Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:57 PM GMT

PDB ID	:	4QHK
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

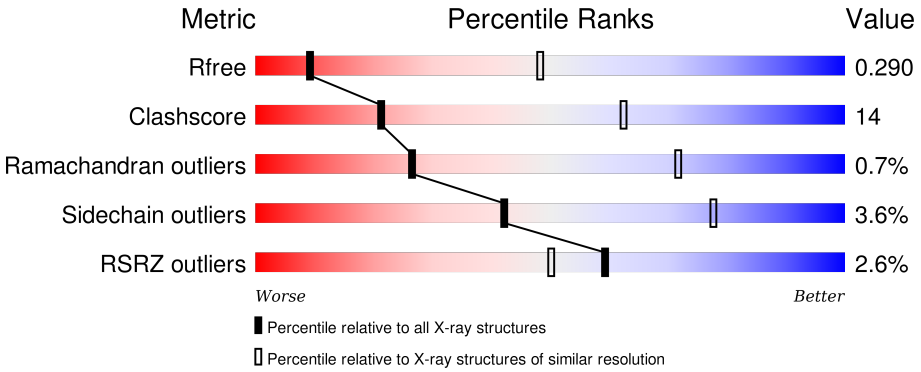
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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 <=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	59% 31% 6%
1	K	232	69% 23% 6%
1	M	232	3% 63% 28% 7%
1	O	232	5% 61% 31% 7%
2	J	213	69% 27%

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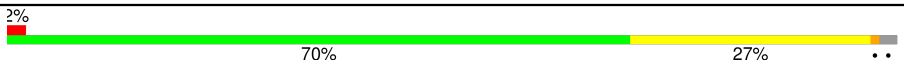
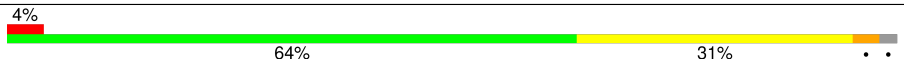
Mol	Chain	Length	Quality of chain
2	L	213	
2	N	213	
2	P	213	

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.

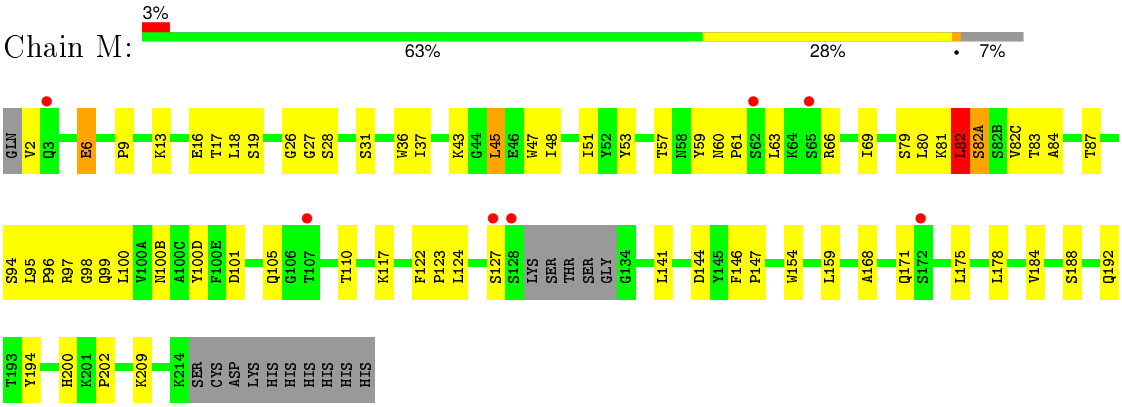
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	J	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	L	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			
2	P	209	Total	C	N	O	S	0	0	0
			1573	988	257	322	6			

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 errors 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.

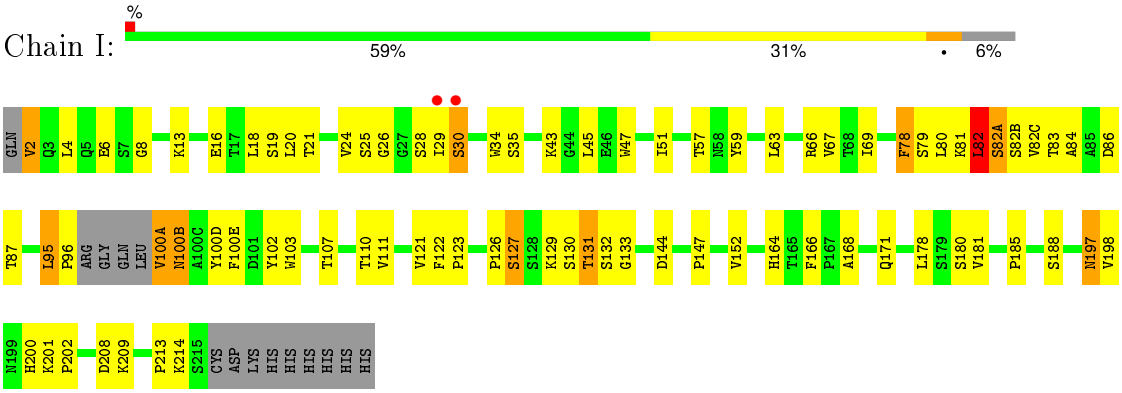
- Molecule 1: UCA heavy chain

Chain M:



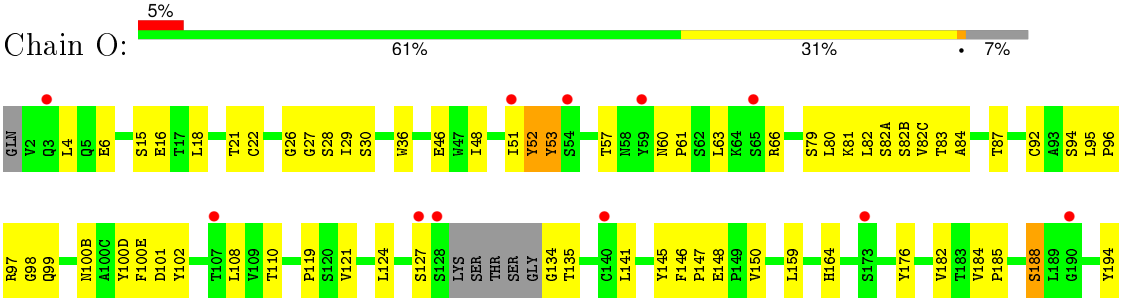
- Molecule 1: UCA heavy chain

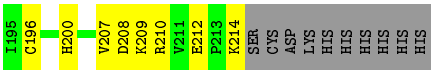
Chain I:



- Molecule 1: UCA heavy chain

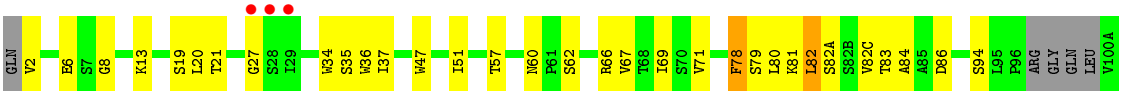
Chain O:

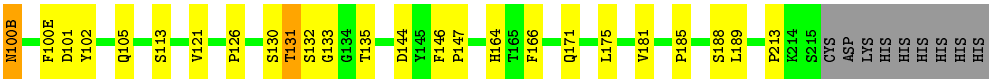




• Molecule 1: UCA heavy chain

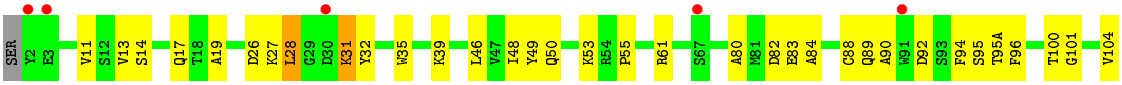
Chain K:

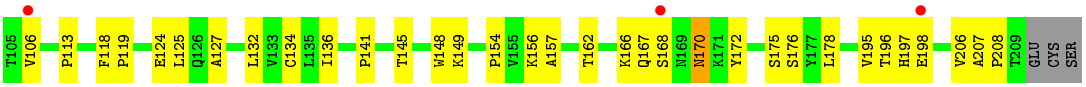




• Molecule 2: UCA light chain

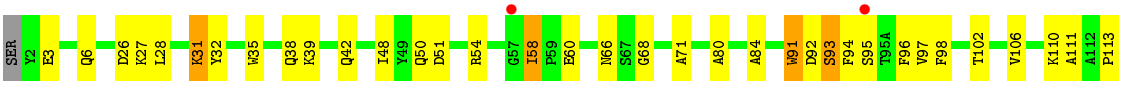
Chain N:





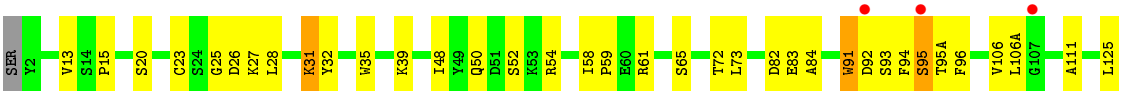
• Molecule 2: UCA light chain

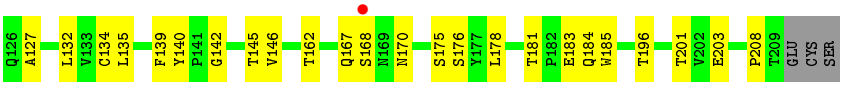
Chain J:



• Molecule 2: UCA light chain

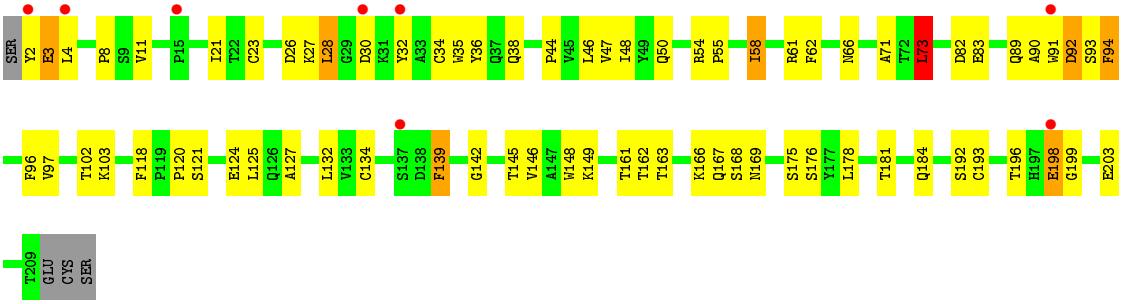
Chain L:





• Molecule 2: UCA light chain

Chain P:


SER Y2 E3 L4 P8 S9 V11 P15 I21 T22 C23 D26 K27 L28 G29 D30 K31 Y32 A33 C34 W35 Y36 Q37 Q38 P44 V45 L46 V47 I48 Y49 Q50 R54 P55 I58 R61 F62 N66 A71 I72 L73 D82 E83 Q89 A90 W91 D92 S93 F94
F96 V97 T102 K103 F118 P119 P120 S121 E124 L125 Q126 A127 L132 V133 C134 S137 D138 F139 G142 T145 V146 A147 W148 K149 T161 T162 T163 K166 Q167 S168 N169 S175 S176 Y177 L178 T181 Q184 S192 C193 T196 H197 E198 G199 E203
T209 GLU CYS SER

4 Data and refinement statistics (i)

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) 90.4 (46.85-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 23851 reflections (0.004%)	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	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(^{o})	Ideal(^{o})
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

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
2:N:35:TRP:HB2	2:N:48:ILE:HB	1.73	0.70
1:I:87:THR:HG23	1:I:110:THR:HA	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:O:164:HIS:CE1	2:P:167:GLN:HE21	2.11	0.69
1:M:87:THR:HG23	1:M:110:THR:HA	1.75	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

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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:156:LYS:NZ	2:P:163:THR:OG1	2.29	0.64
2:N:39:LYS:HD3	2:N:84:ALA:HB2	1.79	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:P:83:GLU:O	2:P:166:LYS:NZ	2.33	0.61
2:J:54:ARG:HB2	2:J:58:ILE:HD11	1.83	0.61
1:M:95:LEU:HD12	1:M:96:PRO:HD2	1.82	0.61
2:P:55:PRO:HG2	2:P:58:ILE:HG13	1.83	0.61
2:J:80:ALA:HA	2:J:106:VAL:HG21	1.82	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: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

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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
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.39	0.55
1:K:34:TRP:HB3	1:K:78:PHE:CE1	2.41	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:166:PHE:HE2	2:J:135:LEU:HD22	1.72	0.55
1:I:127:SER:N	1:I:130:SER:O	2.31	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:K:185:PRO:HG2	1:K:188:SER:HB3	1.88	0.54
1:O:63:LEU:O	1:O:66:ARG:HB3	2.08	0.53
1:M:18:LEU:HB3	1:M:82:LEU:HD13	1.90	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: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

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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: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:31:LYS:HG2	2:J:91:TRP:CE2	2.44	0.51
2:J:93:SER:H	2:J:95:SER:N	2.09	0.51
1:M:100(B):ASN:HB3	2:N:32:TYR:CG	2.45	0.51
1:K:94:SER:OG	1:K:101:ASP:O	2.25	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: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:59:TYR:HE1	1:I:69:ILE:HG13	1.76	0.51
1:I:83:THR:OG1	1:I:84:ALA:N	2.44	0.51
2:L:50:GLN:O	2:L:52:SER:N	2.37	0.50
1:I:47:TRP:CD2	2:J:96:PHE:HB2	2.46	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:O:97:ARG:HG2	1:O:98:GLY:N	2.25	0.50
1:I:123:PRO:CA	1:I:209:LYS:HZ1	2.24	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:47:TRP:CZ3	2:N:95(A):THR:HB	2.47	0.49
1:O:134:GLY:C	1:O:135:THR:HG23	2.33	0.49
1:M:43:LYS:HZ3	2:N:101:GLY:HA3	1.77	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:98:GLY:N	1:O:99:GLN:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:LEU:HB3	1:O:92:CYS:SG	2.52	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
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:97:ARG:C	1:O:99:GLN:HA	2.34	0.48
1:O:29:ILE:HG23	1:O:53:TYR:CZ	2.48	0.48
2:J:125:LEU:C	2:J:127:ALA:H	2.17	0.48
1:I:26:GLY:C	1:I:28:SER:HA	2.33	0.48
2:L:28:LEU:HG	2:L:31:LYS:HD2	1.94	0.47
1:I:59:TYR:CE1	1:I:69:ILE:HG13	2.48	0.47
2:P:89:GLN:HG2	2:P:90:ALA:N	2.29	0.47
1:I:21:THR:HG22	1:I:79:SER:OG	2.14	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
1:I:35:SER:HG	1:I:100(E):PHE:HE1	1.61	0.47
2:P:93:SER:O	2:P:94:PHE:CG	2.67	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:L:93:SER:H	2:L:95:SER:N	2.13	0.47
2:N:53:LYS:HG2	2:J:32:TYR:CE2	2.50	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:N:14:SER:N	2:N:17:GLN:OE1	2.42	0.46
1:K:100(B):ASN:HD22	2:L:50:GLN:HG2	1.80	0.46
1:K:67:VAL:CG2	1:K:80:LEU:HD11	2.46	0.46
2:J:110:LYS:NZ	2:J:198:GLU:OE1	2.35	0.46
2:N:26:ASP:HA	2:N:27:LYS:HA	1.53	0.46
2:N:13:VAL:HG12	2:N:106:VAL:HG12	1.98	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:P:146:VAL:HG11	2:P:161:THR:HG21	1.97	0.46
1:I:214:LYS:HE2	1:I:214:LYS:HB3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:145:THR:HB	2:P:196:THR:OG1	2.16	0.46
1:I:132:SER:HA	1:I:133:GLY:HA2	1.73	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
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
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
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:O:36:TRP:HB3	1:O:48:ILE:HD11	1.98	0.45
1:M:43:LYS:NZ	2:N:100:THR:O	2.39	0.45
2:P:162:THR:CG2	2:P:175:SER:H	2.29	0.45
1:K:60:ASN:OD1	1:K:62:SER:OG	2.21	0.45
1:O:100(E):PHE:N	2:P:36:TYR:OH	2.26	0.45
1:I:45:LEU:HD23	2:J:98:PHE:CD1	2.51	0.45
2:P:167:GLN:HB3	2:P:168:SER:H	1.56	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
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:O:60:ASN:HA	1:O:61:PRO:HD3	1.87	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
2:P:11:VAL:HG21	2:P:21:ILE:HG13	1.98	0.45
2:J:149:LYS:HG2	2:J:154:PRO:HA	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:L:54:ARG:HH22	2:L:59:PRO:C	2.21	0.44
1:M:48:ILE:HG22	1:M:63:LEU:HD22	1.98	0.44
1:K:130:SER:HA	1:K:131:THR:HA	1.64	0.44
1:O:100(B):ASN:HB3	2:P:32:TYR:CD2	2.51	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:K:19:SER:HA	1:K:80:LEU:O	2.17	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:P:2:TYR:O	2:P:3:GLU:HG3	2.18	0.44
2:L:20:SER:HA	2:L:73:LEU:O	2.17	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: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:K:8:GLY:HA3	1:K:20:LEU:HD23	2.00	0.44
1:O:214:LYS:HD2	1:O:214:LYS:HA	1.68	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: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
2:P:198:GLU:CG	2:P:199:GLY:H	2.25	0.44
2:L:162:THR:HG22	2:L:175:SER:H	1.82	0.44
2:P:120:PRO:HD3	2:P:132:LEU:HD13	1.98	0.44
1:K:83:THR:OG1	1:K:84:ALA:N	2.51	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
2:N:94:PHE:N	2:N:95:SER:CA	2.76	0.43
1:I:126:PRO:HD2	1:I:213:PRO:HA	1.99	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
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:92:ASP:O	2:L:95:SER:HB3	2.19	0.43
1:K:71:VAL:HG23	1:K:78:PHE:HB3	2.01	0.43
1:O:196:CYS:O	1:O:208:ASP:HA	2.19	0.43
1:I:96:PRO:HG2	1:I:100(D):TYR:CZ	2.54	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:K:126:PRO:HD2	1:K:213:PRO:HA	2.01	0.43
1:O:15:SER:HA	1:O:82(B):SER:HA	2.00	0.43
1:M:83:THR:OG1	1:M:84:ALA:N	2.50	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
2:L:93:SER:H	2:L:94:PHE:C	2.22	0.42
1:M:100(B):ASN:HB3	2:N:32:TYR:CD2	2.54	0.42
1:I:13:LYS:HB2	1:I:16:GLU:CD	2.39	0.42
2:N:167:GLN:HB3	2:N:168:SER:H	1.53	0.42
1:M:37:ILE:HG21	1:M:45:LEU:HD21	2.00	0.42
2:J:60:GLU:H	2:J:60:GLU:CD	2.23	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
2:L:83:GLU:OE2	2:L:106:VAL:N	2.30	0.42
1:K:146:PHE:HA	1:K:147:PRO:HA	1.79	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
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
1:I:2:VAL:HG23	1:I:25:SER:H	1.85	0.42
1:K:80:LEU:C	1:K:81:LYS:HD2	2.40	0.42
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
1:K:2:VAL:HG22	1:K:102:TYR:CD1	2.55	0.41
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:M:63:LEU:O	1:M:66:ARG:HB3	2.20	0.41
1:K:131:THR:OG1	1:K:135:THR:O	2.34	0.41
1:O:36:TRP:CD2	1:O:80:LEU:HD23	2.55	0.41
2:J:110:LYS:HG2	2:J:111:ALA:N	2.35	0.41
1:M:26:GLY:C	1:M:28:SER:HA	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:34:CYS:SG	2:P:89:GLN:HB3	2.60	0.41
1:O:121:VAL:HB	1:O:209:LYS:NZ	2.35	0.41
2:L:28:LEU:HA	2:L:31:LYS:CD	2.49	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
1:I:8:GLY:HA3	1:I:20:LEU:HD23	2.02	0.41
1:O:184:VAL:HG11	1:O:194:TYR:CE1	2.56	0.41
1:I:43:LYS:HE2	1:I:43:LYS:HB3	1.88	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: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:K:132:SER:HA	1:K:133:GLY:HA2	1.67	0.41
1:I:67:VAL:HG12	1:I:82:LEU:HG	2.03	0.41
2:L:13:VAL:O	2:L:106:VAL:HA	2.19	0.41
1:O:36:TRP:O	1:O:48:ILE:HG12	2.21	0.41
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.56	0.41
1:I:83:THR:O	1:I:111:VAL:HG21	2.20	0.41
1:O:207:VAL:HG11	1:O:209:LYS:NZ	2.35	0.41
2:N:170:ASN:ND2	2:N:170:ASN:O	2.48	0.41
2:N:46:LEU:HG	2:N:55:PRO:HG3	1.98	0.41
1:K:78:PHE:CD2	1:K:78:PHE:N	2.89	0.41
1:I:129:LYS:NZ	1:I:132:SER:HB3	2.36	0.41
2:P:21:ILE:HG12	2:P:102:THR:HG21	2.03	0.41
2:N:28:LEU:HA	2:N:31:LYS:HG3	2.02	0.41
1:O:148:GLU:HG2	1:O:176:TYR:CD2	2.55	0.41
2:N:136:ILE:HG12	2:N:195:VAL:HG21	2.03	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:M:47:TRP:CE2	2:N:96:PHE:HD2	2.38	0.40
1:K:20:LEU:HB2	1:K:36:TRP:CZ3	2.55	0.40
1:O:96:PRO:HG2	1:O:100(D):TYR:CZ	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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 (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	I	214/232 (92%)	194 (91%)	18 (8%)	2 (1%)	21 67
1	K	214/232 (92%)	193 (90%)	21 (10%)	0	100 100
1	M	212/232 (91%)	192 (91%)	19 (9%)	1 (0%)	34 77
1	O	212/232 (91%)	192 (91%)	18 (8%)	2 (1%)	21 67
2	J	207/213 (97%)	175 (84%)	32 (16%)	0	100 100
2	L	207/213 (97%)	173 (84%)	33 (16%)	1 (0%)	34 77
2	N	207/213 (97%)	176 (85%)	30 (14%)	1 (0%)	34 77
2	P	207/213 (97%)	175 (84%)	27 (13%)	5 (2%)	7 46
All	All	1680/1780 (94%)	1470 (88%)	198 (12%)	12 (1%)	26 72

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 (i)

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%)	22	63
1	K	189/202 (94%)	182 (96%)	7 (4%)	41	76
1	M	187/202 (93%)	180 (96%)	7 (4%)	41	76
1	O	187/202 (93%)	180 (96%)	7 (4%)	41	76
2	J	178/182 (98%)	173 (97%)	5 (3%)	51	82
2	L	178/182 (98%)	174 (98%)	4 (2%)	60	85
2	N	178/182 (98%)	174 (98%)	4 (2%)	60	85
2	P	178/182 (98%)	171 (96%)	7 (4%)	39	76
All	All	1464/1536 (95%)	1411 (96%)	53 (4%)	42	78

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

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, 95^{th} 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%)	0.06	2 (0%)	85 79	26, 51, 87, 123	0
1	K	218/232 (93%)	0.17	3 (1%)	78 70	26, 57, 90, 133	0
1	M	216/232 (93%)	0.48	7 (3%)	51 43	36, 80, 110, 132	0
1	O	216/232 (93%)	0.51	11 (5%)	32 26	38, 79, 109, 131	0
2	J	209/213 (98%)	0.05	2 (0%)	84 77	22, 54, 82, 127	0
2	L	209/213 (98%)	0.10	4 (1%)	70 62	23, 55, 83, 128	0
2	N	209/213 (98%)	0.43	8 (3%)	44 37	45, 65, 89, 130	0
2	P	209/213 (98%)	0.47	8 (3%)	44 37	40, 72, 99, 146	0
All	All	1704/1780 (95%)	0.28	45 (2%)	59 50	22, 65, 99, 146	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	128	SER	4.5
1	K	28	SER	3.8
1	M	65	SER	3.8
2	N	2	TYR	3.6
1	I	30	SER	3.4
2	N	106	VAL	3.4
2	P	2	TYR	3.2
1	O	140	CYS	3.1
2	P	30	ASP	3.1
2	P	198	GLU	3.0
1	O	128	SER	3.0
1	M	172	SER	2.9
1	O	107	THR	2.8
1	O	54	SER	2.8
1	O	190	GLY	2.8
2	L	95	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	27	GLY	2.7
1	M	127	SER	2.6
2	N	67	SER	2.6
2	J	95	SER	2.6
2	L	92	ASP	2.6
1	M	62	SER	2.5
1	K	29	ILE	2.5
1	O	127	SER	2.5
1	M	3	GLN	2.5
2	L	107	GLY	2.4
1	I	29	ILE	2.4
2	N	3	GLU	2.4
2	P	91	TRP	2.3
2	N	168	SER	2.3
2	N	30	ASP	2.3
1	O	173	SER	2.3
1	M	107	THR	2.2
2	P	137	SER	2.2
1	O	51	ILE	2.2
2	P	15	PRO	2.2
2	L	168	SER	2.2
2	J	57	GLY	2.2
2	P	4	LEU	2.2
1	O	3	GLN	2.2
2	P	32	TYR	2.1
2	N	198	GLU	2.1
1	O	59	TYR	2.1
2	N	91	TRP	2.1
1	O	65	SER	2.1

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.