



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 01:11 PM EST

PDB ID : 4QHK
Title : UCA (unbound) from CH103 Lineage
Authors : Fera, D.; Harrison, S.C.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

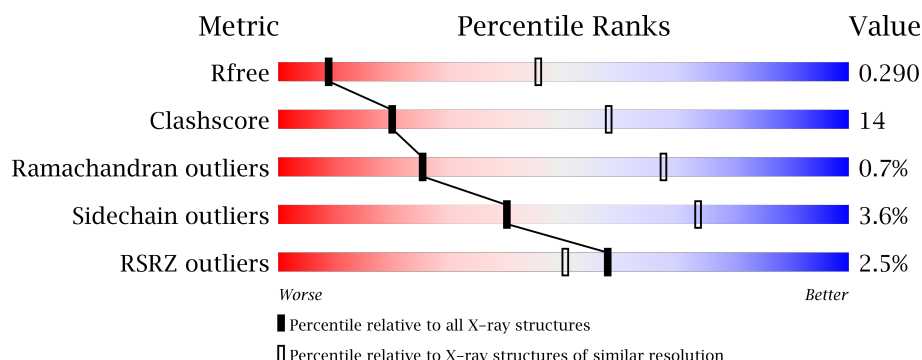
1 Overall quality at a glance

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}	100719	1049 (3.58-3.38)
Clashscore	112137	1096 (3.56-3.40)
Ramachandran outliers	110173	1063 (3.56-3.40)
Sidechain outliers	110143	1064 (3.56-3.40)
RSRZ outliers	101464	1019 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 59%, yellow 31%, orange 6%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 100% 59% 31% 6% </div> </div>
1	K	232	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 23%, orange 6%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 100% 69% 23% 6% </div> </div>
1	M	232	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 63%, yellow 28%, orange 7%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 100% 63% 28% 7% </div> </div>
1	O	232	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 61%, yellow 31%, orange 7%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 100% 61% 31% 7% </div> </div>
2	J	213	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 27%, orange 3%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 100% 69% 27% </div> </div>

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Mol	Chain	Length	Quality of chain
2	L	213	<div><div></div><div>2%</div><div>70%</div><div>27%</div><div>..</div></div>
2	N	213	<div><div></div><div>3%</div><div>67%</div><div>30%</div><div>..</div></div>
2	P	213	<div><div></div><div>4%</div><div>64%</div><div>31%</div><div>..</div></div>

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			

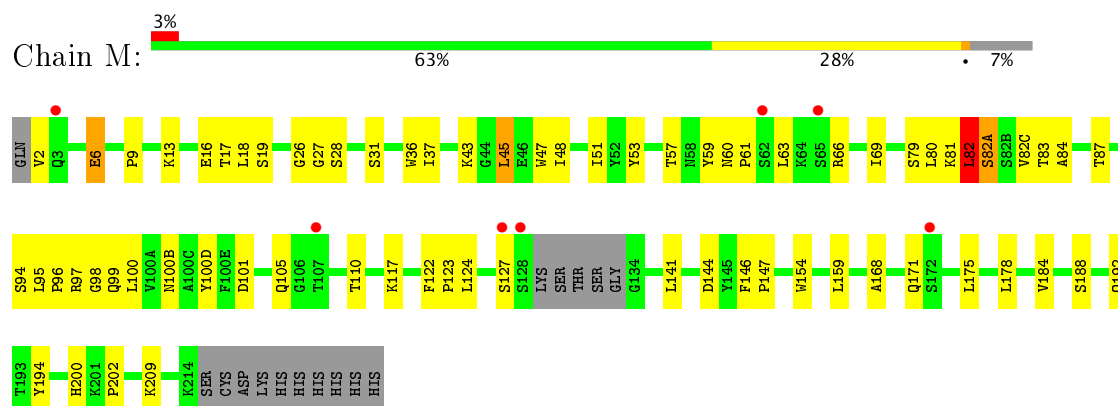
- Molecule 2 is a protein called UCA light chain.

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			

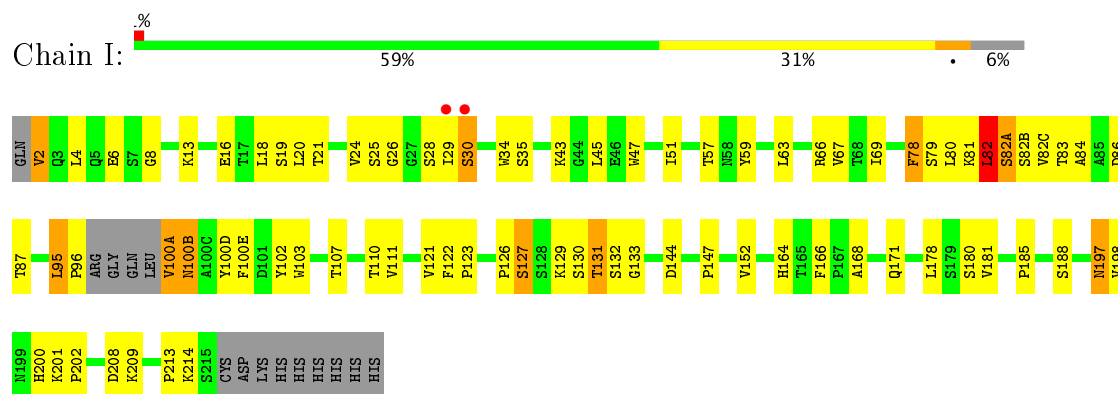
3 Residue-property plots [i](#)

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

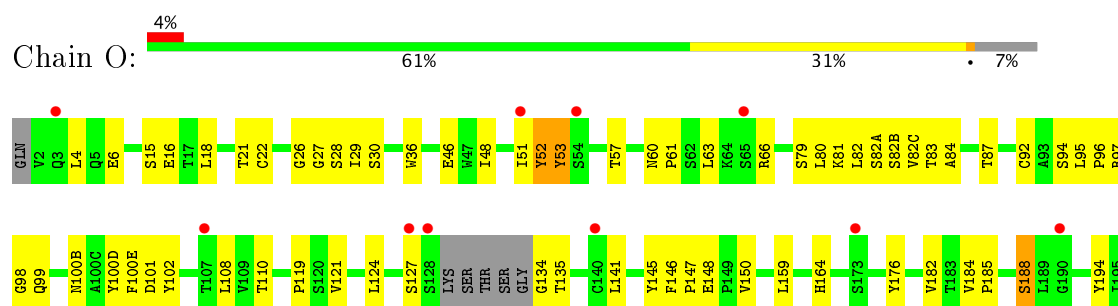
• Molecule 1: UCA heavy chain



• Molecule 1: UCA heavy chain



• Molecule 1: UCA heavy chain

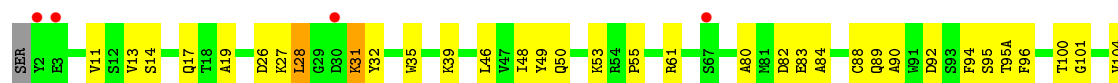




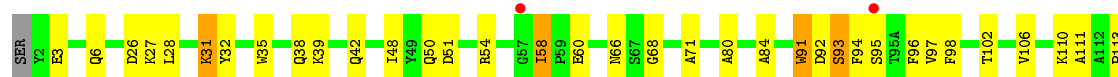
• Molecule 1: UCA heavy chain



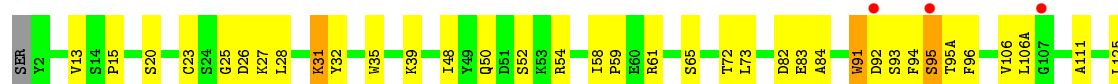
• Molecule 2: UCA light chain



• Molecule 2: UCA light chain

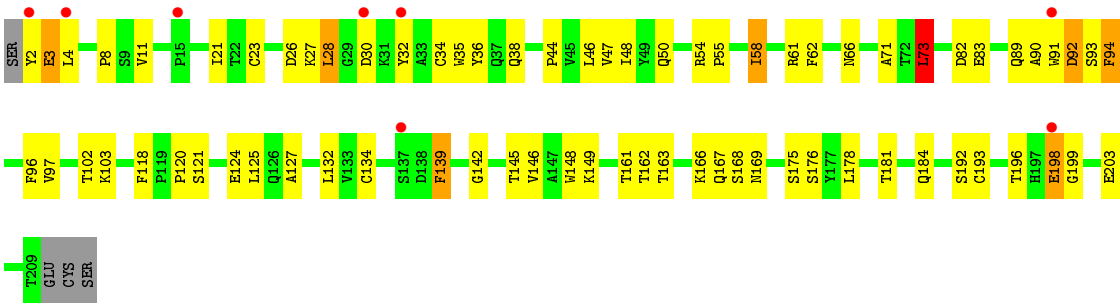


• Molecule 2: UCA light chain



• 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	78.69 Å 71.15 Å 184.40 Å 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) 90.4 (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 3.48 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.269 , 0.285 0.268 , 0.290	Depositor DCC
R_{free} test set	1208 reflections (5.08%)	DCC
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 , 17.9	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/1673	0.60	3/2289 (0.1%)
1	K	0.28	0/1673	0.57	0/2289
1	M	0.28	0/1667	0.58	2/2281 (0.1%)
1	O	0.30	0/1667	0.56	0/2281
2	J	0.29	0/1614	0.54	1/2206 (0.0%)
2	L	0.28	0/1614	0.52	0/2206
2	N	0.28	0/1614	0.53	0/2206
2	P	0.29	0/1614	0.57	1/2206 (0.0%)
All	All	0.29	0/13136	0.56	7/17964 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	73	LEU	CA-CB-CG	6.11	129.34	115.30
1	I	95	LEU	CA-CB-CG	6.04	129.19	115.30
1	M	82(A)	SER	C-N-CA	5.75	136.07	121.70
1	I	82(A)	SER	C-N-CA	5.41	135.22	121.70
1	I	82	LEU	CA-CB-CG	5.32	127.54	115.30
1	M	82	LEU	CA-CB-CG	5.25	127.37	115.30
2	J	93	SER	C-N-CA	5.12	134.50	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1630	0	1600	60	0
1	K	1630	0	1600	43	0
1	M	1624	0	1597	49	0
1	O	1624	0	1597	52	0
2	J	1573	0	1513	44	0
2	L	1573	0	1513	48	1
2	N	1573	0	1513	56	0
2	P	1573	0	1513	45	1
All	All	12800	0	12446	359	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 14.

All (359) 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
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
2:N:13:VAL:HG21	2:N:19:ALA:HB2	1.74	0.70
1:O:87:THR:HG23	1:O:110:THR:HA	1.73	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:123:PRO:HD3	1:M:209:LYS:HE2	1.74	0.69
1:M:36:TRP:HB2	1:M:48:ILE:HD11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:I:82(A):SER:H	1:I:82(C):VAL:N	2.01	0.58
1:M:168:ALA:HA	1:M:178:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:LYS:NZ	2:J:51:ASP:OD2	2.25	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
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:K:2:VAL:HG11	1:K:27:GLY:HA2	1.90	0.54
1:O:21:THR:HG22	1:O:79:SER:HB3	1.90	0.54
1:K:185:PRO:HG2	1:K:188:SER:HB3	1.88	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:L:134:CYS:HB3	2:L:176:SER:HB2	1.91	0.53
2:N:132:LEU:HB2	2:N:178:LEU:HB3	1.90	0.53
2:N:46:LEU:CD2	2:N:55:PRO:HG3	2.39	0.53
1:K:82:LEU:O	1:K:82(C):VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:59:TYR:HE1	1:M:69:ILE:HG13	1.74	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
2:P:35:TRP:CD2	2:P:73:LEU:HD23	2.45	0.52
2:J:31:LYS:HG2	2:J:91:TRP:CE2	2.44	0.51
2:N:156:LYS:HG3	2:N:157:ALA:H	1.74	0.51
1:O:100(B):ASN:ND2	2:P:50:GLN:HE21	2.08	0.51
2:J:93:SER:H	2:J:95:SER:N	2.09	0.51
1:K:94:SER:OG	1:K:101:ASP:O	2.25	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
1:K:35:SER:HG	1:K:100(E):PHE:HE1	1.56	0.51
2:P:28:LEU:O	2:P:30:ASP:N	2.41	0.51
2:P:121:SER:OG	2:P:124:GLU:OE1	2.24	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:N	1:K:100(B):ASN:OD1	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
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
2:N:162:THR:HG22	2:N:175:SER:H	1.77	0.49
1:O:119:PRO:HB3	1:O:145:TYR:HB3	1.94	0.49
1:M:47:TRP:CZ3	2:N:95(A):THR:HB	2.47	0.49
1:M:43:LYS:HZ3	2:N:101:GLY:HA3	1.77	0.49
1:O:134:GLY:C	1:O:135:THR:HG23	2.33	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
1:I:166:PHE:CE2	2:J:135:LEU:HD22	2.47	0.49
1:O:4:LEU:HB3	1:O:92:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:98:GLY:N	1:O:99:GLN:HA	2.28	0.49
1:I:168:ALA:HA	1:I:178:LEU:HB3	1.95	0.48
1:M:43:LYS:NZ	2:N:101:GLY:HA3	2.28	0.48
1:I:185:PRO:HG2	1:I:188:SER:HB3	1.95	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
2:J:125:LEU:C	2:J:127:ALA:H	2.17	0.48
1:M:47:TRP:HZ3	2:N:95(A):THR:HB	1.79	0.48
1:O:29:ILE:HG23	1:O:53:TYR:CZ	2.48	0.48
1:O:97:ARG:C	1:O:99:GLN:HA	2.34	0.48
1:I:26:GLY:C	1:I:28:SER:HA	2.33	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
2:L:28:LEU:HG	2:L:31:LYS:HD2	1.94	0.47
2:P:89:GLN:HG2	2:P:90:ALA:N	2.29	0.47
1:I:147:PRO:HD2	1:I:202:PRO:HB2	1.96	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
2:P:125:LEU:C	2:P:127:ALA:H	2.17	0.47
1:K:100(B):ASN:HD22	2:L:50:GLN:CG	2.28	0.47
2:N:14:SER:O	2:N:17:GLN:HG2	2.14	0.47
1:O:48:ILE:O	1:O:60:ASN:N	2.36	0.47
2:P:93:SER:O	2:P:94:PHE:CG	2.67	0.47
1:I:35:SER:HG	1:I:100(E):PHE:HE1	1.61	0.47
1:M:192:GLN:CD	1:M:194:TYR:HE2	2.18	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:L:93:SER:H	2:L:95:SER:N	2.13	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
2:J:110:LYS:NZ	2:J:198:GLU:OE1	2.35	0.46
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:N:26:ASP:HA	2:N:27:LYS:HA	1.53	0.46
1:I:152:VAL:HA	1:I:197:ASN:O	2.14	0.46
1:I:47:TRP:CE3	2:J:96:PHE:HB2	2.51	0.46
1:M:117:LYS:HD3	1:M:175:LEU:HD13	1.97	0.46
2:N:13:VAL:HG12	2:N:106:VAL:HG12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:149:LYS:HG2	2:N:154:PRO:HA	1.97	0.46
1:O:159:LEU:HD23	1:O:182:VAL:HG21	1.98	0.46
1:O:22:CYS:HB2	1:O:36:TRP:CH2	2.51	0.46
2:J:35:TRP:HB2	2:J:48:ILE:HB	1.98	0.46
2:J:139:PHE:HE2	2:J:142:GLY:HA2	1.81	0.46
2:J:38:GLN:O	2:J:84:ALA:HB1	2.15	0.46
1:I:168:ALA:HB2	1:I:178:LEU:HD23	1.98	0.46
2:L:125:LEU:C	2:L:127:ALA:H	2.20	0.46
2:P:26:ASP:HA	2:P:27:LYS:HA	1.46	0.45
2:J:93:SER:HB3	2:J:94:PHE:CB	2.42	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:P:148:TRP:CZ3	2:P:193:CYS:HB2	2.51	0.45
1:I:45:LEU:HD23	2:J:98:PHE:CD1	2.51	0.45
1:K:60:ASN:OD1	1:K:62:SER:OG	2.21	0.45
1:M:43:LYS:NZ	2:N:100:THR:O	2.39	0.45
1:O:36:TRP:HB3	1:O:48:ILE:HD11	1.98	0.45
2:P:162:THR:CG2	2:P:175:SER:H	2.29	0.45
1:O:100(E):PHE:N	2:P:36:TYR:OH	2.26	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
2:N:134:CYS:HB3	2:N:176:SER:HB3	1.98	0.45
1:O:83:THR:OG1	1:O:84:ALA:N	2.50	0.45
1:I:130:SER:HA	1:I:131:THR:HA	1.70	0.45
2:N:141:PRO:HD2	2:N:198:GLU:OE2	2.17	0.45
1:O:60:ASN:HA	1:O:61:PRO:HD3	1.87	0.45
2:P:11:VAL:HG21	2:P:21:ILE:HG13	1.98	0.45
1:I:123:PRO:O	2:J:121:SER:HB3	2.17	0.45
1:I:34:TRP:HB3	1:I:78:PHE:CE1	2.52	0.45
2:J:149:LYS:HG2	2:J:154:PRO:HA	1.98	0.45
2:L:54:ARG:HH22	2:L:59:PRO:C	2.21	0.44
1:K:130:SER:HA	1:K:131:THR:HA	1.64	0.44
1:K:19:SER:HA	1:K:80:LEU:O	2.17	0.44
1:M:48:ILE:HG22	1:M:63:LEU:HD22	1.98	0.44
2:N:162:THR:CG2	2:N:175:SER:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100(B):ASN:HB3	2:P:32:TYR:CD2	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
1:O:52:TYR:OH	1:O:97:ARG:NH1	2.51	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:35:SER:C	1:K:36:TRP:HD1	2.20	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
2:L:26:ASP:HA	2:L:27:LYS:HA	1.63	0.44
2:N:119:PRO:HG3	2:N:206:VAL:HG11	2.00	0.44
1:O:185:PRO:HG2	1:O:188:SER:HB3	2.00	0.44
1:O:27:GLY:N	1:O:28:SER:HA	2.31	0.44
1:I:4:LEU:HD23	1:I:24:VAL:HG12	2.00	0.44
1:K:21:THR:HG22	1:K:79:SER:HB2	2.00	0.44
1:K:8:GLY:HA3	1:K:20:LEU:HD23	2.00	0.44
1:M:154:TRP:HB2	1:M:159:LEU:HB2	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
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
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
2:J:148:TRP:HB2	2:J:155:VAL:HG12	2.00	0.43
1:K:47:TRP:CD2	2:L:96:PHE:HB2	2.54	0.43
2:L:93:SER:HB3	2:L:94:PHE:CB	2.44	0.43
1:O:26:GLY:C	1:O:28:SER:HA	2.39	0.43
1:I:96:PRO:HG2	1:I:100(D):TYR:CZ	2.54	0.43
1:K:71:VAL:HG23	1:K:78:PHE:HB3	2.01	0.43
2:L:92:ASP:O	2:L:95:SER:HB3	2.19	0.43
2:N:125:LEU:C	2:N:127:ALA:H	2.22	0.43
2:N:145:THR:HB	2:N:196:THR:OG1	2.19	0.43
1:O:196:CYS:O	1:O:208:ASP:HA	2.19	0.43
1:K:126:PRO:HD2	1:K:213:PRO:HA	2.01	0.43
1:M:83:THR:OG1	1:M:84:ALA:N	2.50	0.43
1:O:15:SER:HA	1:O:82(B):SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:PRO:HA	2:J:139:PHE:HB3	2.00	0.43
1:M:146:PHE:HA	1:M:147:PRO:HA	1.77	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
1:O:146:PHE:HA	1:O:147:PRO:HA	1.86	0.42
1:I:13:LYS:HB2	1:I:16:GLU:CD	2.39	0.42
2:J:60:GLU:H	2:J:60:GLU:CD	2.23	0.42
2:L:93:SER:H	2:L:94:PHE:C	2.22	0.42
1:M:37:ILE:HG21	1:M:45:LEU:HD21	2.00	0.42
2:N:167:GLN:HB3	2:N:168:SER:H	1.53	0.42
1:M:100(B):ASN:HB3	2:N:32:TYR:CD2	2.54	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: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
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
2:N:13:VAL:HG22	2:N:17:GLN:HG3	2.02	0.42
1:O:150:VAL:HG22	1:O:200:HIS:CD2	2.55	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:L:185:TRP:O	2:L:208:PRO:HG3	2.19	0.42
2:N:207:ALA:HA	2:N:208:PRO:HD2	1.77	0.42
1:K:80:LEU:C	1:K:81:LYS:HD2	2.40	0.42
1:I:35:SER:HB2	1:I:47:TRP:HE1	1.84	0.41
2:J:124:GLU:HG2	2:J:129:LYS:O	2.20	0.41
2:J:26:ASP:HA	2:J:27:LYS:HA	1.56	0.41
1:K:2:VAL:HG22	1:K:102:TYR:CD1	2.55	0.41
1:M:36:TRP:CG	1:M:80:LEU:HD12	2.55	0.41
2:P:46:LEU:O	2:P:55:PRO:HG3	2.20	0.41
2:J:110:LYS:HG2	2:J:111:ALA:N	2.35	0.41
1:K:131:THR:OG1	1:K:135:THR:O	2.34	0.41
2:L:111:ALA:HB3	2:L:140:TYR:H	1.85	0.41
1:M:26:GLY:C	1:M:28:SER:HA	2.40	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:O:121:VAL:HB	1:O:209:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100(B):ASN:HB3	2:P:32:TYR:CG	2.56	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
2:L:168:SER:C	2:L:170:ASN:H	2.23	0.41
2:L:146:VAL:HG11	2:L:176:SER:OG	2.20	0.41
2:L:28:LEU:HA	2:L:31:LYS:CD	2.49	0.41
1:O:184:VAL:HG11	1:O:194:TYR:CE1	2.56	0.41
2:L:196:THR:HG22	2:L:201:THR:OG1	2.20	0.41
2:L:32:TYR:HD1	2:L:50:GLN:HA	1.85	0.41
1:M:16:GLU:HB3	1:M:17:THR:H	1.66	0.41
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
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
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.56	0.41
1:O:207:VAL:HG11	1:O:209:LYS:NZ	2.35	0.41
1:O:36:TRP:O	1:O:48:ILE:HG12	2.21	0.41
1:K:78:PHE:CD2	1:K:78:PHE:N	2.89	0.41
2:N:170:ASN:ND2	2:N:170:ASN:O	2.48	0.41
2:N:136:ILE:HG12	2:N:195:VAL:HG21	2.03	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
1:O:148:GLU:HG2	1:O:176:TYR:CD2	2.55	0.41
2:P:21:ILE:HG12	2:P:102:THR:HG21	2.03	0.41
1:I:129:LYS:NZ	1:I:132:SER:HB3	2.36	0.41
2:L:65:SER:OG	2:L:72:THR:HG22	2.20	0.41
1:I:164:HIS:HE1	2:J:173:ALA:HB3	1.86	0.41
1:M:9:PRO:HD3	1:M:19:SER:O	2.21	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:I:100(B):ASN:ND2	1:I:100(B):ASN:N	2.69	0.40
1:K:20:LEU:HB2	1:K:36:TRP:CZ3	2.55	0.40
1:M:27:GLY:N	1:M:28:SER:HA	2.36	0.40
2:N:89:GLN:HG2	2:N:90:ALA:N	2.36	0.40
1:M:47:TRP:CE2	2:N:96:PHE:HD2	2.38	0.40
1:O:96:PRO:HG2	1:O:100(D):TYR:CZ	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:SER:O	1:M:97:ARG:HB2	2.22	0.40
2:P:27:LYS:HB2	2:P:28:LEU:H	1.69	0.40
2:J:145:THR:OG1	2:J:196:THR:HB	2.22	0.40
2:J:92:ASP:O	2:J:95:SER:HB3	2.21	0.40
2:N:134:CYS:HB2	2:N:148:TRP:CH2	2.57	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%)	20	63
1	K	214/232 (92%)	193 (90%)	21 (10%)	0	100	100
1	M	212/232 (91%)	192 (91%)	19 (9%)	1 (0%)	32	73
1	O	212/232 (91%)	192 (91%)	18 (8%)	2 (1%)	20	63
2	J	207/213 (97%)	175 (84%)	32 (16%)	0	100	100
2	L	207/213 (97%)	173 (84%)	33 (16%)	1 (0%)	32	73
2	N	207/213 (97%)	176 (85%)	30 (14%)	1 (0%)	32	73
2	P	207/213 (97%)	175 (84%)	27 (13%)	5 (2%)	7	41
All	All	1680/1780 (94%)	1470 (88%)	198 (12%)	12 (1%)	25	67

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%)	177 (94%)	12 (6%)	21	58
1	K	189/202 (94%)	182 (96%)	7 (4%)	39	73
1	M	187/202 (93%)	180 (96%)	7 (4%)	39	73
1	O	187/202 (93%)	180 (96%)	7 (4%)	39	73
2	J	178/182 (98%)	173 (97%)	5 (3%)	49	79
2	L	178/182 (98%)	174 (98%)	4 (2%)	57	83
2	N	178/182 (98%)	174 (98%)	4 (2%)	57	83
2	P	178/182 (98%)	171 (96%)	7 (4%)	37	72
All	All	1464/1536 (95%)	1411 (96%)	53 (4%)	40	73

All (53) 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

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Mol	Chain	Res	Type
1	M	53	TYR
1	M	79	SER
1	M	82	LEU
1	I	2	VAL
1	I	6	GLU
1	I	30	SER
1	I	78	PHE
1	I	82	LEU
1	I	95	LEU
1	I	100(A)	VAL
1	I	100(B)	ASN
1	I	131	THR
1	I	181	VAL
1	I	197	ASN
1	I	208	ASP
1	O	6	GLU
1	O	46	GLU
1	O	52	TYR
1	O	53	TYR
1	O	82	LEU
1	O	108	LEU
1	O	188	SER
1	K	78	PHE
1	K	82	LEU
1	K	100(B)	ASN
1	K	121	VAL
1	K	131	THR
1	K	175	LEU
1	K	181	VAL
2	N	28	LEU
2	N	31	LYS
2	N	88	CYS
2	N	170	ASN
2	J	28	LEU
2	J	31	LYS
2	J	58	ILE
2	J	91	TRP
2	J	155	VAL
2	L	31	LYS
2	L	91	TRP
2	L	183	GLU
2	L	203	GLU

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Mol	Chain	Res	Type
2	P	28	LEU
2	P	58	ILE
2	P	73	LEU
2	P	92	ASP
2	P	97	VAL
2	P	139	PHE
2	P	203	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	100(B)	ASN
1	M	192	GLN
1	I	100(B)	ASN
1	I	164	HIS
1	I	197	ASN
1	O	100(B)	ASN
1	O	164	HIS
1	K	171	GLN
2	N	128	ASN
2	N	167	GLN
2	J	38	GLN
2	J	42	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	I	218/232 (93%)	0.03	2 (0%) 84 78	26, 51, 87, 123	0
1	K	218/232 (93%)	0.14	3 (1%) 75 68	26, 57, 90, 133	0
1	M	216/232 (93%)	0.44	7 (3%) 48 42	36, 80, 110, 132	0
1	O	216/232 (93%)	0.47	10 (4%) 33 28	38, 79, 109, 131	0
2	J	209/213 (98%)	0.03	2 (0%) 82 76	22, 54, 82, 127	0
2	L	209/213 (98%)	0.07	4 (1%) 67 60	23, 55, 83, 128	0
2	N	209/213 (98%)	0.40	7 (3%) 47 41	45, 65, 89, 130	0
2	P	209/213 (98%)	0.43	8 (3%) 41 36	40, 72, 99, 146	0
All	All	1704/1780 (95%)	0.25	43 (2%) 58 50	22, 65, 99, 146	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	128	SER	4.4
1	K	28	SER	3.7
1	M	65	SER	3.7
2	N	2	TYR	3.5
1	I	30	SER	3.3
2	N	106	VAL	3.3
2	P	2	TYR	3.1
1	O	140	CYS	3.0
2	P	30	ASP	3.0
2	P	198	GLU	3.0
1	O	128	SER	2.9
1	M	172	SER	2.8
1	O	107	THR	2.7
1	O	54	SER	2.7
1	O	190	GLY	2.7
2	L	95	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	27	GLY	2.6
1	M	127	SER	2.5
2	N	67	SER	2.5
2	J	95	SER	2.5
2	L	92	ASP	2.5
1	K	29	ILE	2.4
1	M	62	SER	2.4
1	M	3	GLN	2.4
1	O	127	SER	2.4
2	L	107	GLY	2.4
1	I	29	ILE	2.3
2	N	3	GLU	2.3
2	P	91	TRP	2.2
2	N	168	SER	2.2
2	N	30	ASP	2.2
1	O	173	SER	2.2
1	O	51	ILE	2.2
1	M	107	THR	2.2
2	P	137	SER	2.1
2	L	168	SER	2.1
2	P	15	PRO	2.1
1	O	3	GLN	2.1
2	J	57	GLY	2.1
2	P	4	LEU	2.1
2	N	198	GLU	2.0
2	P	32	TYR	2.0
1	O	65	SER	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 carbohydrates 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.