13	GLN	C-N-CA	8.83	130.88	119.84
2	B	207	LYS	CA-C-N	-8.60	110.88	119.56
2	B	207	LYS	C-N-CA	-8.60	110.88	119.56
2	D	100	GLY	N-CA-C	8.13	123.17	112.77
1	A	43	ALA	CA-C-N	-7.98	112.49	120.31
1	A	43	ALA	C-N-CA	-7.98	112.49	120.31
1	C	58	ILE	CA-C-N	7.96	128.02	119.90
1	C	58	ILE	C-N-CA	7.96	128.02	119.90
1	K	125	LEU	N-CA-C	-7.67	102.57	112.23
1	C	43	ALA	CA-C-N	7.66	127.70	119.89
1	C	43	ALA	C-N-CA	7.66	127.70	119.89
2	H	89	GLU	N-CA-C	-6.92	102.96	113.89
1	K	133	VAL	CA-C-N	6.91	134.14	121.70
1	K	133	VAL	C-N-CA	6.91	134.14	121.70
1	O	43	ALA	CA-C-N	-6.89	113.56	120.31
1	O	43	ALA	C-N-CA	-6.89	113.56	120.31
1	M	192	TYR	N-CA-C	6.81	119.52	110.53
2	B	31	ILE	CB-CA-C	-6.69	103.28	112.04
1	G	163	VAL	N-CA-C	6.54	118.20	108.46
2	L	13	GLN	CA-C-N	6.52	127.99	119.84
2	L	13	GLN	C-N-CA	6.52	127.99	119.84
1	O	101	GLY	N-CA-C	6.37	118.00	111.95
2	F	40	ALA	CA-C-N	6.17	127.56	119.84
2	F	40	ALA	C-N-CA	6.17	127.56	119.84
2	D	103	ASP	N-CA-C	6.09	116.28	108.24
2	D	217	VAL	N-CA-C	6.04	116.21	108.12
1	K	108	ARG	N-CA-C	6.02	123.63	110.80
1	I	209	PHE	N-CA-C	6.01	117.99	108.79
1	I	196	VAL	N-CA-C	5.99	116.50	107.75
2	B	145	GLY	N-CA-C	5.99	118.94	110.74
2	L	218	GLU	N-CA-C	5.97	119.61	110.36
1	I	58	ILE	CA-C-N	5.96	127.29	119.84
1	I	58	ILE	C-N-CA	5.96	127.29	119.84
2	N	197	THR	N-CA-C	-5.94	106.19	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	192	SER	N-CA-C	5.89	123.36	110.80
2	D	43	LYS	N-CA-C	5.89	118.83	109.65
1	E	203	SER	N-CA-C	5.87	113.42	108.13
1	K	123	GLU	N-CA-C	5.82	115.69	108.19
2	B	192	SER	N-CA-C	5.76	123.06	110.80
1	M	66	GLY	N-CA-C	5.74	118.97	110.60
1	A	72	THR	N-CA-C	5.73	117.74	108.34
2	P	82	GLN	CA-C-N	5.72	131.99	121.70
2	P	82	GLN	C-N-CA	5.72	131.99	121.70
1	K	107	LYS	N-CA-C	5.70	117.84	109.24
1	K	201	LEU	N-CA-C	5.69	116.42	108.00
1	K	108	ARG	CA-C-N	5.68	131.92	121.70
1	K	108	ARG	C-N-CA	5.68	131.92	121.70
1	M	122	ASP	N-CA-C	-5.67	102.25	110.64
2	J	165	LEU	N-CA-C	-5.65	103.81	111.55
2	B	31	ILE	N-CA-C	5.55	116.20	110.82
2	F	13	GLN	CA-C-N	5.55	125.55	119.89
2	F	13	GLN	C-N-CA	5.55	125.55	119.89
1	M	179	LEU	CA-C-N	5.55	131.69	121.70
1	M	179	LEU	C-N-CA	5.55	131.69	121.70
1	G	2	ILE	N-CA-C	5.52	116.20	109.30
1	A	161	GLU	N-CA-C	5.51	117.56	109.24
1	G	63	SER	N-CA-C	5.48	117.73	109.23
1	K	202	SER	N-CA-C	5.45	117.09	107.61
2	F	74	ASN	N-CA-C	5.43	117.06	111.03
1	M	179	LEU	N-CA-C	-5.43	100.85	109.59
2	P	3	GLN	N-CA-C	5.38	117.83	110.24
2	P	31	ILE	CB-CA-C	-5.38	104.97	112.02
1	A	201	LEU	N-CA-C	5.35	117.89	108.75
2	B	49	SER	N-CA-C	5.33	116.94	108.79
2	P	112	GLY	N-CA-C	5.32	118.69	111.72
2	P	56	GLY	CA-C-N	5.31	131.26	121.70
2	P	56	GLY	C-N-CA	5.31	131.26	121.70
2	D	64	VAL	N-CA-C	5.31	116.38	111.81
1	E	137	ASN	N-CA-C	5.31	118.46	109.76
2	F	145	GLY	N-CA-C	5.30	118.28	110.80
2	L	32	TYR	CA-C-N	5.30	125.76	120.14
2	L	32	TYR	C-N-CA	5.30	125.76	120.14
2	P	85	SER	CA-C-N	5.29	131.23	121.70
2	P	85	SER	C-N-CA	5.29	131.23	121.70
2	F	3	GLN	N-CA-C	5.29	117.12	108.76
2	N	146	CYS	N-CA-C	5.29	116.86	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	165	GLU	N-CA-C	-5.28	103.92	110.41
2	B	12	VAL	N-CA-C	5.26	115.85	108.17
1	I	43	ALA	CA-C-N	-5.25	115.17	120.21
1	I	43	ALA	C-N-CA	-5.25	115.17	120.21
2	L	60	TYR	N-CA-C	5.23	121.95	110.80
1	M	43	ALA	CA-C-N	-5.18	113.37	119.84
1	M	43	ALA	C-N-CA	-5.18	113.37	119.84
2	N	102	ASN	N-CA-C	5.17	122.50	114.64
2	H	175	VAL	CB-CA-C	-5.16	103.82	110.84
2	N	124	GLY	CA-C-N	5.12	126.24	119.84
2	N	124	GLY	C-N-CA	5.12	126.24	119.84
1	M	178	THR	N-CA-C	5.11	116.51	107.61
1	A	71	PHE	N-CA-C	5.10	117.75	109.24
1	I	36	TYR	N-CA-C	5.08	116.66	108.34
1	M	190	LYS	N-CA-C	5.07	121.59	110.80
1	E	66	GLY	N-CA-C	5.06	117.45	111.63
1	M	58	ILE	CA-C-N	5.06	126.16	119.84
1	M	58	ILE	C-N-CA	5.06	126.16	119.84
2	J	177	GLN	N-CA-C	5.05	116.46	110.19
2	L	32	TYR	N-CA-C	5.04	116.84	109.84
2	F	117	VAL	N-CA-C	5.03	114.81	107.37
1	C	160	GLN	N-CA-C	5.02	116.48	107.80
2	P	57	ILE	N-CA-CB	5.01	120.02	111.50

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	58	0
1	E	1640	0	1589	69	0
1	G	1640	0	1589	47	0
1	I	1640	0	1589	77	0
1	K	1605	0	1556	120	0
1	M	1597	0	1552	116	0
1	O	1640	0	1589	73	0
2	B	1672	0	1622	60	0
2	D	1672	0	1622	58	0
2	F	1663	0	1609	63	0
2	H	1663	0	1609	85	0
2	J	1663	0	1609	79	0
2	L	1663	0	1609	86	0
2	N	1663	0	1609	113	0
2	P	1657	0	1598	103	0
All	All	26358	0	25529	1146	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 22.

All (1146) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:94:TRP:NE1	2:J:104:TRP:HE1	1.58	0.99
2:L:30:SER:HA	2:L:74:ASN:ND2	1.77	0.99
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:HD22	2:L:161:ASN:H	1.08	0.94
2:N:130:LEU:CD1	2:N:160:TRP:CH2	2.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:35:PHE:HE2	2:B:99:GLU:HB3	1.37	0.87
2:B:201:THR:HG22	2:B:216:THR:HB	1.55	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:HH21	1:M:24:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:20:LEU:HG	2:B:83:MET:HE2	1.62	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:HG12	1:K:115:VAL:O	1.80	0.79
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
1:M:4:MET:HE2	1:M:90:GLN:HB3	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:36:TYR:HH	2:D:106:PHE:HD2	1.33	0.75
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:HE3	2:J:104:TRP:H	1.34	0.75
2:L:161:ASN:HD22	2:L:161:ASN:N	1.85	0.74
1:I:150:VAL:HB	1:I:155:GLN:CD	2.12	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
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:F:73:ASP:CG	2:F:76:LYS:HG3	2.14	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:HH21	1:K:108:ARG:CG	2.00	0.72
1:O:158:ASN:HD22	1:O:158:ASN:H	1.35	0.72
1:G:158:ASN:H	1:G:158:ASN:HD22	1.36	0.72
2:H:80:TYR:HE2	2:N:102:ASN:CG	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:SER:HA	1:I:8:PRO:C	2.13	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
2:F:73:ASP:C	2:F:76:LYS:HG2	2.16	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:HG13	1:M:150:VAL:O	1.91	0.70
2:D:199:THR:OG1	1:K:125:LEU:HB2	1.91	0.70
1:C:158:ASN:HD22	1:C:158:ASN:H	1.39	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
2:F:198:GLN:HA	2:F:198:GLN:NE2	2.06	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:C:19:ALA:CB	1:C:78:LEU:HD21	2.22	0.69
1:E:158:ASN:HD22	1:E:158:ASN:N	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
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:166:THR:OG1	2:J:167:SER:N	2.22	0.69
2:J:189:THR:O	2:J:190:VAL:HG13	1.93	0.69
1:G:62:PHE:CE1	1:G:75:ILE:HG12	2.27	0.69
2:J:103:ASP:O	2:J:105:TYR:N	2.23	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:51:ILE:HD13	2:P:59:LYS:HB2	1.76	0.68
2:P:137:THR:HB	2:P:139:GLU:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:186:TYR:CE1	1:K:187:GLU:HG2	2.29	0.68
2:N:101:HIS:C	2:N:103:ASP:HB2	2.11	0.68
1:M:119:PRO:HD3	2:N:133:CYS:HB2	1.74	0.68
1:M:124:GLN:HA	1:M:124:GLN:NE2	2.09	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:L:103:ASP:O	2:L:104:TRP:HB2	1.93	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:HD23	1:M:179:LEU:H	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
2:L:97:ALA:O	2:L:98:ARG:HB3	1.94	0.67
1:M:155:GLN:HE21	1:M:155:GLN:HA	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:HD22	1:O:158:ASN:N	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:P:99:GLU:N	2:P:99:GLU:CD	2.50	0.66
2:L:161:ASN:ND2	2:L:161:ASN:N	2.39	0.66
1:A:79:GLN:NE2	1:O:81:GLU:HG2	2.10	0.66
1:A:198:HIS:CD2	1:A:200:GLY:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:80:TYR:CE2	2:N:102:ASN:CG	2.74	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
1:K:106:ILE:HG22	1:K:107:LYS:N	2.07	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
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
1:K:64:GLY:HA2	1:K:72:THR:O	1.98	0.64
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
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
2:H:76:LYS:CD	1:M:32:TYR:CE2	2.80	0.63
1:I:147:GLN:HB3	1:I:195:GLU:HB3	1.81	0.63
2:F:75:SER:C	2:F:76:LYS:HD3	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:49:TYR:HB2	1:O:54:ARG:C	2.24	0.63
1:E:4:MET:HE2	1:E:90:GLN:HB3	1.80	0.62
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:D:19:ARG:HD3	2:P:102:ASN:CG	2.25	0.62
2:J:3:GLN:HE21	2:J:3:GLN:HA	1.64	0.62
2:L:31:ILE:O	2:L:53:PRO:HB3	1.99	0.62
2:L:123:LYS:O	2:L:151:TYR:HA	2.00	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
2:F:62:ASP:C	2:F:64:VAL:H	2.08	0.62
1:O:165:GLU:OE1	1:O:165:GLU:HA	1.99	0.62
2:J:60:TYR:HE1	2:J:68:PHE:O	1.84	0.61
1:M:155:GLN:HE21	1:M:155:GLN:CA	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
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:CG1	1:E:104:VAL:O	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
1:E:183:LYS:HG2	1:E:187:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:98:ARG:HH21	2:D:107:ASP:CG	2.09	0.60
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:L:155:PRO:O	2:L:156:VAL:HB	2.00	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
2:F:74:ASN:C	2:F:76:LYS:H	2.09	0.59
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:O	1:I:143:GLU:HG3	2.02	0.59
1:K:155:GLN:HG2	1:K:156:SER:N	2.17	0.59
1:E:203:SER:HB2	1:E:204:PRO:HD2	1.84	0.59
1:G:125:LEU:C	1:G:127:SER:H	2.10	0.59
2:H:99:GLU:OE2	2:H:103:ASP:HB3	2.03	0.59
2:D:78:THR:HG21	1:O:93:LYS:HZ3	1.67	0.59
1:A:79:GLN:NE2	1:O:81:GLU:H	2.01	0.59
1:G:62:PHE:CD1	1:G:75:ILE:HG12	2.38	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:11:LEU:CD2	2:F:122:THR:HG22	2.32	0.58
2:F:106:PHE:HD2	2:F:109:TRP:CZ2	2.21	0.58
1:E:93:LYS:HB2	1:E:93:LYS:NZ	2.18	0.58
1:E:104:VAL:O	1:E:104:VAL:HG13	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:130:LEU:HD22	2:N:217:VAL:CG1	2.25	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
2:P:54:SER:O	2:P:55:GLY:C	2.47	0.58
1:K:187:GLU:OE1	1:K:187:GLU:HA	2.03	0.58
1:M:192:TYR:O	1:M:208:SER:HA	2.03	0.58
1:M:198:HIS:O	1:M:200:GLY:N	2.37	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:HD1	1:M:192:TYR:N	2.02	0.58
2:D:88:ALA:HA	2:D:117:VAL:HB	1.85	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
2:L:101:HIS:CG	2:L:102:ASN:N	2.72	0.58
2:P:83:MET:HE1	2:P:115:VAL:HG21	1.84	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:OD2	2:H:103:ASP:N	2.36	0.57
2:N:64:VAL:O	2:N:67:ARG:HG3	2.04	0.57
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
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:61:ALA:O	2:N:64:VAL:N	2.33	0.57
2:N:111:ARG:HG3	2:N:111:ARG:HH11	1.67	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
1:I:94:TRP:CE2	2:J:104:TRP:CD1	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:120:ALA:O	2:L:121:SER:C	2.47	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:HG2	1:K:108:ARG:NH2	2.05	0.56
2:L:179:SER:HB3	2:L:181:LEU:HD12	1.86	0.56
2:N:209:SER:C	2:N:211:THR:H	2.10	0.56
2:B:62:ASP:C	2:B:64:VAL:H	2.11	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
2:H:62:ASP:C	2:H:64:VAL:H	2.12	0.56
1:I:61:ARG:HH21	1:I:82:ASP:CG	2.12	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:34:MET:HB3	2:D:79:LEU:HD22	1.87	0.56
2:D:137:THR:HA	2:D:138:SER:HB3	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
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:HG12	2:P:64:VAL:O	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:L:51:ILE:HG21	2:L:72:ARG:HD2	1.88	0.56
2:N:194:ASN:CG	2:N:197:THR:HB	2.31	0.56
2:B:97:ALA:HB1	2:B:106:PHE:HB3	1.87	0.56
1:M:124:GLN:CD	2:N:128:PHE:CG	2.84	0.56
1:O:2:ILE:O	1:O:3:GLN:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:LEU:CD2	2:N:144:LEU:HB3	2.09	0.55
2:N:132:PRO:HD2	2:N:133:CYS:H	1.71	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: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:M:192:TYR:N	1:M:192:TYR:CD1	2.74	0.55
2:P:194:ASN:C	2:P:196:GLY:H	2.15	0.55
1:A:79:GLN:HE22	1:O:81:GLU:H	1.55	0.55
1:A:106:ILE:H	1:A:166:GLN:NE2	2.04	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:OD2	2:F:103:ASP:N	2.41	0.54
1:G:115:VAL:CG1	1:G:207:LYS:HG2	2.37	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
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:30:SER:CB	2:L:74:ASN:ND2	2.70	0.54
2:L:206:HIS:CD2	2:L:209:SER:HB2	2.43	0.54
2:P:110:GLY:O	2:P:111:ARG:HG3	2.07	0.54
1:G:125:LEU:C	1:G:127:SER:N	2.65	0.54
2:J:53:PRO:O	2:J:54:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:ARG:NH2	1:I:82:ASP:OD1	2.35	0.54
1:I:148:TRP:CE3	1:I:179:LEU:HD22	2.42	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:A:175:LEU:C	1:A:175:LEU:HD23	2.33	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:H:4:LEU:HD22	2:H:22:CYS:SG	2.48	0.53
1:K:108:ARG:HD3	1:K:108:ARG:C	2.33	0.53
2:L:51:ILE:HG23	2:L:52:GLY:O	2.08	0.53
2:F:76:LYS:HD2	1:I:32:TYR:OH	2.08	0.53
1:M:124:GLN:CD	2:N:128:PHE:CD2	2.87	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
2:J:198:GLN:O	2:J:199:THR:C	2.51	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
1:M:198:HIS:C	1:M:200:GLY:H	2.17	0.53
2:D:122:THR:CG2	2:P:74:ASN:HB3	2.37	0.53
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
1:E:198:HIS:HD2	1:E:200:GLY:H	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:N:111:ARG:CG	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:H:76:LYS:HD2	1:M:32:TYR:CE2	2.44	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
1:E:196:VAL:O	1:E:204:PRO:HA	2.09	0.52
1:M:47:LEU:HA	1:M:58:ILE:HG13	1.90	0.52
1:M:155:GLN:HA	1:M:155:GLN:NE2	2.23	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:O:49:TYR:H	1:O:53:ASN:C	2.18	0.52
1:E:84:ALA:N	1:E:104:VAL:HG12	2.24	0.52
1:E:95:PRO:HB3	2:F:47:TRP:CZ3	2.43	0.52
1:E:108:ARG:NH1	1:E:111:ALA:HB2	2.24	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:K:145:LYS:HB2	1:K:198:HIS:HD1	1.74	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: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
2:N:102:ASN:H	2:N:103:ASP:CG	2.13	0.52
2:P:103:ASP:HB2	2:P:105:TYR:CE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:39:LYS:O	1:O:40:PRO:C	2.52	0.52
1:E:95:PRO:CB	2:F:47:TRP:CZ3	2.93	0.51
2:H:184:LEU:HD12	2:H:184:LEU:C	2.34	0.51
2:J:163:GLY:O	2:J:164:ALA:C	2.53	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
1:C:40:PRO:C	1:C:42:GLN:H	2.18	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:H:13:GLN:O	2:H:14:PRO:C	2.51	0.51
1:M:186:TYR:C	1:M:188:LYS:H	2.18	0.51
2:B:40:ALA:HB3	2:B:43:LYS:HD2	1.91	0.51
2:B:144:LEU:HD12	2:B:217:VAL:HG21	1.92	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
1:C:79:GLN:C	1:C:81:GLU:H	2.19	0.51
2:B:60:TYR:CE1	2:B:69:THR:HA	2.45	0.51
1:M:152:ASN:CG	1:M:152:ASN:O	2.54	0.51
2:N:130:LEU:HG	2:N:145:GLY:CA	2.40	0.51
2:P:219:ARG:O	2:P:219:ARG:NE	2.37	0.51
2:J:207:LYS:H	2:J:207:LYS:HZ2	1.59	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:6:GLN:NE2	1:A:86:TYR:O	2.41	0.51
1:A:28:SER:HA	1:A:68:GLY:O	2.11	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
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.18	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:49:TYR:CD2	1:O:55:ALA:HA	2.46	0.51
1:O:108:ARG:HG2	1:O:109:THR:N	2.26	0.51
2:F:201:THR:HA	2:F:216:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:VAL:HG12	1:G:207:LYS:HG2	1.92	0.51
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:D:193:SER:C	2:D:195:PHE:H	2.19	0.50
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:O	1:I:191:VAL:HG13	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
2:H:101:HIS:O	2:H:102:ASN:C	2.54	0.50
2:L:20:LEU:O	2:L:80:TYR:HA	2.12	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:O:31:SER:C	1:O:33:LEU:H	2.19	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:H:218:GLU:O	2:H:219:ARG:C	2.54	0.50
2:J:64:VAL:HG13	2:J:68:PHE:HB2	1.92	0.50
2:N:102:ASN:O	2:N:102:ASN:ND2	2.44	0.50
1:A:210:ASN:H	1:A:210:ASN:ND2	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:K:159:SER:HB2	1:K:160:GLN:C	2.36	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:I:90:GLN:C	1:I:90:GLN:CD	2.79	0.49
1:O:19:ALA:HB2	1:O:78:LEU:HD21	1.94	0.49
1:O:32:TYR:HA	1:O:50:ASP:OD1	2.12	0.49
1:O:90:GLN:HG2	1:O:91:TYR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:PHE:HB2	1:K:211:ARG:HG3	1.94	0.49
1:G:125:LEU:HD23	1:G:130:ALA:HB2	1.93	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
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
2:N:184:LEU:C	2:N:184:LEU:HD12	2.37	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
2:L:65:LYS:C	2:L:67:ARG:H	2.20	0.49
1:M:7:SER:O	1:M:22:SER:HB2	2.11	0.49
2:P:59:LYS:C	2:P:60:TYR:HD2	2.20	0.49
1:C:15:PRO:C	1:C:17:GLU:H	2.21	0.49
1:C:24:ARG:CG	1:C:70:GLU:HG2	2.42	0.49
1:C:125:LEU:O	1:C:127:SER:N	2.46	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
1:M:150:VAL:O	1:M:151:ASP:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:E:13:LEU:O	1:E:107:LYS:N	2.45	0.48
1:G:135:LEU:C	1:G:136:LEU:HD23	2.39	0.48
2:J:137:THR:CA	2:J:138:SER:HB3	2.34	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
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:2:ILE:HD12	1:K:2:ILE:H	1.79	0.48
1:K:145:LYS:HD2	1:K:198:HIS:ND1	2.29	0.48
2:N:123:LYS:HD2	2:N:124:GLY:H	1.79	0.48
1:C:125:LEU:C	1:C:127:SER:H	2.21	0.48
2:J:68:PHE:CD2	2:J:83:MET:HG2	2.48	0.48
2:P:54:SER:O	2:P:56:GLY:N	2.47	0.48
2:P:176:LEU:HD23	2:P:177:GLN:O	2.13	0.48
1:A:34:ALA:O	1:A:88:CYS:HA	2.14	0.48
1:A:146:VAL:HA	1:A:195:GLU:O	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:81:GLU:CD	1:K:81:GLU:H	2.22	0.48
1:K:181:LEU:CG	1:K:182:SER:H	2.25	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: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
1:I:94:TRP:H	1:I:94:TRP:CD1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:129:PRO:O	2:N:130:LEU:C	2.56	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
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:94:TRP:HA	1:I:95:PRO:O	2.14	0.47
1:I:201:LEU:O	1:I:202:SER:CB	2.63	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
2:H:18:LEU:HB2	2:H:83:MET:HE3	1.96	0.47
1:K:108:ARG:CG	1:K:108:ARG:NH2	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:C:150:VAL:HB	1:C:155:GLN:NE2	2.29	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
2:H:207:LYS:N	2:H:208:PRO:CD	2.78	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
2:B:195:PHE:O	2:B:196:GLY:C	2.58	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
1:M:126:LYS:C	1:M:126:LYS:HE2	2.40	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:4:MET:HE3	1:A:23:CYS:SG	2.55	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: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
2:B:97:ALA:O	2:B:98:ARG:CB	2.50	0.46
2:B:190:VAL:O	2:B:195:PHE:HZ	1.98	0.46
1:E:193:ALA:CB	1:E:208:SER:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:LEU:HD11	2:P:108:LEU:O	2.16	0.46
2:P:104:TRP:HA	2:P:104:TRP:CE3	2.50	0.46
1:A:56:THR:HG23	1:A:57:GLY:N	2.29	0.46
1:C:83:PHE:CD2	1:C:106:ILE:HG12	2.51	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:N	1:E:21:LEU:CD1	2.78	0.46
2:F:140:SER:O	2:F:192:SER:OG	2.33	0.46
1:G:1:ASP:OD1	1:G:1:ASP:C	2.57	0.46
2:L:32:TYR:HA	2:L:33:PRO:HD3	1.78	0.46
2:F:62:ASP:C	2:F:64:VAL:N	2.70	0.46
1:I:159:SER:O	1:I:160:GLN:HG3	2.15	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
2:J:163:GLY:O	2:J:165:LEU:N	2.48	0.46
1:M:186:TYR:O	1:M:188:LYS:N	2.41	0.46
2:N:61:ALA:O	2:N:62:ASP:C	2.59	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:L:102:ASN:CA	2:L:103:ASP:CB	2.75	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:HD12	1:K:2:ILE:N	2.31	0.46
2:P:125:PRO:CB	2:P:151:TYR:HB3	2.37	0.46
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.30	0.46
1:I:94:TRP:HA	1:I:95:PRO:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:163:GLY:O	2:N:164:ALA:HB2	2.16	0.46
1:E:203:SER:O	1:E:204:PRO:C	2.58	0.45
2:H:60:TYR:OH	2:H:70:ILE:N	2.36	0.45
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:J:169:VAL:H	2:J:188:VAL:HA	1.81	0.45
2:N:209:SER:C	2:N:211:THR:N	2.74	0.45
1:O:30:SER:HB3	1:O:31:SER:H	1.44	0.45
1:C:48:ILE:HG23	1:C:53:ASN:O	2.16	0.45
1:C:158:ASN:HD22	1:C:158:ASN:N	2.01	0.45
2:F:38:ARG:HD3	2:F:94:TYR:CE2	2.51	0.45
2:F:76:LYS:CD	1:I:32:TYR:OH	2.64	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:4:MET:CE	1:M:90:GLN:HB3	2.43	0.45
1:M:179:LEU:HA	1:M:180:THR:HB	1.99	0.45
2:D:19:ARG:NH1	2:P:102:ASN:OD1	2.50	0.45
2:D:152:PHE:HA	2:D:153:PRO:HA	1.73	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:CD1	2:B:106:PHE:N	2.85	0.45
1:I:47:LEU:HD23	1:I:58:ILE:HD12	1.99	0.45
1:I:48:ILE:HA	1:I:53:ASN:O	2.16	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
1:M:27:GLN:O	1:M:28:SER:C	2.59	0.45
2:P:104:TRP:HA	2:P:104:TRP:HE3	1.81	0.45
1:E:175:LEU:C	1:E:175:LEU:HD23	2.42	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
2:P:59:LYS:C	2:P:60:TYR:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:126:SER:HB2	2:N:128:PHE:HE2	1.82	0.45
1:O:36:TYR:OH	1:O:89:GLN:NE2	2.50	0.45
1:O:136:LEU:N	1:O:136:LEU:HD23	2.32	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:36:TYR:HA	1:I:45:ARG:O	2.17	0.44
1:I:108:ARG:NH1	1:I:111:ALA:HB2	2.32	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
1:M:198:HIS:C	1:M:200:GLY:N	2.75	0.44
2:N:137:THR:HA	2:N:138:SER:HA	1.74	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
1:K:197:THR:C	1:K:198:HIS:CG	2.94	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
2:F:70:ILE:HD11	2:F:79:LEU:HD11	1.99	0.44
2:H:53:PRO:O	2:H:72:ARG:HD3	2.17	0.44
2:H:62:ASP:C	2:H:64:VAL:N	2.76	0.44
2:H:174:ALA:HA	2:H:184:LEU:HB3	1.99	0.44
2:B:137:THR:HB	2:B:138:SER:C	2.43	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:54:ARG:HB3	1:O:58:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:151:ASP:HA	1:O:191:VAL:HG12	2.00	0.44
1:K:48:ILE:HA	1:K:53:ASN:O	2.18	0.44
1:K:159:SER:HA	1:K:160:GLN:CB	2.40	0.44
1:O:46:LEU:HD23	1:O:55:ALA:HB2	1.99	0.44
2:B:65:LYS:C	2:B:67:ARG:H	2.25	0.44
2:D:198:GLN:NE2	1:M:61:ARG:HD3	2.32	0.44
2:H:35:PHE:CZ	2:H:104:TRP:NE1	2.84	0.44
2:J:88:ALA:C	2:J:90:ASP:H	2.26	0.44
1:K:183:LYS:C	1:K:186:TYR:CD2	2.95	0.44
2:N:191:PRO:O	2:N:193:SER:N	2.51	0.44
1:O:55:ALA:O	1:O:56:THR:C	2.61	0.44
1:E:95:PRO:HB3	2:F:47:TRP:HZ3	1.83	0.44
1:E:203:SER:HB2	1:E:204:PRO:CD	2.48	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
2:L:100:GLY:O	2:L:101:HIS:C	2.61	0.44
1:M:37:GLN:O	1:M:44:PRO:HA	2.18	0.44
1:M:149:LYS:HB2	1:M:193:ALA:HB3	2.00	0.44
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
1:C:27:GLN:O	1:C:28:SER:C	2.61	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:K:186:TYR:CD1	1:K:186:TYR:C	2.96	0.43
2:F:76:LYS:HD2	1:I:32:TYR:CE2	2.53	0.43
1:I:147:GLN:HE21	1:I:154:LEU:HD11	1.83	0.43
1:I:151:ASP:C	1:I:153:ALA:H	2.21	0.43
1:I:195:GLU:OE2	1:I:206:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:177:GLN:C	2:N:179:SER:N	2.76	0.43
1:O:193:ALA:CB	1:O:208:SER:HB3	2.48	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:N	1:K:210:ASN:ND2	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: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
1:K:186:TYR:C	1:K:186:TYR:HD1	2.27	0.43
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
2:B:50:TRP:CG	2:B:51:ILE:N	2.87	0.43
2:J:106:PHE:N	2:J:106:PHE:CD1	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:126:LYS:HE3	2:L:128:PHE:HE1	1.84	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:HA	1:C:125:LEU:HD23	1.76	0.42
1:I:108:ARG:HD2	1:I:170:ASP:O	2.19	0.42
1:I:115:VAL:C	1:I:116:PHE:CD1	2.97	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
1:M:143:GLU:CD	1:M:198:HIS:CG	2.97	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
2:J:64:VAL:O	2:J:65:LYS:C	2.61	0.42
1:M:124:GLN:CG	2:N:128:PHE:CG	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:183:LYS:O	1:O:186:TYR:N	2.52	0.42
2:P:6:GLU:H	2:P:6:GLU:HG2	1.47	0.42
2:P:50:TRP:CZ3	2:P:59:LYS:CG	3.01	0.42
2:P:86:LEU:HD23	2:P:86:LEU:HA	1.76	0.42
2:P:102:ASN:HD22	2:P:102:ASN:HA	1.64	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
2:B:18:LEU:CB	2:B:83:MET:HE3	2.49	0.42
1:G:125:LEU:O	1:G:126:LYS:C	2.62	0.42
2:L:22:CYS:HB3	2:L:79:LEU:HB3	2.00	0.42
1:M:50:ASP:O	1:M:51:ALA:HB3	2.19	0.42
1:M:124:GLN:HG3	2:N:128:PHE:CG	2.54	0.42
2:B:35:PHE:CZ	2:B:104:TRP:CD1	3.08	0.42
2:B:62:ASP:C	2:B:64:VAL:N	2.77	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
1:E:170:ASP:C	1:E:170:ASP:OD1	2.61	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:151:ASP:O	1:M:189:HIS:ND1	2.53	0.42
1:M:155:GLN:CA	1:M:155:GLN:NE2	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: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
2:N:214:ASP:OD1	2:N:214:ASP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:179:LEU:C	1:K:181:LEU:H	2.27	0.42
2:L:207:LYS:HA	2:L:207:LYS:HE2	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:F:65:LYS:C	2:F:67:ARG:H	2.28	0.41
2:F:198:GLN:CD	2:F:199:THR:H	2.28	0.41
1:G:10:THR:HG22	1:G:11:LEU:N	2.34	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
2:P:54:SER:C	2:P:56:GLY:N	2.77	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
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
1:C:189:HIS:O	1:C:211:ARG:HD3	2.20	0.41
2:D:133:CYS:C	2:D:135:ARG:H	2.28	0.41
1:E:30:SER:HB3	1:E:31:SER:H	1.73	0.41
1:E:136:LEU:HD11	1:E:196:VAL:CG1	2.49	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:20:LEU:HB2	2:B:81:LEU:HB3	2.03	0.41
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.02	0.41
2:H:137:THR:HB	2:H:139:GLU:CD	2.45	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
1:G:109:THR:O	1:G:110:VAL:C	2.63	0.41
2:H:195:PHE:O	2:H:196:GLY:C	2.63	0.41
2:J:87:ARG:O	2:J:90:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:TYR:OH	2:N:106:PHE:HD1	2.03	0.41
1:M:163:VAL:CG2	1:M:175:LEU:HG	2.43	0.41
2:N:160:TRP:O	2:N:161:ASN:C	2.63	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:C:175:LEU:C	1:C:175:LEU:HD23	2.45	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
1:A:96:LEU:HD11	2:B:104:TRP:HB3	2.02	0.41
1:A:210:ASN:H	1:A:210:ASN:HD22	1.68	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:I:211:ARG:O	1:I:213:GLU:N	2.53	0.41
1:K:122:ASP:OD1	1:K:123:GLU:N	2.54	0.41
1:M:54:ARG:HD3	1:M:59:PRO:O	2.21	0.41
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:HD12	1:M:46:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:140:SER:C	2:J:192:SER:HB2	2.47	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
1:O:95:PRO:O	1:O:96:LEU:C	2.64	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
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:C:20:THR:HG22	1:C:72:THR:HG21	2.03	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
1:K:208:SER:O	1:K:210:ASN:ND2	2.55	0.40
2:L:87:ARG:O	2:L:88:ALA:C	2.65	0.40
2:P:109:TRP:CD1	2:P:109:TRP:N	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%)	6	12
1	C	211/214 (99%)	183 (87%)	24 (11%)	4 (2%)	6	12
1	E	211/214 (99%)	195 (92%)	14 (7%)	2 (1%)	14	28
1	G	211/214 (99%)	190 (90%)	19 (9%)	2 (1%)	14	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	211/214 (99%)	183 (87%)	19 (9%)	9 (4%)	2	2
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	0
2	B	218/227 (96%)	185 (85%)	26 (12%)	7 (3%)	3	4
2	D	218/227 (96%)	187 (86%)	23 (11%)	8 (4%)	2	3
2	F	217/227 (96%)	191 (88%)	18 (8%)	8 (4%)	2	3
2	H	217/227 (96%)	184 (85%)	22 (10%)	11 (5%)	1	1
2	J	217/227 (96%)	178 (82%)	24 (11%)	15 (7%)	1	1
2	L	217/227 (96%)	175 (81%)	22 (10%)	20 (9%)	0	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%)	0	0
All	All	3415/3528 (97%)	2882 (84%)	351 (10%)	182 (5%)	1	1

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	149 (81%)	35 (19%)	1	2
1	C	184/185 (100%)	155 (84%)	29 (16%)	2	4
1	E	184/185 (100%)	151 (82%)	33 (18%)	2	3
1	G	184/185 (100%)	154 (84%)	30 (16%)	2	4
1	I	184/185 (100%)	159 (86%)	25 (14%)	3	6
1	K	180/185 (97%)	140 (78%)	40 (22%)	1	1
1	M	180/185 (97%)	142 (79%)	38 (21%)	1	1
1	O	184/185 (100%)	160 (87%)	24 (13%)	4	7
2	B	186/193 (96%)	155 (83%)	31 (17%)	2	3
2	D	186/193 (96%)	156 (84%)	30 (16%)	2	4
2	F	185/193 (96%)	154 (83%)	31 (17%)	2	3
2	H	185/193 (96%)	148 (80%)	37 (20%)	1	2
2	J	185/193 (96%)	153 (83%)	32 (17%)	2	3
2	L	185/193 (96%)	146 (79%)	39 (21%)	1	1
2	N	185/193 (96%)	151 (82%)	34 (18%)	1	2
2	P	184/193 (95%)	154 (84%)	30 (16%)	2	4
All	All	2945/3024 (97%)	2427 (82%)	518 (18%)	2	3

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	11	LEU
1	A	18	ARG
1	A	22	SER
1	A	26	SER
1	A	33	LEU
1	A	56	THR
1	A	67	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

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Mol	Chain	Res	Type
1	A	108	ARG
1	A	121	SER
1	A	126	LYS
1	A	129	THR
1	A	132	VAL
1	A	136	LEU
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	205	VAL
1	A	210	ASN
1	A	211	ARG
1	A	213	GLU
2	B	12	VAL
2	B	30	SER
2	B	64	VAL
2	B	65	LYS
2	B	75	SER
2	B	78	THR
2	B	87	ARG
2	B	93	THR
2	B	106	PHE
2	B	111	ARG
2	B	122	THR
2	B	126	SER
2	B	127	VAL
2	B	134	SER
2	B	139	GLU
2	B	144	LEU
2	B	146	CYS
2	B	157	THR
2	B	188	VAL
2	B	190	VAL
2	B	192	SER
2	B	198	GLN

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Mol	Chain	Res	Type
2	B	199	THR
2	B	201	THR
2	B	202	CYS
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	21	LEU
1	C	27	GLN
1	C	30	SER
1	C	56	THR
1	C	70	GLU
1	C	75	ILE
1	C	85	VAL
1	C	89	GLN
1	C	93	LYS
1	C	102	THR
1	C	107	LYS
1	C	109	THR
1	C	129	THR
1	C	132	VAL
1	C	136	LEU
1	C	149	LYS
1	C	158	ASN
1	C	169	LYS
1	C	180	THR
1	C	187	GLU
1	C	190	LYS
1	C	191	VAL
1	C	202	SER
1	C	203	SER
2	D	2	VAL
2	D	12	VAL
2	D	18	LEU
2	D	25	SER

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Mol	Chain	Res	Type
2	D	31	ILE
2	D	47	TRP
2	D	64	VAL
2	D	65	LYS
2	D	71	SER
2	D	89	GLU
2	D	111	ARG
2	D	119	SER
2	D	122	THR
2	D	126	SER
2	D	135	ARG
2	D	137	THR
2	D	141	THR
2	D	146	CYS
2	D	154	GLU
2	D	157	THR
2	D	183	SER
2	D	185	SER
2	D	188	VAL
2	D	190	VAL
2	D	197	THR
2	D	198	GLN
2	D	205	ASP
2	D	212	LYS
2	D	216	THR
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
1	E	37	GLN
1	E	42	GLN
1	E	70	GLU
1	E	78	LEU
1	E	79	GLN
1	E	80	SER
1	E	89	GLN
1	E	93	LYS
1	E	94	TRP

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Mol	Chain	Res	Type
1	E	97	THR
1	E	104	VAL
1	E	107	LYS
1	E	108	ARG
1	E	114	SER
1	E	133	VAL
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	6	GLU
2	F	47	TRP
2	F	57	ILE
2	F	63	SER
2	F	64	VAL
2	F	65	LYS
2	F	69	THR
2	F	71	SER
2	F	76	LYS
2	F	78	THR
2	F	79	LEU
2	F	93	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
2	F	185	SER
2	F	188	VAL
2	F	192	SER

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Mol	Chain	Res	Type
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	22	SER
1	G	27	GLN
1	G	30	SER
1	G	33	LEU
1	G	45	ARG
1	G	56	THR
1	G	70	GLU
1	G	78	LEU
1	G	79	GLN
1	G	93	LYS
1	G	96	LEU
1	G	106	ILE
1	G	108	ARG
1	G	132	VAL
1	G	142	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	180	THR
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	12	VAL
2	H	13	GLN
2	H	22	CYS
2	H	31	ILE
2	H	43	LYS
2	H	54	SER

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Mol	Chain	Res	Type
2	H	57	ILE
2	H	62	ASP
2	H	64	VAL
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	114	LEU
2	H	121	SER
2	H	122	THR
2	H	135	ARG
2	H	139	GLU
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	217	VAL
2	H	219	ARG
1	I	6	GLN
1	I	24	ARG
1	I	29	VAL
1	I	33	LEU
1	I	54	ARG
1	I	70	GLU
1	I	74	THR
1	I	78	LEU
1	I	79	GLN
1	I	81	GLU
1	I	89	GLN

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Mol	Chain	Res	Type
1	I	103	LYS
1	I	121	SER
1	I	126	LYS
1	I	132	VAL
1	I	142	ARG
1	I	143	GLU
1	I	145	LYS
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
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	64	VAL
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	149	LYS
2	J	166	THR
2	J	177	GLN
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

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Mol	Chain	Res	Type
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
1	K	21	LEU
1	K	23	CYS
1	K	24	ARG
1	K	27	GLN
1	K	33	LEU
1	K	48	ILE
1	K	50	ASP
1	K	54	ARG
1	K	67	SER
1	K	78	LEU
1	K	79	GLN
1	K	80	SER
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	124	GLN
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	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

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Mol	Chain	Res	Type
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	28	THR
2	L	49	SER
2	L	51	ILE
2	L	54	SER
2	L	64	VAL
2	L	65	LYS
2	L	69	THR
2	L	71	SER
2	L	74	ASN
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	156	VAL
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	216	THR
1	M	3	GLN

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Mol	Chain	Res	Type
1	M	11	LEU
1	M	17	GLU
1	M	20	THR
1	M	24	ARG
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	63	SER
1	M	69	THR
1	M	74	THR
1	M	79	GLN
1	M	81	GLU
1	M	97	THR
1	M	108	ARG
1	M	109	THR
1	M	126	LYS
1	M	129	THR
1	M	131	SER
1	M	136	LEU
1	M	137	ASN
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	187	GLU
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	6	GLU
2	N	11	LEU

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Mol	Chain	Res	Type
2	N	18	LEU
2	N	49	SER
2	N	64	VAL
2	N	67	ARG
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
2	N	140	SER
2	N	146	CYS
2	N	149	LYS
2	N	158	VAL
2	N	165	LEU
2	N	166	THR
2	N	167	SER
2	N	169	VAL
2	N	187	VAL
2	N	201	THR
2	N	202	CYS
2	N	212	LYS
2	N	216	THR
2	N	217	VAL
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	69	THR
1	O	71	PHE
1	O	78	LEU
1	O	79	GLN
1	O	80	SER
1	O	114	SER

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Mol	Chain	Res	Type
1	O	131	SER
1	O	132	VAL
1	O	136	LEU
1	O	156	SER
1	O	158	ASN
1	O	163	VAL
1	O	169	LYS
1	O	191	VAL
1	O	199	GLN
1	O	203	SER
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
2	P	54	SER
2	P	59	LYS
2	P	60	TYR
2	P	62	ASP
2	P	78	THR
2	P	82	GLN
2	P	87	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	79	GLN
1	A	89	GLN
1	A	158	ASN
1	A	198	HIS
1	A	210	ASN
2	B	74	ASN
2	B	77	ASN
2	B	170	HIS
2	B	206	HIS
1	C	37	GLN
1	C	89	GLN
1	C	137	ASN
1	C	147	GLN
1	C	155	GLN
1	C	158	ASN
1	C	198	HIS
2	D	74	ASN
2	D	177	GLN
2	D	194	ASN
2	D	198	GLN
2	D	206	HIS
1	E	27	GLN
1	E	42	GLN
1	E	79	GLN
1	E	89	GLN
1	E	137	ASN
1	E	158	ASN
1	E	166	GLN
1	E	198	HIS
1	E	210	ASN
2	F	3	GLN
2	F	102	ASN
2	F	177	GLN
2	F	198	GLN
2	F	206	HIS
2	F	210	ASN
1	G	27	GLN
1	G	79	GLN
1	G	158	ASN
1	G	166	GLN
1	G	198	HIS

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Mol	Chain	Res	Type
1	G	199	GLN
2	H	77	ASN
2	H	177	GLN
2	H	206	HIS
1	I	42	GLN
1	I	79	GLN
1	I	89	GLN
1	I	152	ASN
1	I	166	GLN
1	I	198	HIS
1	I	210	ASN
2	J	3	GLN
2	J	77	ASN
2	J	206	HIS
1	K	27	GLN
1	K	53	ASN
1	K	137	ASN
1	K	147	GLN
1	K	152	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
2	L	210	ASN
1	M	38	GLN
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	39	GLN
2	N	82	GLN
2	N	102	ASN

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Mol	Chain	Res	Type
2	N	170	HIS
1	O	38	GLN
1	O	42	GLN
1	O	79	GLN
1	O	89	GLN
1	O	137	ASN
1	O	155	GLN
1	O	158	ASN
1	O	166	GLN
1	O	198	HIS
2	P	3	GLN
2	P	82	GLN
2	P	177	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 oligosaccharides 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%)	-0.02	0 100 100	27, 47, 64, 73	0
1	C	213/214 (99%)	0.20	0 100 100	40, 57, 68, 75	0
1	E	213/214 (99%)	-0.22	0 100 100	25, 39, 53, 64	0
1	G	213/214 (99%)	-0.34	0 100 100	18, 35, 49, 66	0
1	I	213/214 (99%)	0.20	8 (3%) 44 39	18, 41, 74, 83	0
1	K	209/214 (97%)	0.56	29 (13%) 6 5	26, 49, 89, 100	0
1	M	208/214 (97%)	0.36	6 (2%) 53 48	33, 55, 72, 78	0
1	O	213/214 (99%)	0.26	13 (6%) 27 22	27, 46, 73, 83	0
2	B	220/227 (96%)	-0.00	2 (0%) 81 78	29, 47, 67, 76	0
2	D	220/227 (96%)	0.13	6 (2%) 56 51	37, 47, 70, 81	0
2	F	219/227 (96%)	0.08	7 (3%) 50 45	25, 42, 61, 73	0
2	H	219/227 (96%)	-0.03	5 (2%) 61 56	28, 38, 65, 72	0
2	J	219/227 (96%)	0.08	8 (3%) 45 40	26, 44, 67, 77	0
2	L	219/227 (96%)	0.31	8 (3%) 45 40	31, 50, 71, 85	0
2	N	219/227 (96%)	0.53	14 (6%) 25 21	32, 56, 80, 86	0
2	P	219/227 (96%)	0.39	18 (8%) 17 14	35, 51, 74, 78	0
All	All	3449/3528 (97%)	0.15	124 (3%) 46 41	18, 47, 72, 100	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	195	PHE	6.4
1	K	209	PHE	6.2
2	H	137	THR	5.1
2	N	145	GLY	4.7
1	O	30	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	136	SER	4.3
1	K	109	THR	4.3
1	M	191	VAL	4.3
2	F	197	THR	4.2
2	D	136	SER	4.1
2	N	136	SER	4.1
2	P	64	VAL	4.1
1	O	94	TRP	4.0
1	K	116	PHE	4.0
1	K	197	THR	4.0
2	F	137	THR	4.0
2	L	136	SER	4.0
1	K	125	LEU	3.9
2	F	196	GLY	3.9
1	O	32	TYR	3.9
1	O	92	ASP	3.9
2	P	137	THR	3.8
1	O	50	ASP	3.8
1	M	198	HIS	3.8
2	J	137	THR	3.8
1	I	201	LEU	3.8
1	K	189	HIS	3.8
2	N	102	ASN	3.7
2	P	136	SER	3.6
1	K	195	GLU	3.6
2	N	196	GLY	3.5
1	O	91	TYR	3.5
1	O	49	TYR	3.5
2	P	61	ALA	3.5
1	K	205	VAL	3.4
1	O	31	SER	3.4
2	H	103	ASP	3.4
2	N	163	GLY	3.3
2	F	195	PHE	3.2
1	K	157	GLY	3.2
2	D	137	THR	3.2
1	K	201	LEU	3.1
1	K	120	PRO	3.1
2	P	53	PRO	3.1
2	D	197	THR	3.1
2	P	60	TYR	3.1
2	D	195	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	131	ALA	3.1
1	I	191	VAL	3.1
1	K	193	ALA	3.0
1	O	184	ALA	3.0
1	O	2	ILE	3.0
2	P	58	THR	3.0
1	K	112	ALA	3.0
2	P	195	PHE	3.0
1	K	204	PRO	2.9
2	N	101	HIS	2.9
2	N	129	PRO	2.9
2	J	136	SER	2.9
2	P	57	ILE	2.9
1	K	158	ASN	2.8
1	K	196	VAL	2.8
2	J	102	ASN	2.8
1	K	200	GLY	2.8
1	K	94	TRP	2.8
2	P	54	SER	2.8
1	O	48	ILE	2.8
2	L	140	SER	2.7
1	I	30	SER	2.7
2	F	42	GLY	2.7
2	P	194	ASN	2.7
2	J	195	PHE	2.6
1	K	203	SER	2.6
2	N	128	PHE	2.6
2	P	104	TRP	2.6
1	K	121	SER	2.5
2	N	130	LEU	2.5
1	K	202	SER	2.5
2	L	159	SER	2.5
1	M	94	TRP	2.5
1	I	153	ALA	2.5
1	K	126	LYS	2.5
1	I	147	GLN	2.5
2	B	137	THR	2.5
2	L	103	ASP	2.5
1	K	123	GLU	2.4
2	L	137	THR	2.4
2	P	15	GLY	2.4
2	J	198	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	195	PHE	2.4
2	P	52	GLY	2.4
1	K	186	TYR	2.4
1	K	159	SER	2.4
2	L	133	CYS	2.4
1	O	33	LEU	2.3
2	L	195	PHE	2.3
1	O	212	GLY	2.3
2	N	138	SER	2.3
1	M	124	GLN	2.3
2	N	140	SER	2.2
2	J	164	ALA	2.2
2	P	88	ALA	2.2
1	K	199	GLN	2.2
2	P	205	ASP	2.2
2	J	138	SER	2.2
2	H	193	SER	2.1
1	K	180	THR	2.1
1	M	186	TYR	2.1
2	N	167	SER	2.1
1	M	200	GLY	2.1
1	I	24	ARG	2.1
2	L	141	THR	2.1
1	K	184	ALA	2.0
2	D	134	SER	2.0
2	H	136	SER	2.0
2	P	119	SER	2.0
1	I	152	ASN	2.0
1	I	212	GLY	2.0
2	B	56	GLY	2.0
2	F	135	ARG	2.0
2	P	193	SER	2.0
2	J	166	THR	2.0
1	K	212	GLY	2.0
2	D	196	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.