



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:37 PM UTC

PDB ID : 4QHK / pdb_00004qhk
Title : UCA (unbound) from CH103 Lineage
Authors : Fera, D.; Harrison, S.C.
Deposited on : 2014-05-28
Resolution : 3.49 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

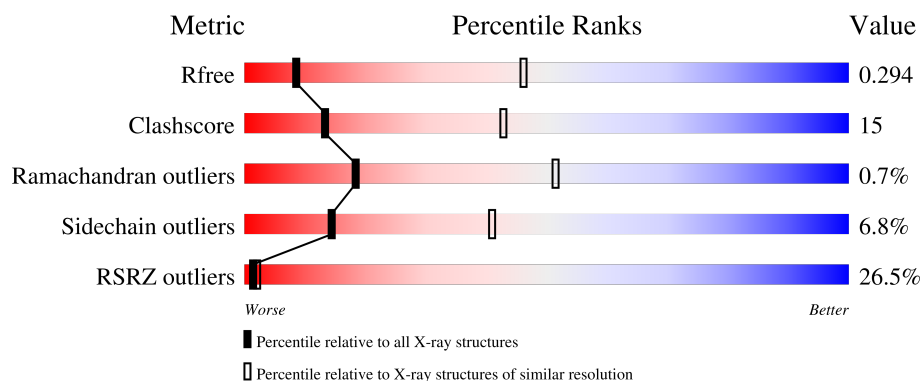
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	I	232	19% 56% 32% 5% 6%
1	K	232	24% 65% 27% • 6%
1	M	232	30% 61% 29% • 7%
1	O	232	28% 59% 31% • 7%
2	J	213	21% 66% 30% ••

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Mol	Chain	Length	Quality of chain
2	L	213	20%67%27%••
2	N	213	28%64%31%••
2	P	213	32%61%32%5%•

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12800 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 UCA heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	216	Total	C	N	O	S	0	0	0
			1624	1036	264	320	4			
1	I	218	Total	C	N	O	S	0	0	0
			1630	1038	263	325	4			
1	O	216	Total	C	N	O	S	0	0	0
			1624	1036	264	320	4			
1	K	218	Total	C	N	O	S	0	0	0
			1630	1038	263	325	4			

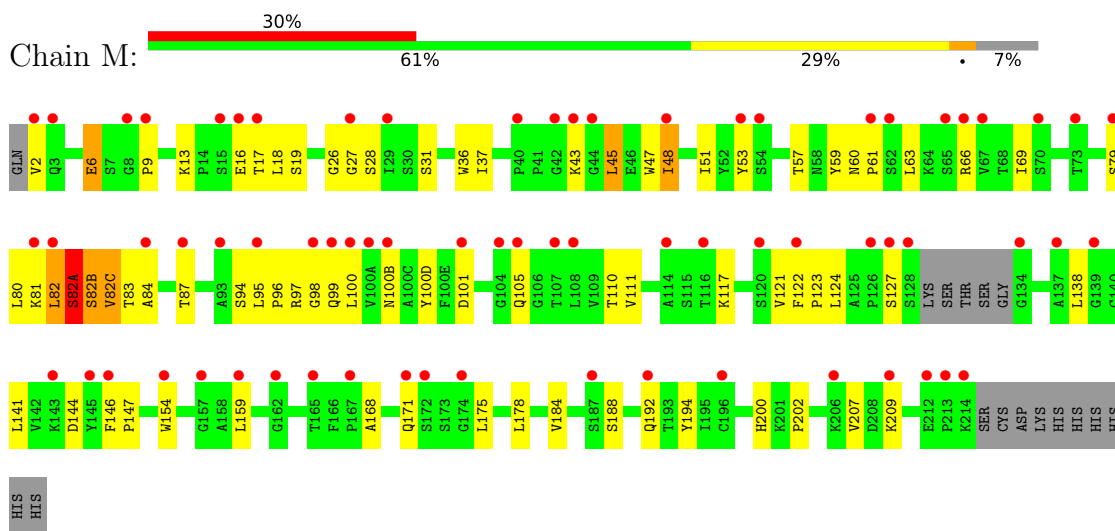
- Molecule 2 is a protein called UCA light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	J	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	L	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	P	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			

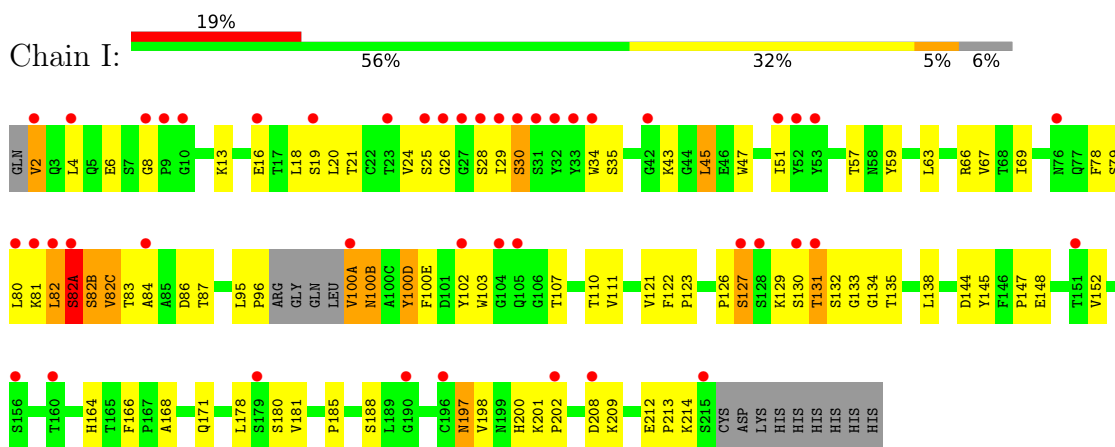
3 Residue-property plots [i](#)

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.

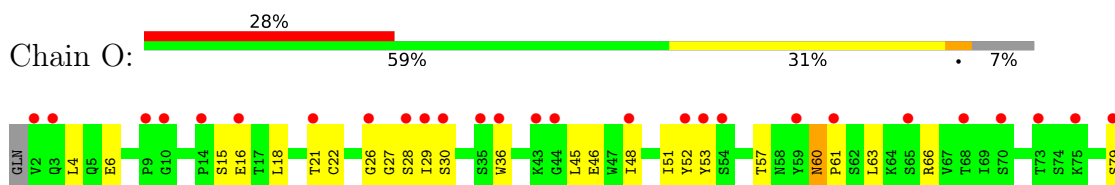
• Molecule 1: UCA heavy chain

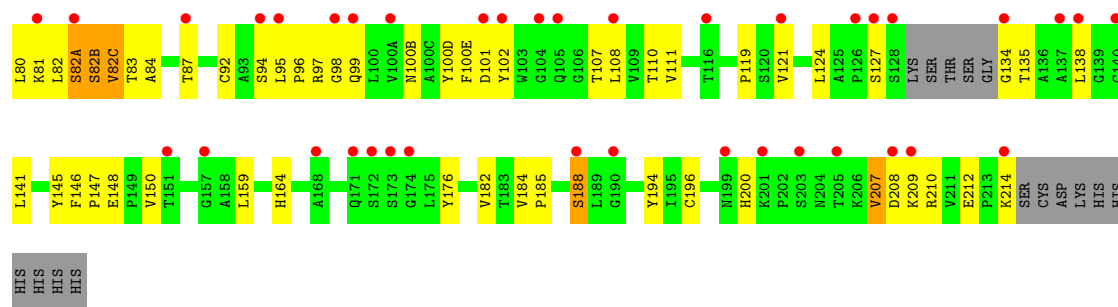


• Molecule 1: UCA heavy chain

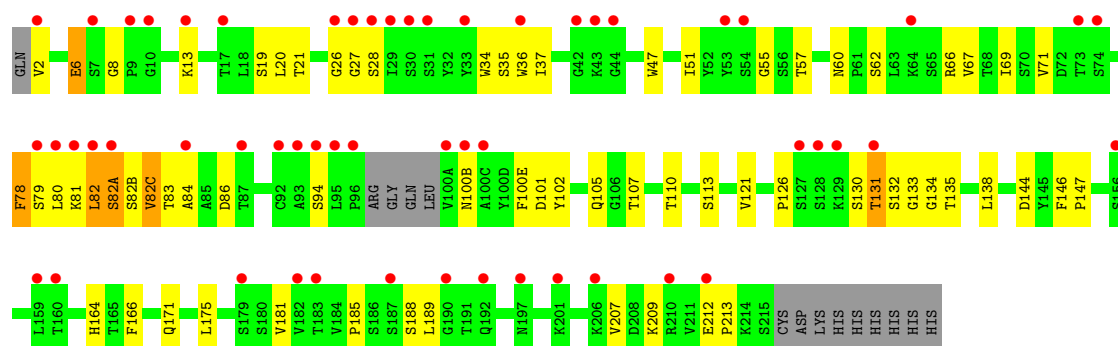


• Molecule 1: UCA heavy chain

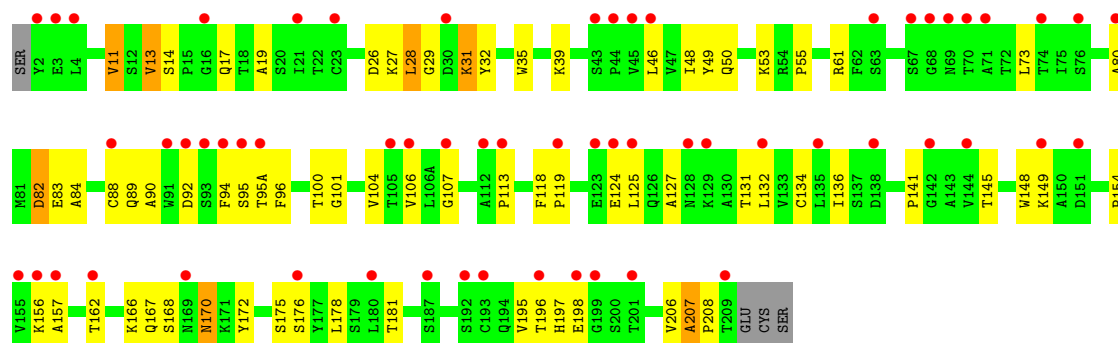




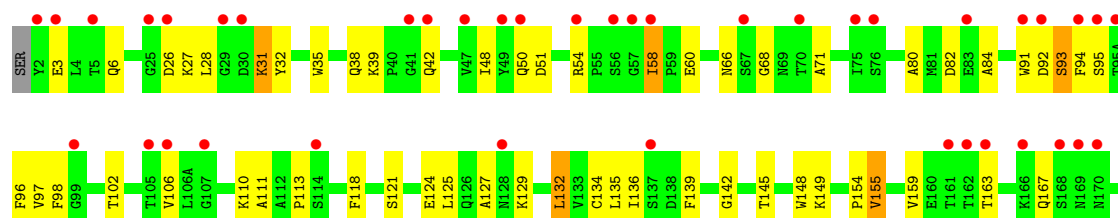
• Molecule 1: UCA heavy chain

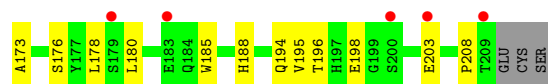


• Molecule 2: UCA light chain

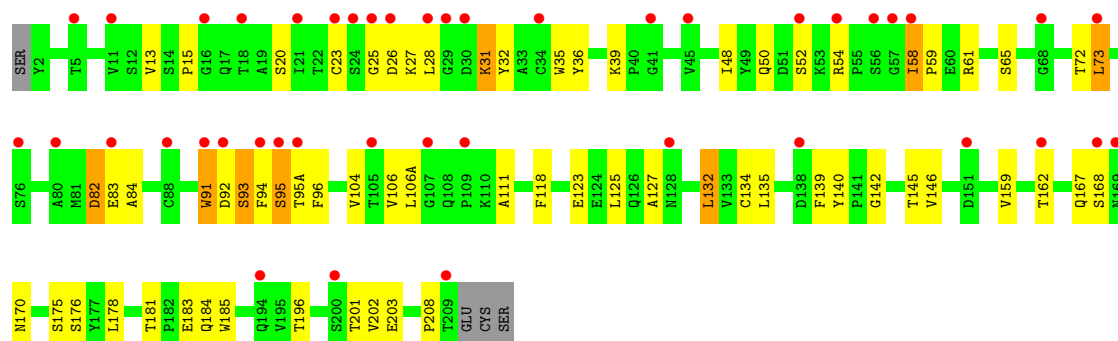


• Molecule 2: UCA light chain

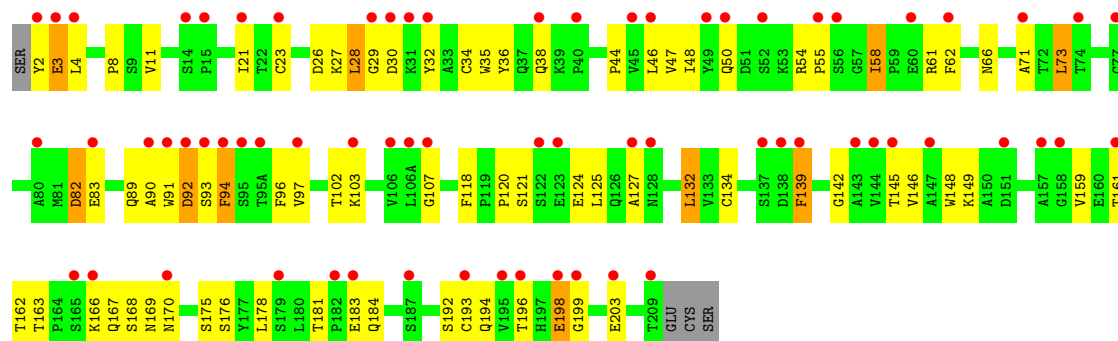




• Molecule 2: UCA light chain



• Molecule 2: UCA light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.69Å 71.15Å 184.40Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	46.85 – 3.49 46.85 – 3.49	Depositor EDS
% Data completeness (in resolution range)	90.1 (46.85-3.49) 90.3 (46.85-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.269 , 0.285 0.273 , 0.294	Depositor DCC
R_{free} test set	1210 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12800	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4918e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	I	0.38	0/1673	0.86	4/2289 (0.2%)
1	K	0.36	0/1673	0.84	2/2289 (0.1%)
1	M	0.36	0/1667	0.84	1/2281 (0.0%)
1	O	0.38	0/1667	0.81	2/2281 (0.1%)
2	J	0.37	0/1614	0.84	6/2206 (0.3%)
2	L	0.34	0/1614	0.83	4/2206 (0.2%)
2	N	0.35	0/1614	0.83	5/2206 (0.2%)
2	P	0.38	0/1614	0.87	1/2206 (0.0%)
All	All	0.37	0/13136	0.84	25/17964 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	55	GLY	N-CA-C	-7.36	105.93	114.69
2	J	93	SER	CA-C-N	7.11	134.50	121.70
2	J	93	SER	C-N-CA	7.11	134.50	121.70
2	L	93	SER	CA-C-N	6.88	134.08	121.70
2	L	93	SER	C-N-CA	6.88	134.08	121.70
1	I	134	GLY	N-CA-C	-5.98	107.57	114.69
2	L	118	PHE	CA-C-N	5.95	126.50	120.38
2	L	118	PHE	C-N-CA	5.95	126.50	120.38
1	M	82(A)	SER	C-N-CA	5.75	136.07	121.70
2	J	118	PHE	CA-C-N	5.66	126.21	120.38
2	J	118	PHE	C-N-CA	5.66	126.21	120.38
1	I	82(A)	SER	C-N-CA	5.41	135.22	121.70
2	N	207	ALA	CA-C-N	5.39	126.58	119.84
2	N	207	ALA	C-N-CA	5.39	126.58	119.84
2	N	107	GLY	N-CA-C	-5.38	105.61	114.76
1	K	134	GLY	N-CA-C	-5.29	108.39	114.69
1	I	212	GLU	CA-C-N	5.25	126.40	119.84
1	I	212	GLU	C-N-CA	5.25	126.40	119.84
2	N	181	THR	CA-C-N	5.25	126.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	181	THR	C-N-CA	5.25	126.40	119.84
1	O	60	ASN	CA-C-N	5.21	124.83	119.05
1	O	60	ASN	C-N-CA	5.21	124.83	119.05
2	J	163	THR	CA-C-N	5.12	126.24	119.84
2	J	163	THR	C-N-CA	5.12	126.24	119.84
2	P	107	GLY	N-CA-C	-5.07	106.14	114.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1630	0	1600	61	0
1	K	1630	0	1600	45	0
1	M	1624	0	1597	51	0
1	O	1624	0	1597	52	0
2	J	1573	0	1513	46	0
2	L	1573	0	1513	51	1
2	N	1573	0	1513	58	0
2	P	1573	0	1513	50	1
All	All	12800	0	12446	373	1

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 15.

All (373) 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)
1:I:100(B):ASN:ND2	1:I:100(B):ASN:O	2.08	0.86
1:M:61:PRO:HD3	2:N:95(A):THR:HG21	1.57	0.85
2:L:25:GLY:H	2:L:28:LEU:HD11	1.43	0.84
2:N:94:PHE:H	2:N:95:SER:HA	1.43	0.81
2:N:94:PHE:N	2:N:95:SER:HA	1.95	0.80
2:J:93:SER:HB3	2:J:94:PHE:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:198:GLU:HG2	2:P:199:GLY:H	1.51	0.75
1:O:97:ARG:HG2	1:O:98:GLY:H	1.51	0.75
2:L:93:SER:HB3	2:L:94:PHE:HB2	1.68	0.75
2:J:39:LYS:HB2	2:J:42:GLN:HE21	1.53	0.72
2:J:194:GLN:HG2	2:J:203:GLU:HG2	1.72	0.71
2:P:132:LEU:HB2	2:P:178:LEU:HB3	1.70	0.71
1:M:144:ASP:OD1	1:M:171:GLN:NE2	2.24	0.71
1:I:87:THR:HG23	1:I:110:THR:HA	1.73	0.70
2:N:35:TRP:HB2	2:N:48:ILE:HB	1.73	0.70
1:O:87:THR:HG23	1:O:110:THR:HA	1.73	0.70
2:N:13:VAL:HG21	2:N:19:ALA:HB2	1.74	0.70
2:N:83:GLU:OE1	2:N:170:ASN:ND2	2.24	0.70
1:M:87:THR:HG23	1:M:110:THR:HA	1.75	0.69
1:O:164:HIS:CE1	2:P:167:GLN:HE21	2.11	0.69
1:M:36:TRP:HB2	1:M:48:ILE:HD11	1.75	0.69
1:M:123:PRO:HD3	1:M:209:LYS:HE2	1.74	0.69
1:K:144:ASP:OD1	1:K:171:GLN:NE2	2.25	0.68
1:O:94:SER:OG	1:O:101:ASP:O	2.12	0.68
1:I:30:SER:HA	1:I:34:TRP:HE1	1.57	0.68
2:P:35:TRP:HB2	2:P:48:ILE:HB	1.76	0.68
1:I:66:ARG:NH2	1:I:86:ASP:OD2	2.27	0.67
2:J:149:LYS:NZ	2:J:194:GLN:OE1	2.24	0.67
1:I:200:HIS:CD2	1:I:202:PRO:HD2	2.31	0.66
2:L:132:LEU:HB2	2:L:178:LEU:HB3	1.78	0.66
1:K:131:THR:OG1	1:K:132:SER:N	2.23	0.66
1:K:51:ILE:HG13	1:K:57:THR:HG22	1.78	0.66
1:I:164:HIS:CE1	2:J:167:GLN:HG3	2.32	0.65
2:N:46:LEU:HG	2:N:55:PRO:CG	2.26	0.65
2:J:134:CYS:HB3	2:J:176:SER:HB3	1.79	0.65
1:O:51:ILE:HG13	1:O:57:THR:HG22	1.79	0.65
2:N:39:LYS:HD3	2:N:84:ALA:HB2	1.79	0.64
2:N:156:LYS:NZ	2:P:163:THR:OG1	2.29	0.64
2:P:61:ARG:NH1	2:P:82:ASP:OD2	2.30	0.64
1:M:97:ARG:HH11	1:M:98:GLY:H	1.44	0.64
2:L:54:ARG:NH2	2:L:58:ILE:O	2.31	0.64
1:K:66:ARG:NH2	1:K:86:ASP:OD2	2.32	0.63
1:I:121:VAL:HG11	1:I:198:VAL:HG21	1.80	0.63
2:L:28:LEU:HA	2:L:31:LYS:HD2	1.80	0.63
2:J:178:LEU:HG	2:J:180:LEU:HD13	1.81	0.63
2:N:61:ARG:NH1	2:N:82:ASP:OD2	2.31	0.63
1:M:94:SER:OG	1:M:101:ASP:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:LEU:HG	2:N:55:PRO:HG2	1.79	0.62
1:K:164:HIS:CD2	2:L:167:GLN:HG3	2.34	0.62
1:K:189:LEU:HD22	1:K:213:PRO:HD3	1.81	0.62
2:J:132:LEU:HB2	2:J:178:LEU:HB3	1.81	0.62
1:K:13:LYS:NZ	1:K:113:SER:O	2.34	0.61
2:J:54:ARG:HB2	2:J:58:ILE:HD11	1.83	0.61
2:P:83:GLU:O	2:P:166:LYS:NZ	2.33	0.61
1:M:95:LEU:HD12	1:M:96:PRO:HD2	1.82	0.61
2:J:80:ALA:HA	2:J:106:VAL:HG21	1.82	0.61
2:P:55:PRO:HG2	2:P:58:ILE:HG13	1.83	0.61
1:I:100(B):ASN:HD22	1:I:100(B):ASN:C	2.06	0.61
1:M:6:GLU:OE1	1:M:105:GLN:N	2.35	0.60
1:O:48:ILE:HG22	1:O:63:LEU:HD22	1.82	0.60
1:M:51:ILE:HG13	1:M:57:THR:HG22	1.83	0.60
1:M:48:ILE:O	1:M:60:ASN:N	2.34	0.59
2:J:32:TYR:HD1	2:J:50:GLN:HA	1.65	0.59
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.82	0.59
2:P:91:TRP:CD1	2:P:92:ASP:H	2.21	0.59
1:M:184:VAL:HG11	1:M:194:TYR:CE1	2.38	0.58
1:M:200:HIS:CD2	1:M:202:PRO:HD2	2.38	0.58
1:M:168:ALA:HA	1:M:178:LEU:HB3	1.85	0.58
1:I:82(A):SER:H	1:I:82(C):VAL:N	2.01	0.58
1:M:100(B):ASN:ND2	2:N:50:GLN:HE21	2.02	0.58
2:L:167:GLN:HG2	2:L:168:SER:H	1.68	0.58
1:I:51:ILE:HD13	1:I:57:THR:HG22	1.86	0.57
1:O:124:LEU:HD11	1:O:141:LEU:HB2	1.86	0.57
2:N:11:VAL:HG13	2:N:104:VAL:HA	1.86	0.57
1:K:6:GLU:OE1	1:K:105:GLN:N	2.35	0.57
1:I:30:SER:HA	1:I:34:TRP:NE1	2.19	0.57
1:O:28:SER:OG	1:O:29:ILE:N	2.37	0.57
1:O:82(A):SER:H	1:O:82(C):VAL:N	2.02	0.56
1:K:130:SER:HB2	1:K:131:THR:HG22	1.85	0.56
2:P:47:VAL:HA	2:P:58:ILE:HD12	1.86	0.56
1:K:166:PHE:HE2	2:L:135:LEU:HD22	1.70	0.56
1:K:166:PHE:CE2	2:L:135:LEU:HD22	2.41	0.56
2:P:139:PHE:CE2	2:P:142:GLY:HA2	2.41	0.56
2:J:136:ILE:HG12	2:J:195:VAL:HG21	1.88	0.55
1:M:82(A):SER:H	1:M:82(C):VAL:N	2.04	0.55
1:I:152:VAL:HG11	1:I:180:SER:HB2	1.89	0.55
1:K:34:TRP:HB3	1:K:78:PHE:CE1	2.41	0.55
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:PRO:HD3	2:N:95(A):THR:CG2	2.33	0.55
1:O:30:SER:HA	1:O:53:TYR:HE2	1.71	0.55
1:I:127:SER:N	1:I:130:SER:O	2.31	0.55
1:I:166:PHE:HE2	2:J:135:LEU:HD22	1.72	0.55
1:M:188:SER:OG	1:M:192:GLN:NE2	2.40	0.55
2:P:38:GLN:HE21	2:P:44:PRO:HG3	1.71	0.55
1:O:18:LEU:O	1:O:81:LYS:HA	2.08	0.54
1:K:66:ARG:HG3	1:K:82(A):SER:OG	2.07	0.54
2:P:91:TRP:HA	2:P:96:PHE:HA	1.89	0.54
1:O:21:THR:HG22	1:O:79:SER:HB3	1.90	0.54
1:K:2:VAL:HG11	1:K:27:GLY:HA2	1.90	0.54
1:O:134:GLY:C	1:O:135:THR:HG23	2.33	0.54
1:K:185:PRO:HG2	1:K:188:SER:HB3	1.88	0.54
1:K:209:LYS:NZ	2:L:123:GLU:OE2	2.33	0.54
1:M:18:LEU:HB3	1:M:82:LEU:HD13	1.90	0.53
1:O:63:LEU:O	1:O:66:ARG:HB3	2.08	0.53
1:I:30:SER:CA	1:I:34:TRP:HE1	2.21	0.53
2:L:39:LYS:HG2	2:L:84:ALA:HB2	1.91	0.53
2:J:66:ASN:HA	2:J:71:ALA:HA	1.91	0.53
2:N:53:LYS:NZ	2:J:51:ASP:OD2	2.25	0.53
1:I:26:GLY:C	1:I:28:SER:HA	2.33	0.53
2:N:46:LEU:CD2	2:N:55:PRO:HG3	2.39	0.53
2:N:132:LEU:HB2	2:N:178:LEU:HB3	1.90	0.53
2:L:134:CYS:HB3	2:L:176:SER:HB2	1.91	0.53
1:K:82:LEU:O	1:K:82(C):VAL:HG23	2.09	0.53
1:M:59:TYR:HE1	1:M:69:ILE:HG13	1.74	0.53
2:J:125:LEU:C	2:J:127:ALA:H	2.17	0.53
1:O:134:GLY:O	1:O:135:THR:HG23	2.09	0.52
1:O:210:ARG:NE	1:O:212:GLU:OE2	2.42	0.52
1:I:144:ASP:OD1	1:I:171:GLN:NE2	2.41	0.52
1:I:18:LEU:O	1:I:81:LYS:HA	2.10	0.52
1:K:94:SER:OG	1:K:101:ASP:O	2.25	0.52
1:M:192:GLN:CD	1:M:194:TYR:HE2	2.18	0.52
1:O:97:ARG:C	1:O:99:GLN:HA	2.34	0.52
2:P:35:TRP:CD2	2:P:73:LEU:HD23	2.45	0.52
1:O:100(B):ASN:ND2	2:P:50:GLN:HE21	2.08	0.51
2:N:156:LYS:HG3	2:N:157:ALA:H	1.74	0.51
2:J:31:LYS:HG2	2:J:91:TRP:CE2	2.44	0.51
1:M:100(B):ASN:HB3	2:N:32:TYR:CG	2.45	0.51
1:M:124:LEU:HD11	1:M:141:LEU:HB2	1.92	0.51
2:J:93:SER:H	2:J:95:SER:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:28:LEU:O	2:P:30:ASP:N	2.41	0.51
2:P:125:LEU:C	2:P:127:ALA:H	2.17	0.51
2:P:134:CYS:HB3	2:P:176:SER:HB2	1.92	0.51
2:N:80:ALA:HA	2:N:106:VAL:HG21	1.93	0.51
1:I:59:TYR:HE1	1:I:69:ILE:HG13	1.76	0.51
1:K:100(B):ASN:OD1	1:K:100(B):ASN:N	2.31	0.51
2:N:166:LYS:NZ	2:N:172:TYR:OH	2.44	0.51
1:I:83:THR:OG1	1:I:84:ALA:N	2.44	0.51
1:I:47:TRP:CD2	2:J:96:PHE:HB2	2.46	0.50
2:L:50:GLN:O	2:L:52:SER:N	2.37	0.50
2:L:125:LEU:C	2:L:127:ALA:H	2.20	0.50
1:M:18:LEU:O	1:M:81:LYS:HA	2.12	0.50
2:P:54:ARG:NH1	2:P:62:PHE:O	2.44	0.50
1:I:123:PRO:CA	1:I:209:LYS:HZ1	2.24	0.50
1:O:97:ARG:HG2	1:O:98:GLY:N	2.25	0.50
1:I:16:GLU:O	1:I:82(B):SER:N	2.45	0.50
2:L:91:TRP:CZ3	2:L:95(A):THR:HA	2.47	0.50
1:I:19:SER:HA	1:I:80:LEU:O	2.12	0.50
1:I:197:ASN:N	1:I:197:ASN:HD22	2.10	0.49
1:O:119:PRO:HB3	1:O:145:TYR:HB3	1.94	0.49
2:N:162:THR:HG22	2:N:175:SER:H	1.77	0.49
1:M:43:LYS:HZ3	2:N:101:GLY:HA3	1.77	0.49
1:M:47:TRP:CZ3	2:N:95(A):THR:HB	2.47	0.49
1:K:69:ILE:HG12	1:K:80:LEU:CD1	2.43	0.49
1:I:107:THR:HG23	1:I:201:LYS:NZ	2.28	0.49
2:L:54:ARG:HH22	2:L:59:PRO:C	2.21	0.49
1:I:166:PHE:CE2	2:J:135:LEU:HD22	2.47	0.49
1:K:35:SER:C	1:K:36:TRP:HD1	2.20	0.49
1:O:4:LEU:HB3	1:O:92:CYS:SG	2.52	0.49
1:O:98:GLY:N	1:O:99:GLN:HA	2.28	0.49
1:M:43:LYS:NZ	2:N:101:GLY:HA3	2.28	0.48
1:I:168:ALA:HA	1:I:178:LEU:HB3	1.95	0.48
1:I:185:PRO:HG2	1:I:188:SER:HB3	1.95	0.48
1:I:13:LYS:HB2	1:I:16:GLU:CD	2.39	0.48
2:L:25:GLY:H	2:L:28:LEU:CD1	2.22	0.48
1:I:29:ILE:HG13	1:I:30:SER:OG	2.14	0.48
1:M:47:TRP:HZ3	2:N:95(A):THR:HB	1.79	0.48
1:O:26:GLY:C	1:O:28:SER:HA	2.39	0.48
1:O:29:ILE:HG23	1:O:53:TYR:CZ	2.48	0.48
1:I:21:THR:HG22	1:I:79:SER:OG	2.14	0.47
1:I:59:TYR:CE1	1:I:69:ILE:HG13	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:28:LEU:HG	2:L:31:LYS:HD2	1.94	0.47
2:L:93:SER:H	2:L:94:PHE:C	2.22	0.47
1:I:147:PRO:HD2	1:I:202:PRO:HB2	1.96	0.47
2:N:125:LEU:C	2:N:127:ALA:H	2.22	0.47
1:I:122:PHE:HA	1:I:209:LYS:HE3	1.95	0.47
2:L:31:LYS:HE2	2:L:31:LYS:HB3	1.64	0.47
1:K:100(B):ASN:HD22	2:L:50:GLN:CG	2.28	0.47
1:K:100(E):PHE:H	2:L:36:TYR:HH	1.58	0.47
1:O:48:ILE:O	1:O:60:ASN:N	2.36	0.47
2:N:14:SER:O	2:N:17:GLN:HG2	2.14	0.47
2:P:93:SER:O	2:P:94:PHE:CG	2.67	0.47
2:P:162:THR:HG22	2:P:175:SER:H	1.79	0.47
2:N:53:LYS:HG2	2:J:32:TYR:CE2	2.50	0.47
2:J:60:GLU:CD	2:J:60:GLU:H	2.23	0.47
2:L:93:SER:H	2:L:95:SER:N	2.13	0.47
2:P:89:GLN:HG2	2:P:90:ALA:N	2.29	0.47
2:L:139:PHE:HE1	2:L:142:GLY:HA2	1.80	0.47
2:P:4:LEU:HB3	2:P:23:CYS:SG	2.54	0.47
1:K:67:VAL:CG2	1:K:80:LEU:HD11	2.46	0.46
1:K:100(B):ASN:HD22	2:L:50:GLN:HG2	1.80	0.46
2:N:14:SER:N	2:N:17:GLN:OE1	2.42	0.46
2:J:110:LYS:NZ	2:J:198:GLU:OE1	2.35	0.46
1:K:80:LEU:C	1:K:81:LYS:HD2	2.40	0.46
2:N:26:ASP:HA	2:N:27:LYS:HA	1.53	0.46
1:M:117:LYS:HD3	1:M:175:LEU:HD13	1.97	0.46
1:I:47:TRP:CE3	2:J:96:PHE:HB2	2.51	0.46
1:I:152:VAL:HA	1:I:197:ASN:O	2.14	0.46
2:N:13:VAL:HG12	2:N:106:VAL:HG12	1.98	0.46
1:M:26:GLY:C	1:M:28:SER:HA	2.40	0.46
1:I:214:LYS:HE2	1:I:214:LYS:HB3	1.70	0.46
2:P:146:VAL:HG11	2:P:161:THR:HG21	1.97	0.46
1:I:132:SER:HA	1:I:133:GLY:HA2	1.73	0.46
2:P:145:THR:HB	2:P:196:THR:OG1	2.16	0.46
1:M:100(D):TYR:CD2	2:N:49:TYR:HB2	2.51	0.46
1:O:22:CYS:HB2	1:O:36:TRP:CH2	2.51	0.46
1:O:159:LEU:HD23	1:O:182:VAL:HG21	1.98	0.46
2:N:149:LYS:HG2	2:N:154:PRO:HA	1.97	0.46
2:J:35:TRP:HB2	2:J:48:ILE:HB	1.98	0.46
2:J:38:GLN:O	2:J:84:ALA:HB1	2.15	0.46
2:J:139:PHE:HE2	2:J:142:GLY:HA2	1.81	0.46
1:I:168:ALA:HB2	1:I:178:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:168:SER:C	2:L:170:ASN:H	2.23	0.46
2:P:26:ASP:HA	2:P:27:LYS:HA	1.46	0.45
1:K:130:SER:CB	1:K:131:THR:HG22	2.47	0.45
1:K:164:HIS:NE2	2:L:167:GLN:HG3	2.31	0.45
2:J:93:SER:HB3	2:J:94:PHE:CB	2.42	0.45
2:P:148:TRP:CZ3	2:P:193:CYS:HB2	2.51	0.45
1:M:43:LYS:NZ	2:N:100:THR:O	2.39	0.45
1:I:45:LEU:HD23	2:J:98:PHE:CD1	2.51	0.45
1:O:36:TRP:HB3	1:O:48:ILE:HD11	1.98	0.45
1:O:100(E):PHE:N	2:P:36:TYR:OH	2.26	0.45
1:K:60:ASN:OD1	1:K:62:SER:OG	2.21	0.45
2:P:162:THR:CG2	2:P:175:SER:H	2.29	0.45
2:J:6:GLN:NE2	2:J:102:THR:OG1	2.48	0.45
2:L:145:THR:HB	2:L:196:THR:OG1	2.17	0.45
2:P:167:GLN:HB3	2:P:168:SER:H	1.56	0.45
1:M:100:LEU:HG	1:M:100(B):ASN:OD1	2.16	0.45
2:P:149:LYS:HB2	2:P:192:SER:OG	2.17	0.45
1:O:83:THR:OG1	1:O:84:ALA:N	2.50	0.45
2:N:134:CYS:HB3	2:N:176:SER:HB3	1.98	0.45
1:I:130:SER:HA	1:I:131:THR:HA	1.70	0.45
1:O:60:ASN:HA	1:O:61:PRO:HD3	1.87	0.45
2:N:141:PRO:HD2	2:N:198:GLU:OE2	2.17	0.45
2:P:11:VAL:HG21	2:P:21:ILE:HG13	1.98	0.45
1:I:34:TRP:HB3	1:I:78:PHE:CE1	2.52	0.45
1:I:123:PRO:O	2:J:121:SER:HB3	2.17	0.45
2:J:149:LYS:HG2	2:J:154:PRO:HA	1.98	0.45
2:P:194:GLN:HB3	2:P:203:GLU:CD	2.42	0.45
1:M:48:ILE:HG22	1:M:63:LEU:HD22	1.98	0.44
1:O:100(B):ASN:HB3	2:P:32:TYR:CD2	2.51	0.44
1:K:19:SER:HA	1:K:80:LEU:O	2.17	0.44
1:K:130:SER:HA	1:K:131:THR:HA	1.64	0.44
2:N:162:THR:CG2	2:N:175:SER:H	2.30	0.44
1:O:52:TYR:OH	1:O:97:ARG:NH1	2.51	0.44
2:N:32:TYR:OH	2:J:68:GLY:O	2.35	0.44
2:L:20:SER:HA	2:L:73:LEU:O	2.17	0.44
2:P:2:TYR:O	2:P:3:GLU:HG3	2.18	0.44
1:I:63:LEU:O	1:I:66:ARG:HB3	2.17	0.44
1:K:26:GLY:C	1:K:28:SER:HA	2.42	0.44
2:N:29:GLY:O	2:J:27:LYS:NZ	2.29	0.44
2:N:118:PHE:HA	2:N:119:PRO:HD3	1.82	0.44
1:I:82:LEU:HA	1:I:82(A):SER:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:119:PRO:HG3	2:N:206:VAL:HG11	2.00	0.44
2:L:26:ASP:HA	2:L:27:LYS:HA	1.63	0.44
1:O:27:GLY:N	1:O:28:SER:HA	2.31	0.44
1:O:185:PRO:HG2	1:O:188:SER:HB3	2.00	0.44
1:M:154:TRP:HB2	1:M:159:LEU:HB2	2.00	0.44
1:I:4:LEU:HD23	1:I:24:VAL:HG12	2.00	0.44
1:O:16:GLU:O	1:O:82(B):SER:N	2.51	0.44
1:O:214:LYS:HD2	1:O:214:LYS:HA	1.68	0.44
1:K:8:GLY:HA3	1:K:20:LEU:HD23	2.00	0.44
1:K:21:THR:HG22	1:K:79:SER:HB2	2.00	0.44
1:M:82(A):SER:H	1:M:82(B):SER:C	2.26	0.44
2:J:93:SER:H	2:J:94:PHE:C	2.26	0.44
2:L:162:THR:HG22	2:L:175:SER:H	1.82	0.44
2:P:198:GLU:CG	2:P:199:GLY:H	2.25	0.44
1:K:83:THR:OG1	1:K:84:ALA:N	2.51	0.44
2:P:120:PRO:HD3	2:P:132:LEU:HD13	1.98	0.44
2:L:25:GLY:N	2:L:28:LEU:HD11	2.21	0.43
1:M:97:ARG:C	1:M:99:GLN:HA	2.43	0.43
2:J:3:GLU:HA	2:J:97:VAL:CG2	2.47	0.43
2:L:15:PRO:HD3	2:L:106(A):LEU:O	2.18	0.43
1:I:126:PRO:HD2	1:I:213:PRO:HA	1.99	0.43
2:N:94:PHE:N	2:N:95:SER:CA	2.76	0.43
1:K:47:TRP:CD2	2:L:96:PHE:HB2	2.54	0.43
2:J:148:TRP:HB2	2:J:155:VAL:HG12	2.00	0.43
2:L:93:SER:HB3	2:L:94:PHE:CB	2.44	0.43
2:P:168:SER:C	2:P:170:ASN:H	2.26	0.43
1:I:96:PRO:HG2	1:I:100(D):TYR:CZ	2.54	0.43
1:O:196:CYS:O	1:O:208:ASP:HA	2.19	0.43
1:K:71:VAL:HG23	1:K:78:PHE:HB3	2.01	0.43
2:N:145:THR:HB	2:N:196:THR:OG1	2.19	0.43
2:L:92:ASP:O	2:L:95:SER:HB3	2.19	0.43
1:O:15:SER:HA	1:O:82(B):SER:HA	2.00	0.43
1:K:126:PRO:HD2	1:K:213:PRO:HA	2.01	0.43
1:M:146:PHE:HA	1:M:147:PRO:HA	1.77	0.43
2:J:113:PRO:HA	2:J:139:PHE:HB3	2.00	0.43
1:I:103:TRP:CD1	1:I:103:TRP:N	2.86	0.43
2:P:66:ASN:HA	2:P:71:ALA:HA	2.01	0.43
1:M:98:GLY:N	1:M:99:GLN:HA	2.34	0.42
1:O:95:LEU:HD12	1:O:96:PRO:HD2	2.01	0.42
2:P:181:THR:O	2:P:184:GLN:N	2.51	0.42
1:I:100(A):VAL:HB	1:I:100(B):ASN:H	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:146:PHE:HA	1:O:147:PRO:HA	1.86	0.42
1:M:37:ILE:HG21	1:M:45:LEU:HD21	2.00	0.42
1:M:100(B):ASN:HB3	2:N:32:TYR:CD2	2.54	0.42
2:N:167:GLN:HB3	2:N:168:SER:H	1.53	0.42
2:J:31:LYS:HE2	2:J:31:LYS:HB2	1.90	0.42
1:O:124:LEU:HB3	2:P:118:PHE:CD1	2.55	0.42
1:M:184:VAL:HG11	1:M:194:TYR:HE1	1.84	0.42
1:O:150:VAL:HG22	1:O:200:HIS:HD2	1.84	0.42
1:K:146:PHE:HA	1:K:147:PRO:HA	1.79	0.42
2:L:83:GLU:OE2	2:L:106:VAL:N	2.30	0.42
2:P:121:SER:OG	2:P:124:GLU:OE1	2.24	0.42
1:O:150:VAL:HG22	1:O:200:HIS:CD2	2.55	0.42
2:N:13:VAL:HG22	2:N:17:GLN:HG3	2.02	0.42
2:L:92:ASP:HA	2:L:93:SER:HB2	2.02	0.42
1:I:2:VAL:HG23	1:I:25:SER:H	1.85	0.42
2:N:207:ALA:HA	2:N:208:PRO:HD2	1.77	0.42
2:L:185:TRP:O	2:L:208:PRO:HG3	2.19	0.42
2:N:168:SER:C	2:N:170:ASN:H	2.28	0.42
1:M:36:TRP:CG	1:M:80:LEU:HD12	2.55	0.41
1:I:35:SER:HB2	1:I:47:TRP:HE1	1.84	0.41
1:K:2:VAL:HG22	1:K:102:TYR:CD1	2.55	0.41
2:J:26:ASP:HA	2:J:27:LYS:HA	1.56	0.41
2:J:124:GLU:HG2	2:J:129:LYS:O	2.20	0.41
2:P:46:LEU:O	2:P:55:PRO:HG3	2.20	0.41
1:M:63:LEU:O	1:M:66:ARG:HB3	2.20	0.41
1:O:36:TRP:CD2	1:O:80:LEU:HD23	2.55	0.41
1:K:131:THR:OG1	1:K:135:THR:O	2.34	0.41
2:J:110:LYS:HG2	2:J:111:ALA:N	2.35	0.41
2:L:111:ALA:HB3	2:L:140:TYR:H	1.85	0.41
1:O:100(B):ASN:HB3	2:P:32:TYR:CG	2.56	0.41
1:O:121:VAL:HB	1:O:209:LYS:NZ	2.35	0.41
2:P:34:CYS:SG	2:P:89:GLN:HB3	2.60	0.41
1:I:8:GLY:HA3	1:I:20:LEU:HD23	2.02	0.41
1:I:43:LYS:HE2	1:I:43:LYS:HB3	1.88	0.41
1:O:184:VAL:HG11	1:O:194:TYR:CE1	2.56	0.41
2:L:28:LEU:HA	2:L:31:LYS:CD	2.49	0.41
2:L:146:VAL:HG11	2:L:176:SER:OG	2.20	0.41
1:M:16:GLU:HB3	1:M:17:THR:H	1.66	0.41
2:L:32:TYR:HD1	2:L:50:GLN:HA	1.85	0.41
2:L:196:THR:HG22	2:L:201:THR:OG1	2.20	0.41
1:I:145:TYR:OH	1:I:148:GLU:OE1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ILE:HD11	1:K:100(E):PHE:CD1	2.56	0.41
2:N:113:PRO:HD3	2:N:197:HIS:ND1	2.36	0.41
2:L:145:THR:HB	2:L:196:THR:HG1	1.86	0.41
1:I:67:VAL:HG12	1:I:82:LEU:HG	2.03	0.41
1:K:132:SER:HA	1:K:133:GLY:HA2	1.67	0.41
2:L:13:VAL:O	2:L:106:VAL:HA	2.19	0.41
1:I:83:THR:O	1:I:111:VAL:HG21	2.20	0.41
1:O:36:TRP:O	1:O:48:ILE:HG12	2.21	0.41
1:O:207:VAL:HG11	1:O:209:LYS:NZ	2.35	0.41
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.56	0.41
2:P:29:GLY:HA2	2:P:66:ASN:CG	2.45	0.41
1:I:129:LYS:NZ	1:I:132:SER:HB3	2.36	0.41
1:O:148:GLU:HG2	1:O:176:TYR:CD2	2.55	0.41
1:K:78:PHE:N	1:K:78:PHE:CD2	2.89	0.41
2:N:28:LEU:HA	2:N:31:LYS:HG3	2.02	0.41
2:N:46:LEU:HG	2:N:55:PRO:HG3	1.98	0.41
2:N:136:ILE:HG12	2:N:195:VAL:HG21	2.03	0.41
2:N:170:ASN:ND2	2:N:170:ASN:O	2.48	0.41
2:L:65:SER:OG	2:L:72:THR:HG22	2.20	0.41
2:P:21:ILE:HG12	2:P:102:THR:HG21	2.03	0.41
1:M:9:PRO:HD3	1:M:19:SER:O	2.21	0.41
1:I:164:HIS:HE1	2:J:173:ALA:HB3	1.86	0.41
2:P:91:TRP:CG	2:P:92:ASP:H	2.38	0.41
1:M:122:PHE:CD2	2:N:124:GLU:HB3	2.56	0.40
2:P:8:PRO:O	2:P:103:LYS:HB2	2.21	0.40
1:M:27:GLY:N	1:M:28:SER:HA	2.36	0.40
1:M:47:TRP:CE2	2:N:96:PHE:HD2	2.38	0.40
1:I:100(B):ASN:ND2	1:I:100(B):ASN:N	2.69	0.40
1:O:96:PRO:HG2	1:O:100(D):TYR:CZ	2.56	0.40
1:K:20:LEU:HB2	1:K:36:TRP:CZ3	2.55	0.40
2:N:89:GLN:HG2	2:N:90:ALA:N	2.36	0.40
1:M:31:SER:O	1:M:97:ARG:HB2	2.22	0.40
1:M:83:THR:OG1	1:M:84:ALA:N	2.50	0.40
2:J:185:TRP:O	2:J:208:PRO:HG3	2.21	0.40
2:L:181:THR:O	2:L:184:GLN:N	2.54	0.40
2:P:27:LYS:HB2	2:P:28:LEU:H	1.69	0.40
2:N:134:CYS:HB2	2:N:148:TRP:CH2	2.57	0.40
2:J:92:ASP:O	2:J:95:SER:HB3	2.21	0.40
2:J:145:THR:OG1	2:J:196:THR:HB	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:28:LEU:O	2:P:32:TYR:OH[2_646]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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	I	214/232 (92%)	194 (91%)	18 (8%)	2 (1%)	14	47
1	K	214/232 (92%)	193 (90%)	21 (10%)	0	100	100
1	M	212/232 (91%)	192 (91%)	19 (9%)	1 (0%)	24	58
1	O	212/232 (91%)	192 (91%)	18 (8%)	2 (1%)	14	47
2	J	207/213 (97%)	175 (84%)	32 (16%)	0	100	100
2	L	207/213 (97%)	173 (84%)	33 (16%)	1 (0%)	24	58
2	N	207/213 (97%)	176 (85%)	30 (14%)	1 (0%)	24	58
2	P	207/213 (97%)	175 (84%)	27 (13%)	5 (2%)	4	29
All	All	1680/1780 (94%)	1470 (88%)	198 (12%)	12 (1%)	18	51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	102	TYR
2	P	92	ASP
2	P	94	PHE
2	N	92	ASP
2	P	3	GLU
1	M	127	SER
1	I	127	SER
1	O	127	SER
2	L	95	SER
1	O	102	TYR
2	P	169	ASN
2	P	198	GLU

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	I	189/202 (94%)	170 (90%)	19 (10%)	7	28
1	K	189/202 (94%)	174 (92%)	15 (8%)	11	36
1	M	187/202 (93%)	172 (92%)	15 (8%)	11	36
1	O	187/202 (93%)	174 (93%)	13 (7%)	14	40
2	J	178/182 (98%)	170 (96%)	8 (4%)	24	51
2	L	178/182 (98%)	167 (94%)	11 (6%)	16	44
2	N	178/182 (98%)	169 (95%)	9 (5%)	21	48
2	P	178/182 (98%)	169 (95%)	9 (5%)	21	48
All	All	1464/1536 (95%)	1365 (93%)	99 (7%)	14	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	2	VAL
1	M	6	GLU
1	M	13	LYS
1	M	45	LEU
1	M	48	ILE
1	M	53	TYR
1	M	79	SER
1	M	82	LEU
1	M	82(A)	SER
1	M	82(B)	SER
1	M	82(C)	VAL
1	M	111	VAL
1	M	121	VAL
1	M	138	LEU
1	M	207	VAL
1	I	2	VAL
1	I	6	GLU
1	I	30	SER
1	I	45	LEU

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Mol	Chain	Res	Type
1	I	82	LEU
1	I	82(A)	SER
1	I	82(B)	SER
1	I	82(C)	VAL
1	I	95	LEU
1	I	100(A)	VAL
1	I	100(B)	ASN
1	I	100(D)	TYR
1	I	100(E)	PHE
1	I	131	THR
1	I	135	THR
1	I	138	LEU
1	I	181	VAL
1	I	197	ASN
1	I	208	ASP
1	O	6	GLU
1	O	45	LEU
1	O	46	GLU
1	O	82	LEU
1	O	82(A)	SER
1	O	82(B)	SER
1	O	82(C)	VAL
1	O	107	THR
1	O	108	LEU
1	O	111	VAL
1	O	138	LEU
1	O	188	SER
1	O	207	VAL
1	K	6	GLU
1	K	78	PHE
1	K	82	LEU
1	K	82(A)	SER
1	K	82(B)	SER
1	K	82(C)	VAL
1	K	107	THR
1	K	110	THR
1	K	121	VAL
1	K	131	THR
1	K	138	LEU
1	K	175	LEU
1	K	181	VAL
1	K	207	VAL

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Mol	Chain	Res	Type
1	K	212	GLU
2	N	11	VAL
2	N	13	VAL
2	N	28	LEU
2	N	31	LYS
2	N	73	LEU
2	N	82	ASP
2	N	88	CYS
2	N	131	THR
2	N	170	ASN
2	J	28	LEU
2	J	31	LYS
2	J	58	ILE
2	J	82	ASP
2	J	132	LEU
2	J	155	VAL
2	J	159	VAL
2	J	188	HIS
2	L	31	LYS
2	L	58	ILE
2	L	73	LEU
2	L	82	ASP
2	L	91	TRP
2	L	104	VAL
2	L	132	LEU
2	L	159	VAL
2	L	183	GLU
2	L	202	VAL
2	L	203	GLU
2	P	28	LEU
2	P	58	ILE
2	P	73	LEU
2	P	82	ASP
2	P	97	VAL
2	P	132	LEU
2	P	139	PHE
2	P	159	VAL
2	P	183	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	100(B)	ASN
1	M	192	GLN
1	I	58	ASN
1	I	100(B)	ASN
1	I	164	HIS
1	I	197	ASN
1	O	100(B)	ASN
1	O	164	HIS
1	K	100(B)	ASN
1	K	171	GLN
2	N	42	GLN
2	N	69	ASN
2	N	167	GLN
2	J	38	GLN
2	J	42	GLN
2	L	42	GLN
2	P	69	ASN
2	P	167	GLN
2	P	188	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 ⓘ

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	I	218/232 (93%)	1.37	45 (20%) 2 3	26, 51, 87, 123	0
1	K	218/232 (93%)	1.57	55 (25%) 1 2	26, 57, 90, 133	0
1	M	216/232 (93%)	1.68	70 (32%) 1 1	36, 80, 110, 132	0
1	O	216/232 (93%)	1.75	65 (30%) 1 2	38, 79, 109, 131	0
2	J	209/213 (98%)	1.26	45 (21%) 2 3	22, 54, 82, 127	0
2	L	209/213 (98%)	1.31	43 (20%) 2 3	23, 55, 83, 128	0
2	N	209/213 (98%)	1.56	60 (28%) 1 2	45, 65, 89, 130	0
2	P	209/213 (98%)	1.63	68 (32%) 1 1	40, 72, 99, 146	0
All	All	1704/1780 (95%)	1.52	451 (26%) 1 2	22, 65, 99, 146	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	30	SER	7.6
1	O	190	GLY	6.5
1	M	128	SER	6.4
2	P	95	SER	6.1
2	L	95	SER	5.8
1	M	42	GLY	5.6
1	K	127	SER	5.3
1	O	134	GLY	5.3
2	J	107	GLY	5.1
1	O	128	SER	5.1
1	M	15	SER	5.1
1	O	140	CYS	5.1
2	J	57	GLY	4.7
2	L	107	GLY	4.7
1	K	96	PRO	4.5
1	M	172	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	P	91	TRP	4.4
2	J	95	SER	4.4
1	I	102	TYR	4.4
1	K	2	VAL	4.4
1	K	31	SER	4.3
1	O	104	GLY	4.3
2	P	31	LYS	4.3
2	P	30	ASP	4.3
2	N	106	VAL	4.3
1	O	173	SER	4.2
1	K	80	LEU	4.2
1	I	100(A)	VAL	4.2
1	I	31	SER	4.0
2	N	196	THR	4.0
1	K	36	TRP	4.0
1	K	29	ILE	4.0
1	K	28	SER	4.0
1	K	33	TYR	4.0
1	I	42	GLY	3.9
1	K	42	GLY	3.9
1	O	3	GLN	3.9
2	L	168	SER	3.9
2	L	92	ASP	3.8
1	O	209	LYS	3.8
2	N	95	SER	3.8
2	L	91	TRP	3.8
1	I	8	GLY	3.8
2	J	76	SER	3.8
2	N	30	ASP	3.8
2	L	57	GLY	3.7
2	N	67	SER	3.7
2	P	137	SER	3.7
1	K	100(B)	ASN	3.6
1	M	137	ALA	3.6
2	J	83	GLU	3.6
2	P	90	ALA	3.6
1	I	82(A)	SER	3.6
1	O	172	SER	3.6
2	P	198	GLU	3.6
2	P	158	GLY	3.6
1	K	79	SER	3.6
1	M	99	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	116	THR	3.6
1	M	187	SER	3.5
1	I	29	ILE	3.5
1	I	25	SER	3.5
1	I	127	SER	3.5
2	N	92	ASP	3.5
2	P	92	ASP	3.5
2	N	2	TYR	3.5
1	O	43	LYS	3.5
2	J	41	GLY	3.5
1	I	33	TYR	3.5
1	I	131	THR	3.5
1	K	160	THR	3.5
2	J	183	GLU	3.4
1	O	54	SER	3.4
1	O	26	GLY	3.4
1	I	23	THR	3.4
2	N	43	SER	3.4
1	O	2	VAL	3.4
1	O	208	ASP	3.4
1	K	81	LYS	3.4
1	M	65	SER	3.3
1	O	174	GLY	3.3
2	N	16	GLY	3.3
2	P	2	TYR	3.3
1	K	100(A)	VAL	3.3
1	O	99	GLN	3.3
1	K	131	THR	3.3
1	O	9	PRO	3.3
2	J	91	TRP	3.3
1	M	82	LEU	3.2
2	N	155	VAL	3.2
1	M	62	SER	3.2
1	K	73	THR	3.2
1	I	84	ALA	3.2
1	O	100(A)	VAL	3.2
2	N	76	SER	3.2
2	L	169	ASN	3.2
1	I	28	SER	3.2
2	L	24	SER	3.2
1	O	116	THR	3.2
2	N	138	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	67	VAL	3.1
1	O	53	TYR	3.1
2	P	182	PRO	3.1
2	P	80	ALA	3.1
1	O	73	THR	3.1
2	N	162	THR	3.1
2	J	95(A)	THR	3.1
1	K	82(A)	SER	3.1
1	M	196	CYS	3.1
2	J	128	ASN	3.1
1	O	98	GLY	3.0
2	L	83	GLU	3.0
1	M	98	GLY	3.0
1	M	100(B)	ASN	3.0
1	O	157	GLY	3.0
2	N	44	PRO	3.0
1	O	79	SER	3.0
1	M	174	GLY	3.0
2	L	23	CYS	3.0
2	N	3	GLU	3.0
1	O	127	SER	3.0
1	K	206	LYS	3.0
2	L	30	ASP	3.0
1	O	171	GLN	3.0
2	L	95(A)	THR	3.0
1	K	210	ARG	2.9
1	M	214	LYS	2.9
1	O	137	ALA	2.9
1	K	82	LEU	2.9
1	K	156	SER	2.9
1	K	190	GLY	2.9
2	N	107	GLY	2.9
1	I	2	VAL	2.9
1	M	122	PHE	2.9
1	M	127	SER	2.9
1	I	156	SER	2.9
2	J	162	THR	2.9
2	N	187	SER	2.9
2	J	70	THR	2.9
2	L	200	SER	2.8
2	N	157	ALA	2.8
1	I	160	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	170	ASN	2.8
2	L	41	GLY	2.8
2	P	139	PHE	2.8
1	O	65	SER	2.8
1	K	74	SER	2.8
2	J	114	SER	2.8
1	O	126	PRO	2.8
2	L	18	THR	2.8
1	M	167	PRO	2.8
1	I	202	PRO	2.8
2	N	21	ILE	2.8
2	J	94	PHE	2.8
1	I	53	TYR	2.8
1	I	130	SER	2.8
2	J	209	THR	2.8
2	P	4	LEU	2.8
1	O	59	TYR	2.8
2	L	34	CYS	2.8
1	M	3	GLN	2.8
1	M	84	ALA	2.8
2	P	74	THR	2.8
1	M	101	ASP	2.7
1	O	10	GLY	2.7
2	P	107	GLY	2.7
1	K	100(C)	ALA	2.7
2	N	198	GLU	2.7
2	P	196	THR	2.7
1	I	27	GLY	2.7
2	L	16	GLY	2.7
1	I	82	LEU	2.7
2	N	135	LEU	2.7
2	P	203	GLU	2.7
1	O	205	THR	2.7
1	K	26	GLY	2.7
2	N	192	SER	2.7
1	I	26	GLY	2.7
1	M	54	SER	2.7
1	O	201	LYS	2.7
2	N	91	TRP	2.7
1	I	52	TYR	2.7
2	P	83	GLU	2.7
2	L	52	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	144	VAL	2.7
1	I	208	ASP	2.7
2	P	138	ASP	2.7
1	I	9	PRO	2.6
1	O	48	ILE	2.6
1	I	19	SER	2.6
1	O	30	SER	2.6
2	L	21	ILE	2.6
1	K	27	GLY	2.6
2	N	93	SER	2.6
1	K	13	LYS	2.6
1	K	129	LYS	2.6
2	L	109	PRO	2.6
1	O	75	LYS	2.6
1	M	53	TYR	2.6
1	O	52	TYR	2.6
2	L	56	SER	2.6
2	P	165	SER	2.6
2	J	203	GLU	2.6
1	K	17	THR	2.6
2	J	105	THR	2.6
1	K	10	GLY	2.6
2	L	26	ASP	2.6
1	M	93	ALA	2.6
2	N	80	ALA	2.6
2	J	200	SER	2.5
2	P	93	SER	2.5
2	N	45	VAL	2.5
2	N	128	ASN	2.5
2	P	103	LYS	2.5
2	P	32	TYR	2.5
2	N	23	CYS	2.5
1	M	120	SER	2.5
2	J	25	GLY	2.5
2	P	144	VAL	2.5
2	J	26	ASP	2.5
2	P	151	ASP	2.5
1	I	51	ILE	2.5
1	M	9	PRO	2.5
1	O	61	PRO	2.5
1	M	43	LYS	2.5
1	M	108	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	44	GLY	2.5
2	L	29	GLY	2.5
2	P	77	GLY	2.5
1	I	128	SER	2.5
2	L	76	SER	2.5
2	P	71	ALA	2.5
2	J	169	ASN	2.5
1	M	165	THR	2.5
2	J	5	THR	2.5
1	M	206	LYS	2.5
1	O	81	LYS	2.5
2	J	106	VAL	2.5
1	K	94	SER	2.5
2	N	63	SER	2.5
1	I	76	ASN	2.5
2	L	151	ASP	2.5
2	N	4	LEU	2.5
1	O	102	TYR	2.5
1	M	104	GLY	2.5
1	K	192	GLN	2.5
2	P	143	ALA	2.4
2	N	123	GLU	2.4
2	N	209	THR	2.4
2	J	29	GLY	2.4
2	J	58	ILE	2.4
2	P	21	ILE	2.4
1	O	35	SER	2.4
1	K	212	GLU	2.4
2	J	54	ARG	2.4
2	J	166	LYS	2.4
2	J	30	ASP	2.4
2	P	209	THR	2.4
1	K	53	TYR	2.4
1	O	29	ILE	2.4
1	O	168	ALA	2.4
2	P	166	LYS	2.4
1	M	79	SER	2.4
2	N	46	LEU	2.4
2	N	132	LEU	2.4
1	M	107	THR	2.4
2	N	119	PRO	2.4
2	L	128	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	161	THR	2.4
2	P	195	VAL	2.4
2	N	129	LYS	2.4
2	N	94	PHE	2.4
2	P	52	SER	2.4
1	K	87	THR	2.4
1	I	190	GLY	2.4
2	N	142	GLY	2.4
2	L	25	GLY	2.4
1	K	84	ALA	2.4
1	M	171	GLN	2.4
1	I	4	LEU	2.4
1	K	187	SER	2.4
1	M	2	VAL	2.4
2	P	40	PRO	2.4
1	M	27	GLY	2.3
2	P	199	GLY	2.3
1	O	199	ASN	2.3
2	N	69	ASN	2.3
2	J	56	SER	2.3
1	M	87	THR	2.3
1	O	68	THR	2.3
2	N	70	THR	2.3
2	N	199	GLY	2.3
2	L	162	THR	2.3
2	L	209	THR	2.3
1	M	114	ALA	2.3
2	N	88	CYS	2.3
2	J	170	ASN	2.3
2	N	151	ASP	2.3
1	M	146	PHE	2.3
1	O	108	LEU	2.3
2	L	28	LEU	2.3
1	K	182	VAL	2.3
1	O	21	THR	2.3
2	P	56	SER	2.3
1	I	80	LEU	2.3
1	M	105	GLN	2.3
1	M	44	GLY	2.3
1	M	162	GLY	2.3
1	M	17	THR	2.3
2	J	163	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	100	LEU	2.3
1	O	121	VAL	2.3
1	M	157	GLY	2.3
2	N	68	GLY	2.3
2	N	112	ALA	2.3
1	O	28	SER	2.3
1	K	128	SER	2.3
2	J	168	SER	2.3
2	P	97	VAL	2.3
2	L	68	GLY	2.2
2	L	5	THR	2.2
1	K	7	SER	2.2
1	K	54	SER	2.2
1	K	201	LYS	2.2
2	P	49	TYR	2.2
1	O	101	ASP	2.2
2	P	3	GLU	2.2
2	P	55	PRO	2.2
2	P	147	ALA	2.2
1	I	151	THR	2.2
1	O	151	THR	2.2
2	J	161	THR	2.2
2	J	2	TYR	2.2
2	P	122	SER	2.2
2	P	45	VAL	2.2
1	M	192	GLN	2.2
2	P	128	ASN	2.2
2	P	23	CYS	2.2
2	P	123	GLU	2.2
1	M	139	GLY	2.2
1	O	44	GLY	2.2
1	K	159	LEU	2.2
2	J	92	ASP	2.2
1	I	81	LYS	2.2
1	I	34	TRP	2.2
2	N	201	THR	2.2
1	I	32	TYR	2.2
1	I	179	SER	2.2
1	O	94	SER	2.2
1	K	197	ASN	2.2
1	M	159	LEU	2.2
1	O	95	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	14	PRO	2.2
1	K	9	PRO	2.2
2	L	58	ILE	2.2
1	I	16	GLU	2.2
1	M	8	GLY	2.2
1	M	61	PRO	2.2
1	I	104	GLY	2.2
1	O	214	LYS	2.2
2	N	113	PRO	2.2
2	P	29	GLY	2.2
2	L	94	PHE	2.2
1	M	95	LEU	2.1
1	K	95	LEU	2.1
1	M	70	SER	2.1
1	K	30	SER	2.1
1	K	43	LYS	2.1
2	N	149	LYS	2.1
2	P	157	ALA	2.1
2	P	179	SER	2.1
1	O	16	GLU	2.1
2	N	124	GLU	2.1
2	P	183	GLU	2.1
1	M	154	TRP	2.1
1	M	73	THR	2.1
2	N	95(A)	THR	2.1
1	M	29	ILE	2.1
1	O	138	LEU	2.1
2	P	46	LEU	2.1
1	K	93	ALA	2.1
1	M	16	GLU	2.1
1	M	126	PRO	2.1
1	M	212	GLU	2.1
1	M	213	PRO	2.1
2	P	60	GLU	2.1
1	O	36	TRP	2.1
2	L	45	VAL	2.1
2	N	74	THR	2.1
2	N	105	THR	2.1
2	N	180	LEU	2.1
2	P	95(A)	THR	2.1
1	M	145	TYR	2.1
2	L	54	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	42	GLN	2.1
2	P	50	GLN	2.1
2	P	127	ALA	2.1
2	J	67	SER	2.1
2	P	187	SER	2.1
2	N	169	ASN	2.1
2	J	47	VAL	2.1
2	N	156	LYS	2.1
1	O	87	THR	2.1
2	P	145	THR	2.1
2	J	50	GLN	2.1
2	J	3	GLU	2.1
2	P	15	PRO	2.1
2	P	62	PHE	2.1
2	P	94	PHE	2.1
1	O	82(A)	SER	2.1
1	O	188	SER	2.1
1	O	203	SER	2.1
1	M	100(A)	VAL	2.1
1	M	81	LYS	2.1
1	M	209	LYS	2.1
2	L	138	ASP	2.1
2	L	88	CYS	2.1
2	N	71	ALA	2.1
2	J	99	GLY	2.1
2	L	194	GLN	2.1
1	K	64	LYS	2.0
2	L	11	VAL	2.0
1	K	179	SER	2.0
2	N	176	SER	2.0
2	J	137	SER	2.0
2	P	14	SER	2.0
2	L	73	LEU	2.0
1	K	183	THR	2.0
2	J	49	TYR	2.0
2	L	105	THR	2.0
1	K	92	CYS	2.0
1	M	134	GLY	2.0
1	I	105	GLN	2.0
1	M	40	PRO	2.0
1	M	143	LYS	2.0
2	P	106	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	106(A)	LEU	2.0
1	I	215	SER	2.0
1	O	70	SER	2.0
2	J	75	ILE	2.0
2	J	179	SER	2.0
2	L	80	ALA	2.0
1	I	10	GLY	2.0
1	I	196	CYS	2.0
2	N	193	CYS	2.0
2	P	193	CYS	2.0
1	O	105	GLN	2.0
2	P	38	GLN	2.0
1	M	66	ARG	2.0
2	N	125	LEU	2.0
1	M	48	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.