



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:52 AM GMT

PDB ID : 2I2R  
Title : Crystal structure of the KChIP1/Kv4.3 T1 complex  
Authors : Findeisen, F.; Pioletti, M.; Minor Jr., D.L.  
Deposited on : 2006-08-16  
Resolution : 3.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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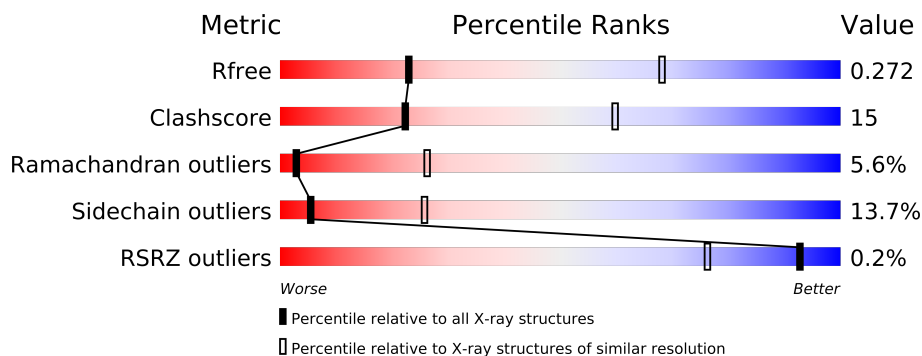
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.35 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))
$R_{free}$	66092	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	144	
1	B	144	
1	C	144	
1	D	144	
1	I	144	
1	J	144	
1	K	144	
1	L	144	
2	E	180	
2	F	180	
2	G	180	
2	H	180	
2	M	180	
2	N	180	

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Mol	Chain	Length	Quality of chain
2	O	180	
2	P	180	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	F	702	-	X
5	NA	H	701	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18970 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Potassium voltage-gated channel subfamily D member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1022	657	166	194	5			
1	B	124	Total	C	N	O	S	0	0	0
			999	643	163	188	5			
1	C	126	Total	C	N	O	S	0	0	0
			1004	646	163	191	4			
1	D	122	Total	C	N	O	S	0	0	0
			983	635	158	186	4			
1	I	133	Total	C	N	O	S	0	0	0
			1047	676	169	197	5			
1	J	129	Total	C	N	O	S	0	0	0
			1018	655	165	193	5			
1	K	132	Total	C	N	O	S	0	0	0
			1037	667	168	197	5			
1	L	138	Total	C	N	O	S	0	0	0
			1082	696	178	203	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP Q62897
A	1	ALA	-	CLONING ARTIFACT	UNP Q62897
B	0	GLY	-	CLONING ARTIFACT	UNP Q62897
B	1	ALA	-	CLONING ARTIFACT	UNP Q62897
C	0	GLY	-	CLONING ARTIFACT	UNP Q62897
C	1	ALA	-	CLONING ARTIFACT	UNP Q62897
D	0	GLY	-	CLONING ARTIFACT	UNP Q62897
D	1	ALA	-	CLONING ARTIFACT	UNP Q62897
I	0	GLY	-	CLONING ARTIFACT	UNP Q62897
I	1	ALA	-	CLONING ARTIFACT	UNP Q62897
J	0	GLY	-	CLONING ARTIFACT	UNP Q62897
J	1	ALA	-	CLONING ARTIFACT	UNP Q62897
K	0	GLY	-	CLONING ARTIFACT	UNP Q62897

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ALA	-	CLONING ARTIFACT	UNP Q62897
L	0	GLY	-	CLONING ARTIFACT	UNP Q62897
L	1	ALA	-	CLONING ARTIFACT	UNP Q62897

- Molecule 2 is a protein called Kv channel-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	179	Total	C	N	O	S	0	0	0
			1380	873	227	272	8			
2	F	180	Total	C	N	O	S	0	0	0
			1393	885	227	272	9			
2	G	174	Total	C	N	O	S	0	0	0
			1341	850	220	265	6			
2	H	174	Total	C	N	O	S	0	0	0
			1360	864	221	268	7			
2	M	170	Total	C	N	O	S	0	0	0
			1309	832	214	257	6			
2	N	168	Total	C	N	O	S	0	0	0
			1308	827	212	261	8			
2	O	168	Total	C	N	O	S	0	0	0
			1311	831	212	260	8			
2	P	172	Total	C	N	O	S	0	0	0
			1348	855	219	265	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
E	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
F	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
F	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
G	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
G	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
H	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
H	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
M	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
M	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
N	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
N	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
O	160	ALA	LYS	ENGINEERED	UNP Q9NZI2
O	167	ALA	LYS	ENGINEERED	UNP Q9NZI2
P	160	ALA	LYS	ENGINEERED	UNP Q9NZI2

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Chain	Residue	Modelled	Actual	Comment	Reference
P	167	ALA	LYS	ENGINEERED	UNP Q9NZI2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0
3	N	2	Total Ca 2 2	0	0
3	O	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	M	2	Total Ca 2 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

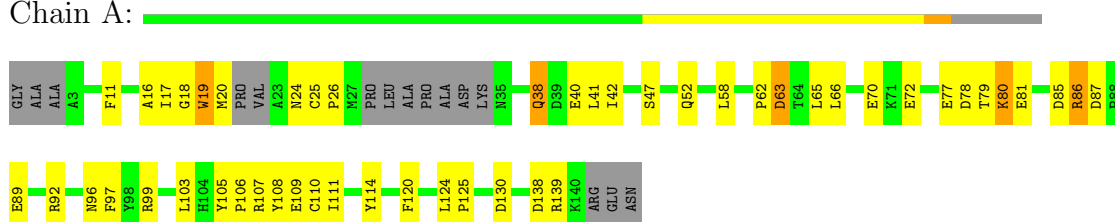
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Na 1	0	0
5	G	1	Total 1	Na 1	0	0
5	F	1	Total 1	Na 1	0	0
5	E	1	Total 1	Na 1	0	0

### 3 Residue-property plots

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.

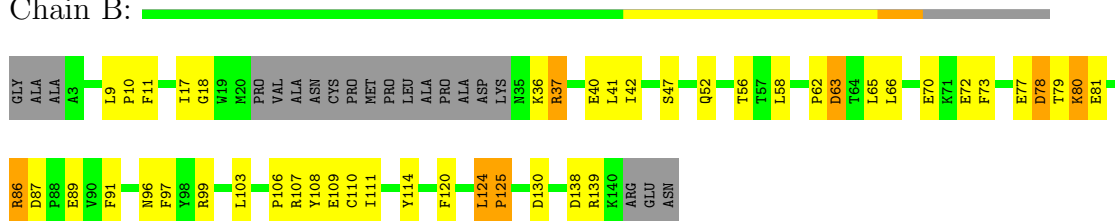
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain A:



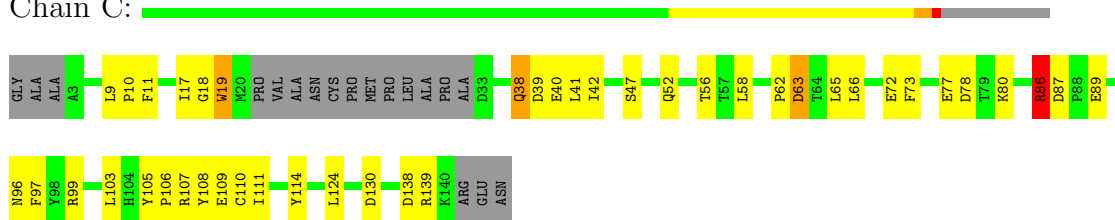
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain B:



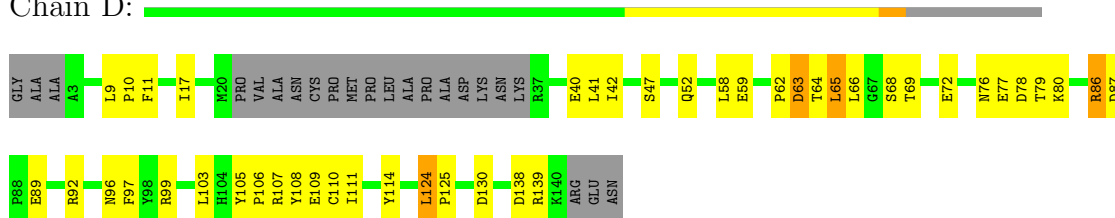
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain C:



- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain D:

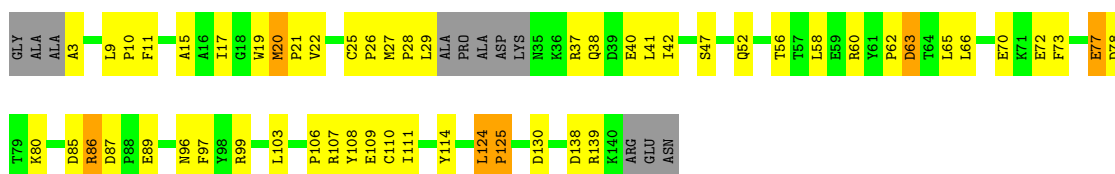


- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain I:

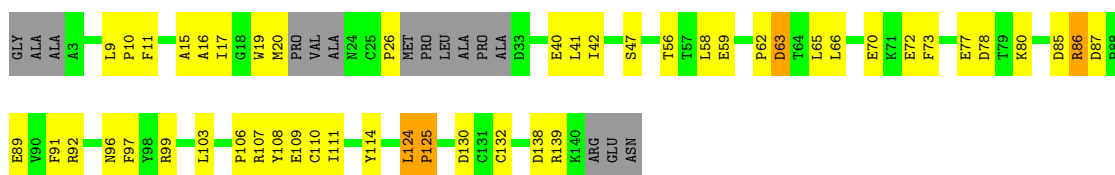






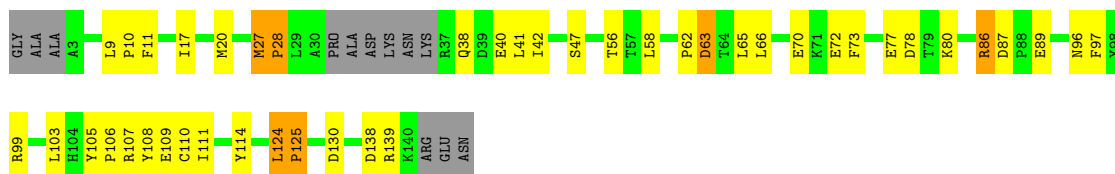
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain J:



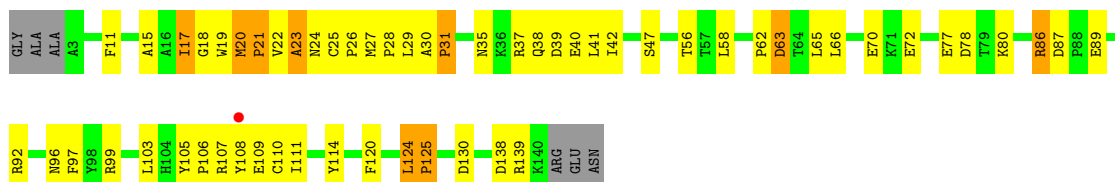
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain K:



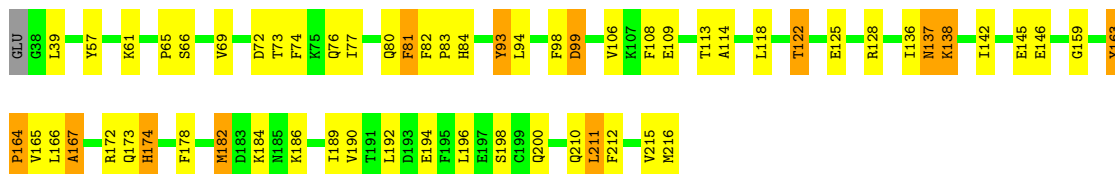
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain L:



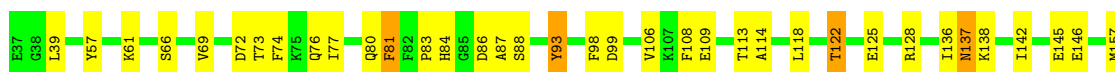
- Molecule 2: Kv channel-interacting protein 1

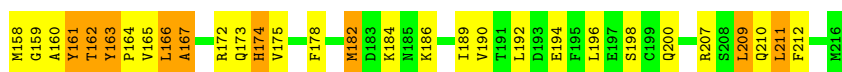
Chain E:



- Molecule 2: Kv channel-interacting protein 1

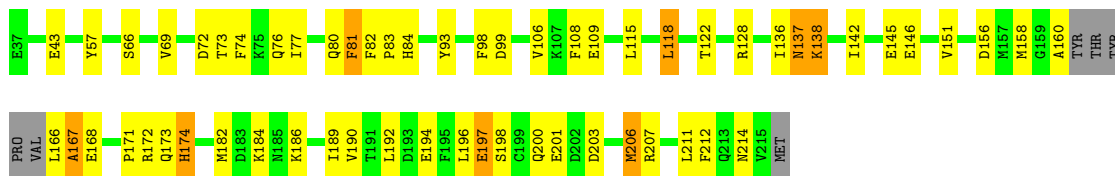
Chain F:





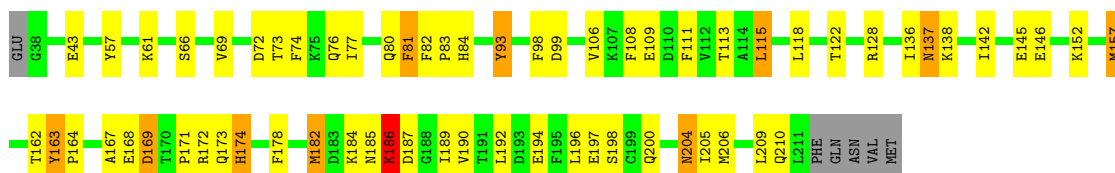
• Molecule 2: Kv channel-interacting protein 1

Chain G:



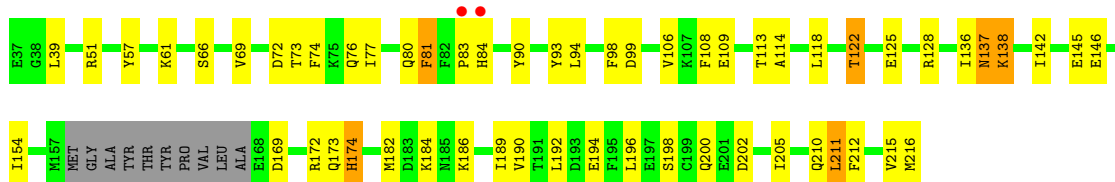
• Molecule 2: Kv channel-interacting protein 1

Chain H:



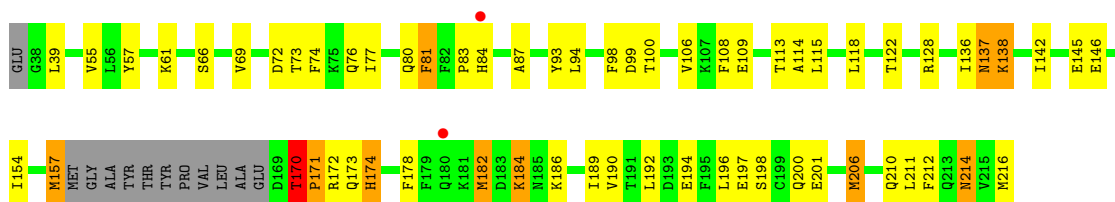
• Molecule 2: Kv channel-interacting protein 1

Chain M:



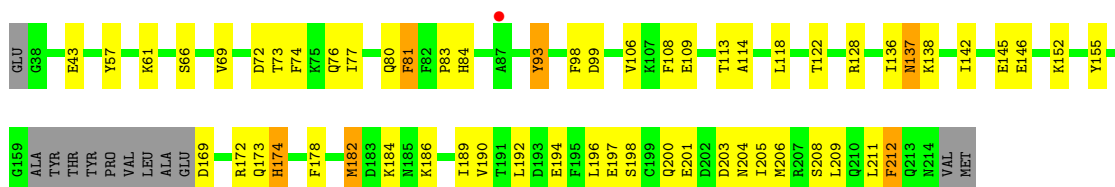
• Molecule 2: Kv channel-interacting protein 1

Chain N:

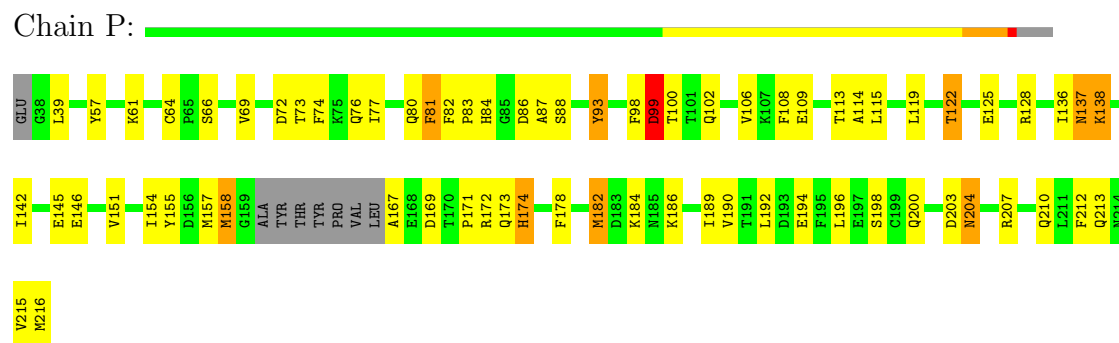


• Molecule 2: Kv channel-interacting protein 1

Chain O:



Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.15Å 98.11Å 97.78Å 91.00° 112.56° 111.77°	Depositor
Resolution (Å)	91.29 – 3.35 57.86 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.9 (91.29-3.35) 96.9 (57.86-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.237 , 0.268 0.247 , 0.272	Depositor DCC
$R_{free}$ test set	2038 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 167.5	EDS
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40632 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.74	0/1049	0.75	1/1424 (0.1%)
1	B	0.70	0/1027	0.73	0/1394
1	C	0.72	0/1032	0.74	1/1403 (0.1%)
1	D	0.69	0/1011	0.73	0/1374
1	I	0.74	0/1078	0.72	0/1469
1	J	0.69	0/1045	0.72	1/1419 (0.1%)
1	K	0.67	0/1066	0.71	0/1451
1	L	0.70	0/1114	0.77	1/1519 (0.1%)
2	E	0.61	0/1408	0.70	0/1912
2	F	0.63	0/1423	0.70	0/1933
2	G	0.58	0/1368	0.70	0/1857
2	H	0.63	0/1390	0.69	0/1888
2	M	0.54	0/1335	0.66	0/1815
2	N	0.52	0/1334	0.73	2/1810 (0.1%)
2	O	0.55	0/1337	0.67	0/1812
2	P	0.62	0/1375	0.70	0/1863
All	All	0.64	0/19392	0.71	6/26343 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	G	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	170	THR	C-N-CD	-11.24	95.87	120.60
1	L	31	PRO	N-CA-CB	6.72	111.37	103.30
1	A	26	PRO	N-CA-CB	6.48	111.07	103.30
2	N	201	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	C	86	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	J	26	PRO	N-CA-CB	5.32	109.69	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	GLN	Peptide
2	G	211	LEU	Peptide
2	G	212	PHE	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1022	0	897	39	0
1	B	999	0	890	36	0
1	C	1004	0	882	35	0
1	D	983	0	877	34	0
1	I	1047	0	925	41	0
1	J	1018	0	888	42	0
1	K	1037	0	923	30	0
1	L	1082	0	957	44	0
2	E	1380	0	1236	44	0
2	F	1393	0	1244	40	0
2	G	1341	0	1190	29	0
2	H	1360	0	1219	42	0
2	M	1309	0	1166	39	0
2	N	1308	0	1161	44	0
2	O	1311	0	1178	34	0
2	P	1348	0	1216	53	0
3	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	1	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	18970	0	16849	534	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (534) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:87:ALA:HB2	2:N:157:MET:HG2	1.25	1.14
2:M:215:VAL:O	2:M:216:MET:HB2	1.45	1.10
1:I:99:ARG:NH2	1:J:47:SER:HB2	1.69	1.07
1:I:47:SER:HB2	1:L:99:ARG:NH2	1.70	1.06
1:B:99:ARG:NH2	1:C:47:SER:HB2	1.68	1.06
1:K:99:ARG:NH2	1:L:47:SER:HB2	1.71	1.06
1:I:47:SER:HB2	1:L:99:ARG:HH22	1.24	1.00
1:B:99:ARG:HH22	1:C:47:SER:HB2	1.25	0.99
2:N:87:ALA:CB	2:N:157:MET:HG2	1.93	0.99
2:F:87:ALA:HB2	2:F:157:MET:HG3	1.45	0.98
1:A:47:SER:HB2	1:D:99:ARG:NH2	1.78	0.97
1:A:99:ARG:NH2	1:B:47:SER:HB2	1.78	0.97
1:A:47:SER:HB2	1:D:99:ARG:HH22	1.29	0.97
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.28	0.97
1:C:99:ARG:NH2	1:D:47:SER:HB2	1.80	0.97
1:I:99:ARG:HH22	1:J:47:SER:HB2	1.23	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:99:ARG:NH2	1:K:47:SER:HB2	1.84	0.93
2:P:87:ALA:HB2	2:P:157:MET:HG3	1.50	0.92
1:K:99:ARG:HH22	1:L:47:SER:HB2	1.30	0.92
2:G:137:ASN:HD22	2:G:137:ASN:H	1.19	0.91
1:A:86:ARG:HH11	1:A:86:ARG:HG3	1.35	0.90
2:M:202:ASP:OD1	2:M:205:ILE:HG12	1.70	0.90
1:J:86:ARG:HG3	1:J:86:ARG:HH11	1.34	0.90
2:N:137:ASN:H	2:N:137:ASN:HD22	1.19	0.89
2:P:137:ASN:HD22	2:P:137:ASN:H	1.19	0.89
2:O:136:ILE:HD12	2:O:146:GLU:HB2	1.55	0.89
2:H:137:ASN:HD22	2:H:137:ASN:H	1.19	0.88
2:M:137:ASN:H	2:M:137:ASN:HD22	1.19	0.88
1:K:86:ARG:HH11	1:K:86:ARG:HG3	1.38	0.88
2:F:137:ASN:H	2:F:137:ASN:HD22	1.19	0.88
2:E:215:VAL:O	2:E:216:MET:HB2	1.75	0.87
2:E:136:ILE:HD12	2:E:146:GLU:HB2	1.57	0.85
1:I:86:ARG:HG3	1:I:86:ARG:HH11	1.39	0.85
2:E:137:ASN:H	2:E:137:ASN:HD22	1.19	0.85
1:B:86:ARG:HH11	1:B:86:ARG:HG3	1.40	0.85
2:H:136:ILE:HD12	2:H:146:GLU:HB2	1.57	0.84
1:C:99:ARG:HH22	1:D:47:SER:HB2	1.38	0.84
2:M:136:ILE:HD12	2:M:146:GLU:HB2	1.58	0.84
2:F:136:ILE:HD12	2:F:146:GLU:HB2	1.59	0.84
2:O:137:ASN:HD22	2:O:137:ASN:H	1.19	0.84
2:P:119:LEU:HD22	2:P:213:GLN:HG3	1.60	0.83
2:E:163:TYR:H	2:E:164:PRO:CD	1.92	0.83
1:A:99:ARG:HH22	1:B:47:SER:HB2	1.42	0.83
2:E:122:THR:HA	2:P:210:GLN:OE1	1.78	0.82
2:G:136:ILE:HD12	2:G:146:GLU:HB2	1.59	0.82
2:N:136:ILE:HD12	2:N:146:GLU:HB2	1.60	0.81
1:L:86:ARG:HG3	1:L:86:ARG:HH11	1.46	0.81
2:P:136:ILE:HD12	2:P:146:GLU:HB2	1.62	0.81
1:K:89:GLU:OE2	1:K:89:GLU:HA	1.82	0.80
2:H:171:PRO:HA	2:H:174:HIS:HB2	1.63	0.80
1:A:89:GLU:OE2	1:A:89:GLU:HA	1.83	0.78
1:C:38:GLN:HG3	1:C:39:ASP:N	1.98	0.78
2:E:163:TYR:H	2:E:164:PRO:HD2	1.51	0.76
1:K:27:MET:H	1:K:28:PRO:HD3	1.49	0.76
2:H:185:ASN:O	2:H:186:LYS:HB2	1.86	0.76
1:J:132:CYS:HG	4:J:606:ZN:ZN	0.99	0.75
1:L:38:GLN:HG2	1:L:39:ASP:H	1.50	0.75
1:J:99:ARG:HH22	1:K:47:SER:HB2	1.48	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:11:PHE:CZ	2:G:115:LEU:HG	2.24	0.73
1:I:89:GLU:OE2	1:I:89:GLU:HA	1.88	0.73
1:C:86:ARG:HH11	1:C:86:ARG:HG3	1.54	0.73
1:J:73:PHE:CE1	2:M:39:LEU:HD13	2.23	0.73
1:A:42:ILE:HD11	1:A:58:LEU:HD12	1.70	0.72
1:A:111:ILE:HG13	1:A:139:ARG:O	1.88	0.72
1:I:42:ILE:HD11	1:I:58:LEU:HD12	1.71	0.72
2:E:194:GLU:O	2:E:198:SER:HB2	1.89	0.72
2:F:160:ALA:HA	2:F:167:ALA:HB3	1.71	0.72
1:B:89:GLU:HA	1:B:89:GLU:OE2	1.88	0.71
1:I:111:ILE:HG13	1:I:139:ARG:O	1.91	0.71
1:D:42:ILE:HD11	1:D:58:LEU:HD12	1.72	0.70
1:I:20:MET:O	1:I:22:VAL:N	2.24	0.70
1:J:89:GLU:HA	1:J:89:GLU:OE2	1.90	0.70
1:L:27:MET:O	1:L:29:LEU:N	2.25	0.68
1:J:15:ALA:HB1	2:N:154:ILE:HD11	1.75	0.68
1:D:89:GLU:OE2	1:D:89:GLU:HA	1.92	0.68
2:N:196:LEU:O	2:N:200:GLN:HG2	1.93	0.68
1:L:89:GLU:HA	1:L:89:GLU:OE2	1.92	0.68
2:P:196:LEU:O	2:P:200:GLN:HG2	1.95	0.67
1:L:42:ILE:HD11	1:L:58:LEU:HD12	1.74	0.67
1:B:70:GLU:OE2	2:E:61:LYS:HE3	1.94	0.67
1:J:97:PHE:CD2	1:J:103:LEU:HB2	2.30	0.67
2:M:202:ASP:CG	2:M:205:ILE:HG12	2.15	0.67
1:C:89:GLU:OE2	1:C:89:GLU:HA	1.95	0.67
1:J:111:ILE:HG13	1:J:139:ARG:O	1.93	0.67
1:B:42:ILE:HD11	1:B:58:LEU:HD12	1.76	0.67
1:D:111:ILE:HG13	1:D:139:ARG:O	1.95	0.67
2:M:196:LEU:O	2:M:200:GLN:HG2	1.95	0.67
1:C:42:ILE:HD11	1:C:58:LEU:HD12	1.75	0.67
1:K:27:MET:N	1:K:28:PRO:HD3	2.10	0.67
1:K:111:ILE:HG13	1:K:139:ARG:O	1.94	0.67
2:E:196:LEU:O	2:E:200:GLN:HG2	1.94	0.66
1:C:19:TRP:CZ3	2:G:151:VAL:HG13	2.30	0.66
1:I:27:MET:O	1:I:29:LEU:N	2.27	0.66
1:J:86:ARG:CG	1:J:86:ARG:HH11	2.08	0.66
2:M:194:GLU:O	2:M:198:SER:HB2	1.96	0.65
1:C:42:ILE:HD11	1:C:58:LEU:CD1	2.26	0.65
1:C:111:ILE:HG13	1:C:139:ARG:O	1.96	0.65
2:F:196:LEU:O	2:F:200:GLN:HG2	1.97	0.65
2:G:196:LEU:O	2:G:200:GLN:HG2	1.97	0.65
2:H:196:LEU:O	2:H:200:GLN:HG2	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:111:ILE:HG13	1:B:139:ARG:O	1.97	0.65
1:D:86:ARG:CG	1:D:86:ARG:HH11	2.04	0.65
2:G:194:GLU:O	2:G:198:SER:HB2	1.97	0.64
1:L:70:GLU:OE2	2:O:61:LYS:HE3	1.97	0.64
2:P:119:LEU:CD2	2:P:213:GLN:HG3	2.27	0.64
2:H:209:LEU:O	2:H:210:GLN:HG3	1.98	0.64
1:L:111:ILE:HG13	1:L:139:ARG:O	1.98	0.64
2:O:155:TYR:CE2	2:O:169:ASP:HA	2.32	0.63
1:I:97:PHE:CD2	1:I:103:LEU:HB2	2.34	0.63
2:M:215:VAL:O	2:M:216:MET:CB	2.33	0.63
1:I:99:ARG:NH2	1:J:47:SER:CB	2.56	0.63
1:B:42:ILE:HD11	1:B:58:LEU:CD1	2.29	0.63
1:C:19:TRP:CD1	1:C:19:TRP:N	2.67	0.62
2:M:69:VAL:HB	2:M:106:VAL:CG2	2.29	0.62
1:C:52:GLN:N	1:D:47:SER:O	2.28	0.62
2:F:194:GLU:O	2:F:198:SER:HB2	1.99	0.62
2:N:194:GLU:O	2:N:198:SER:HB2	2.00	0.62
1:K:70:GLU:OE2	2:N:61:LYS:HE3	2.00	0.61
1:I:42:ILE:HD11	1:I:58:LEU:CD1	2.29	0.61
2:N:87:ALA:HB2	2:N:157:MET:CG	2.14	0.61
1:K:97:PHE:CD2	1:K:103:LEU:HB2	2.34	0.61
1:D:42:ILE:HD11	1:D:58:LEU:CD1	2.30	0.61
1:A:42:ILE:HD11	1:A:58:LEU:CD1	2.30	0.61
2:F:163:TYR:HB3	2:F:164:PRO:HD3	1.81	0.61
1:B:96:ASN:OD1	1:C:87:ASP:HB2	2.01	0.61
1:K:58:LEU:HD13	1:K:66:LEU:HB3	1.83	0.61
2:O:69:VAL:HB	2:O:106:VAL:CG2	2.30	0.61
2:O:196:LEU:O	2:O:200:GLN:HG2	2.01	0.60
1:C:9:LEU:N	1:C:10:PRO:HD2	2.16	0.60
1:J:42:ILE:HD11	1:J:58:LEU:HD12	1.83	0.60
2:F:162:THR:O	2:F:163:TYR:C	2.39	0.60
2:M:73:THR:O	2:M:77:ILE:HG13	2.01	0.60
2:E:69:VAL:HB	2:E:106:VAL:CG2	2.32	0.60
2:P:194:GLU:O	2:P:198:SER:HB2	2.02	0.60
2:H:81:PHE:CB	2:H:82:PHE:CE1	2.85	0.59
2:P:73:THR:O	2:P:77:ILE:HG13	2.02	0.59
2:G:69:VAL:HB	2:G:106:VAL:CG2	2.33	0.59
2:H:164:PRO:HG2	2:H:169:ASP:HB3	1.84	0.59
2:E:73:THR:O	2:E:77:ILE:HG13	2.03	0.59
2:N:69:VAL:HB	2:N:106:VAL:CG2	2.33	0.59
2:P:69:VAL:HB	2:P:106:VAL:CG2	2.33	0.59
1:L:42:ILE:HD11	1:L:58:LEU:CD1	2.32	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:159:GLY:C	2:F:161:TYR:H	2.07	0.59
1:D:97:PHE:CD2	1:D:103:LEU:HB2	2.38	0.59
2:E:212:PHE:HE1	2:P:212:PHE:HE1	1.50	0.58
2:O:194:GLU:O	2:O:198:SER:HB2	2.03	0.58
2:E:212:PHE:CE1	2:P:212:PHE:HE1	2.21	0.58
1:C:97:PHE:CD2	1:C:103:LEU:HB2	2.38	0.58
2:P:119:LEU:HD22	2:P:213:GLN:CG	2.34	0.58
1:A:86:ARG:CG	1:A:86:ARG:HH11	2.08	0.58
1:I:86:ARG:HH11	1:I:86:ARG:CG	2.13	0.58
1:K:86:ARG:HH11	1:K:86:ARG:CG	2.13	0.58
1:C:96:ASN:OD1	1:D:87:ASP:HB2	2.05	0.57
1:J:73:PHE:HE1	2:M:39:LEU:HD13	1.70	0.57
1:J:58:LEU:HD13	1:J:66:LEU:HB3	1.87	0.57
1:D:86:ARG:NH1	1:D:86:ARG:HG3	2.09	0.57
1:L:86:ARG:CG	1:L:86:ARG:HH11	2.16	0.57
2:H:194:GLU:O	2:H:198:SER:HB2	2.05	0.57
1:A:97:PHE:CD2	1:A:103:LEU:HB2	2.39	0.57
1:K:42:ILE:HD11	1:K:58:LEU:HD12	1.87	0.57
2:H:162:THR:O	2:H:163:TYR:CD1	2.58	0.56
2:N:137:ASN:ND2	2:N:137:ASN:H	1.98	0.56
2:P:142:ILE:HB	2:P:190:VAL:HG12	1.87	0.56
1:J:9:LEU:N	1:J:10:PRO:HD2	2.20	0.56
2:F:210:GLN:O	2:F:211:LEU:C	2.44	0.56
2:N:73:THR:O	2:N:77:ILE:HG13	2.04	0.56
2:F:163:TYR:O	2:F:166:LEU:HG	2.04	0.56
1:B:86:ARG:HH11	1:B:86:ARG:CG	2.13	0.56
2:N:206:MET:HG3	2:N:210:GLN:HE21	1.70	0.56
2:P:142:ILE:HB	2:P:190:VAL:CG1	2.36	0.56
1:L:19:TRP:CZ3	2:P:151:VAL:HG13	2.41	0.56
2:N:210:GLN:O	2:N:211:LEU:C	2.43	0.56
2:E:136:ILE:CD1	2:E:146:GLU:HB2	2.34	0.55
1:I:11:PHE:HE2	2:M:114:ALA:HB1	1.70	0.55
2:O:197:GLU:O	2:O:201:GLU:HG3	2.07	0.55
2:F:69:VAL:HB	2:F:106:VAL:CG2	2.36	0.55
1:K:96:ASN:OD1	1:L:87:ASP:HB2	2.07	0.55
2:P:137:ASN:ND2	2:P:137:ASN:H	1.98	0.55
1:L:58:LEU:HD13	1:L:66:LEU:HB3	1.89	0.55
1:L:97:PHE:CD2	1:L:103:LEU:HB2	2.42	0.55
1:A:47:SER:O	1:D:52:GLN:N	2.30	0.55
1:I:87:ASP:HB2	1:L:96:ASN:OD1	2.06	0.55
1:A:87:ASP:HB2	1:D:96:ASN:OD1	2.07	0.55
2:O:137:ASN:ND2	2:O:137:ASN:H	1.98	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:142:ILE:HB	2:O:190:VAL:CG1	2.37	0.54
2:N:212:PHE:CE2	2:N:214:ASN:HB3	2.43	0.54
1:K:42:ILE:HD11	1:K:58:LEU:CD1	2.38	0.54
2:H:80:GLN:O	2:H:81:PHE:C	2.46	0.54
2:O:73:THR:O	2:O:77:ILE:HG13	2.08	0.54
1:D:58:LEU:HD13	1:D:66:LEU:HB3	1.90	0.54
1:L:27:MET:C	1:L:29:LEU:H	2.09	0.54
1:B:120:PHE:O	2:E:61:LYS:NZ	2.32	0.54
2:G:206:MET:HA	2:G:206:MET:CE	2.38	0.54
1:B:99:ARG:NH2	1:C:47:SER:CB	2.58	0.54
2:F:73:THR:O	2:F:77:ILE:HG13	2.08	0.54
2:H:137:ASN:H	2:H:137:ASN:ND2	1.98	0.54
1:A:16:ALA:HB1	1:A:20:MET:HG3	1.89	0.54
1:B:97:PHE:CD2	1:B:103:LEU:HB2	2.43	0.54
2:H:204:ASN:C	2:H:206:MET:H	2.08	0.53
2:F:165:VAL:O	2:F:167:ALA:N	2.41	0.53
1:I:9:LEU:N	1:I:10:PRO:HD2	2.23	0.53
1:I:85:ASP:O	1:L:99:ARG:HD3	2.09	0.53
2:N:55:VAL:HG21	2:N:216:MET:CE	2.39	0.53
2:E:142:ILE:HB	2:E:190:VAL:HG12	1.89	0.53
1:L:120:PHE:O	2:O:61:LYS:NZ	2.40	0.53
2:O:136:ILE:CD1	2:O:146:GLU:HB2	2.34	0.53
1:C:108:TYR:CE1	1:C:109:GLU:HG2	2.44	0.52
1:A:58:LEU:HD13	1:A:66:LEU:HB3	1.91	0.52
2:E:142:ILE:HB	2:E:190:VAL:CG1	2.39	0.52
1:L:18:GLY:O	2:P:178:PHE:HD2	1.92	0.52
2:H:82:PHE:CE1	2:H:157:MET:SD	3.03	0.52
2:M:137:ASN:ND2	2:M:137:ASN:H	1.98	0.52
2:P:87:ALA:HB2	2:P:157:MET:CG	2.30	0.52
2:G:73:THR:O	2:G:77:ILE:HG13	2.10	0.52
1:K:11:PHE:HE2	2:O:114:ALA:HB1	1.75	0.52
2:H:137:ASN:HD22	2:H:137:ASN:N	2.00	0.52
2:O:57:TYR:CE2	2:O:61:LYS:HG3	2.45	0.52
2:P:106:VAL:O	2:P:106:VAL:HG23	2.09	0.52
2:G:156:ASP:HA	2:G:160:ALA:HB2	1.92	0.52
1:I:47:SER:CB	1:L:99:ARG:NH2	2.60	0.51
2:H:163:TYR:N	2:H:164:PRO:HD3	2.25	0.51
2:F:57:TYR:CE2	2:F:61:LYS:HG3	2.46	0.51
2:O:142:ILE:HB	2:O:190:VAL:HG12	1.92	0.51
1:B:106:PRO:O	1:B:108:TYR:N	2.39	0.51
2:E:137:ASN:HD22	2:E:137:ASN:N	2.00	0.51
1:K:70:GLU:OE2	2:N:57:TYR:OH	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:73:PHE:CE1	2:N:39:LEU:HD13	2.45	0.51
1:J:11:PHE:HE2	2:N:114:ALA:HB1	1.76	0.51
2:H:73:THR:O	2:H:77:ILE:HG13	2.11	0.51
2:G:106:VAL:HG23	2:G:106:VAL:O	2.11	0.51
2:G:137:ASN:ND2	2:G:137:ASN:H	1.98	0.51
1:J:42:ILE:HD11	1:J:58:LEU:CD1	2.41	0.51
2:P:57:TYR:CE2	2:P:61:LYS:HG3	2.45	0.51
1:C:38:GLN:CG	1:C:39:ASP:N	2.71	0.51
2:H:80:GLN:O	2:H:82:PHE:N	2.43	0.51
2:E:80:GLN:O	2:E:81:PHE:C	2.48	0.51
1:J:15:ALA:CB	2:N:154:ILE:HD11	2.40	0.51
2:F:136:ILE:CD1	2:F:146:GLU:HB2	2.36	0.51
2:M:128:ARG:HG3	2:M:192:LEU:HD21	1.92	0.50
2:N:142:ILE:HB	2:N:190:VAL:CG1	2.40	0.50
2:N:69:VAL:HB	2:N:106:VAL:HG22	1.94	0.50
1:J:96:ASN:OD1	1:K:87:ASP:HB2	2.11	0.50
2:O:204:ASN:C	2:O:206:MET:H	2.15	0.50
1:A:11:PHE:HE2	2:E:114:ALA:HB1	1.77	0.50
2:M:142:ILE:HB	2:M:190:VAL:CG1	2.41	0.50
2:O:155:TYR:HE2	2:O:169:ASP:HA	1.77	0.50
2:N:57:TYR:CE2	2:N:61:LYS:HG3	2.46	0.50
1:J:11:PHE:HB3	2:N:94:LEU:HD21	1.94	0.50
1:I:106:PRO:O	1:I:108:TYR:N	2.41	0.50
1:B:79:THR:OG1	1:B:81:GLU:HG2	2.12	0.50
1:I:27:MET:C	1:I:29:LEU:H	2.15	0.50
1:L:11:PHE:HE2	2:P:114:ALA:HB1	1.77	0.50
1:I:20:MET:SD	1:I:26:PRO:HB3	2.51	0.50
2:M:57:TYR:CE2	2:M:61:LYS:HG3	2.46	0.50
1:I:96:ASN:OD1	1:J:87:ASP:HB2	2.12	0.49
1:I:3:ALA:HB2	1:I:60:ARG:NH2	2.27	0.49
2:E:57:TYR:CE2	2:E:61:LYS:HG3	2.47	0.49
2:G:80:GLN:O	2:G:81:PHE:C	2.50	0.49
2:H:72:ASP:O	2:H:76:GLN:HG2	2.12	0.49
2:H:178:PHE:O	2:H:182:MET:HB2	2.12	0.49
2:M:72:ASP:O	2:M:76:GLN:HG2	2.12	0.49
1:A:106:PRO:O	1:A:108:TYR:N	2.44	0.49
1:B:58:LEU:HD13	1:B:66:LEU:HB3	1.94	0.49
1:C:58:LEU:HD13	1:C:66:LEU:HB3	1.95	0.49
2:M:69:VAL:HB	2:M:106:VAL:HG22	1.94	0.49
1:D:86:ARG:CG	1:D:86:ARG:NH1	2.72	0.49
2:H:136:ILE:CD1	2:H:146:GLU:HB2	2.36	0.49
2:G:142:ILE:HB	2:G:190:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:185:ASN:ND2	2:H:187:ASP:HB3	2.27	0.48
1:J:97:PHE:HD2	1:J:103:LEU:HB2	1.77	0.48
1:C:18:GLY:C	1:C:19:TRP:HD1	2.17	0.48
2:O:106:VAL:O	2:O:106:VAL:HG23	2.11	0.48
2:F:142:ILE:HB	2:F:190:VAL:CG1	2.43	0.48
2:O:206:MET:C	2:O:208:SER:N	2.66	0.48
2:E:122:THR:HG23	2:E:125:GLU:HB2	1.95	0.48
2:M:136:ILE:CD1	2:M:146:GLU:HB2	2.37	0.48
2:H:172:ARG:C	2:H:174:HIS:H	2.16	0.48
2:N:184:LYS:NZ	2:N:197:GLU:OE1	2.42	0.48
1:A:52:GLN:N	1:B:47:SER:O	2.33	0.48
1:D:89:GLU:O	1:D:92:ARG:HB2	2.14	0.48
1:B:9:LEU:N	1:B:10:PRO:HD2	2.28	0.48
1:J:106:PRO:O	1:J:108:TYR:N	2.45	0.48
2:F:137:ASN:HD22	2:F:137:ASN:N	2.00	0.48
2:G:142:ILE:HB	2:G:190:VAL:HG12	1.96	0.48
2:P:128:ARG:HG3	2:P:192:LEU:HD21	1.96	0.48
1:D:72:GLU:HA	1:D:72:GLU:OE2	2.13	0.48
2:E:72:ASP:O	2:E:76:GLN:HG2	2.14	0.47
1:A:89:GLU:OE2	1:A:89:GLU:CA	2.59	0.47
1:C:86:ARG:HH11	1:C:86:ARG:CG	2.24	0.47
1:I:11:PHE:HB3	2:M:94:LEU:HD21	1.94	0.47
2:M:142:ILE:HB	2:M:190:VAL:HG12	1.96	0.47
1:C:106:PRO:O	1:C:108:TYR:N	2.45	0.47
2:N:142:ILE:HB	2:N:190:VAL:HG12	1.97	0.47
2:P:204:ASN:HA	2:P:207:ARG:HB3	1.96	0.47
1:B:11:PHE:HE2	2:F:114:ALA:HB1	1.79	0.47
1:K:72:GLU:HA	1:K:72:GLU:OE2	2.14	0.47
2:F:212:PHE:HE1	2:O:212:PHE:HE1	1.62	0.47
2:E:128:ARG:HG3	2:E:192:LEU:HD21	1.95	0.47
1:B:18:GLY:O	2:F:178:PHE:HD2	1.98	0.47
2:G:80:GLN:O	2:G:82:PHE:N	2.48	0.47
2:F:142:ILE:HB	2:F:190:VAL:HG12	1.96	0.47
2:O:93:TYR:CD1	2:O:93:TYR:N	2.83	0.47
1:A:85:ASP:O	1:D:99:ARG:HD3	2.15	0.47
1:L:72:GLU:OE2	1:L:72:GLU:HA	2.15	0.47
2:G:69:VAL:HB	2:G:106:VAL:HG22	1.97	0.47
2:N:55:VAL:HG21	2:N:216:MET:HE3	1.95	0.47
1:A:108:TYR:CE1	1:A:109:GLU:HG2	2.49	0.47
1:A:38:GLN:HE22	1:I:77:GLU:HG2	1.80	0.47
1:A:72:GLU:HA	1:A:72:GLU:OE2	2.15	0.47
2:H:57:TYR:CE2	2:H:61:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:172:ARG:C	2:G:174:HIS:H	2.18	0.47
1:A:80:LYS:HG2	1:I:80:LYS:HG2	1.96	0.47
2:E:69:VAL:HB	2:E:106:VAL:HG22	1.97	0.47
1:A:38:GLN:NE2	1:I:77:GLU:HG2	2.30	0.47
1:K:99:ARG:NH2	1:L:47:SER:CB	2.62	0.47
2:G:200:GLN:HA	2:G:206:MET:SD	2.55	0.47
2:F:178:PHE:O	2:F:182:MET:HB2	2.15	0.47
2:H:209:LEU:O	2:H:210:GLN:CG	2.62	0.46
1:C:73:PHE:CE1	2:F:39:LEU:HD13	2.50	0.46
2:F:93:TYR:N	2:F:93:TYR:CD1	2.84	0.46
1:I:124:LEU:HA	1:I:125:PRO:HD2	1.71	0.46
2:F:69:VAL:HB	2:F:106:VAL:HG22	1.97	0.46
1:B:106:PRO:C	1:B:108:TYR:H	2.18	0.46
2:H:69:VAL:HB	2:H:106:VAL:CG2	2.45	0.46
1:L:38:GLN:HG2	1:L:39:ASP:N	2.24	0.46
1:I:70:GLU:OE2	2:P:61:LYS:HE3	2.16	0.46
1:L:62:PRO:O	1:L:63:ASP:OD2	2.32	0.46
2:M:51:ARG:HG2	2:M:216:MET:SD	2.55	0.46
1:J:72:GLU:OE2	1:J:72:GLU:HA	2.15	0.46
2:E:93:TYR:CD1	2:E:93:TYR:N	2.84	0.46
1:B:73:PHE:CE1	2:E:39:LEU:HD13	2.51	0.46
2:H:142:ILE:HB	2:H:190:VAL:CG1	2.45	0.46
2:P:72:ASP:O	2:P:76:GLN:HG2	2.16	0.46
1:L:106:PRO:O	1:L:108:TYR:N	2.48	0.46
2:P:93:TYR:CD1	2:P:93:TYR:N	2.84	0.46
2:N:93:TYR:N	2:N:93:TYR:CD1	2.84	0.46
2:O:57:TYR:HA	2:O:108:PHE:CE1	2.50	0.46
2:M:172:ARG:C	2:M:174:HIS:H	2.19	0.46
1:J:124:LEU:HA	1:J:125:PRO:HD2	1.71	0.46
1:A:96:ASN:OD1	1:B:87:ASP:HB2	2.16	0.46
2:F:161:TYR:O	2:F:162:THR:C	2.54	0.46
1:B:11:PHE:CE2	2:F:114:ALA:HB1	2.51	0.46
2:O:172:ARG:C	2:O:174:HIS:H	2.19	0.46
2:E:172:ARG:C	2:E:174:HIS:H	2.18	0.46
2:F:137:ASN:ND2	2:F:137:ASN:H	1.98	0.46
1:L:108:TYR:CE1	1:L:109:GLU:HG2	2.50	0.46
2:O:128:ARG:HG3	2:O:192:LEU:HD21	1.98	0.46
1:L:20:MET:CG	1:L:25:CYS:HA	2.46	0.46
1:I:62:PRO:O	1:I:63:ASP:OD2	2.33	0.46
2:F:172:ARG:C	2:F:174:HIS:H	2.18	0.46
2:N:87:ALA:HB2	2:N:157:MET:CE	2.47	0.45
2:E:137:ASN:H	2:E:137:ASN:ND2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:58:LEU:HD13	1:I:66:LEU:HB3	1.97	0.45
1:K:9:LEU:N	1:K:10:PRO:HD2	2.31	0.45
2:N:172:ARG:C	2:N:174:HIS:H	2.19	0.45
2:F:80:GLN:O	2:F:81:PHE:C	2.54	0.45
1:B:108:TYR:CE1	1:B:109:GLU:HG2	2.52	0.45
2:H:128:ARG:HG3	2:H:192:LEU:HD21	1.97	0.45
2:G:166:LEU:O	2:G:167:ALA:HB2	2.17	0.45
2:E:210:GLN:O	2:E:211:LEU:C	2.55	0.45
2:G:197:GLU:O	2:G:201:GLU:HG3	2.16	0.45
1:K:124:LEU:HA	1:K:125:PRO:HD2	1.71	0.45
1:I:73:PHE:CE1	2:P:39:LEU:HD13	2.52	0.45
2:E:57:TYR:HA	2:E:108:PHE:CE1	2.52	0.45
2:P:69:VAL:HB	2:P:106:VAL:HG22	1.98	0.45
2:G:128:ARG:HG3	2:G:192:LEU:HD21	1.99	0.45
1:L:105:TYR:HA	1:L:106:PRO:HD2	1.84	0.45
2:G:93:TYR:N	2:G:93:TYR:CD1	2.85	0.45
2:N:136:ILE:CD1	2:N:146:GLU:HB2	2.40	0.45
2:G:72:ASP:O	2:G:76:GLN:HG2	2.17	0.45
1:C:72:GLU:HA	1:C:72:GLU:OE2	2.17	0.45
1:B:37:ARG:HE	1:B:37:ARG:CA	2.30	0.45
1:I:15:ALA:HB1	2:M:154:ILE:HD11	1.98	0.45
1:I:17:ILE:HG23	2:M:205:ILE:CG2	2.47	0.44
1:K:105:TYR:HA	1:K:106:PRO:HD2	1.86	0.44
1:K:106:PRO:C	1:K:108:TYR:H	2.20	0.44
2:G:57:TYR:HA	2:G:108:PHE:CE1	2.52	0.44
2:O:69:VAL:HB	2:O:106:VAL:HG22	1.98	0.44
2:H:108:PHE:O	2:H:111:PHE:HB3	2.18	0.44
2:M:93:TYR:N	2:M:93:TYR:CD1	2.84	0.44
2:N:137:ASN:HD22	2:N:137:ASN:N	2.00	0.44
2:H:142:ILE:HB	2:H:190:VAL:HG12	1.98	0.44
1:I:108:TYR:CE1	1:I:109:GLU:HG2	2.53	0.44
2:P:172:ARG:C	2:P:174:HIS:H	2.21	0.44
1:I:99:ARG:HD3	1:J:85:ASP:O	2.17	0.44
1:A:66:LEU:H	1:A:66:LEU:HD12	1.82	0.44
2:F:128:ARG:HG3	2:F:192:LEU:HD21	2.00	0.44
2:E:165:VAL:O	2:E:167:ALA:N	2.50	0.44
2:G:206:MET:HA	2:G:206:MET:HE2	1.98	0.44
1:J:10:PRO:CG	2:N:115:LEU:HD21	2.48	0.44
2:N:128:ARG:HG3	2:N:192:LEU:HD21	2.00	0.44
1:K:89:GLU:CA	1:K:89:GLU:OE2	2.58	0.44
1:L:11:PHE:CE2	2:P:114:ALA:HB1	2.53	0.44
1:L:21:PRO:C	1:L:23:ALA:H	2.20	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:72:ASP:O	2:O:76:GLN:HG2	2.18	0.44
1:A:89:GLU:O	1:A:92:ARG:HB2	2.17	0.44
1:B:120:PHE:HA	2:E:65:PRO:HB3	1.98	0.44
2:F:159:GLY:C	2:F:161:TYR:N	2.69	0.44
2:H:93:TYR:N	2:H:93:TYR:CD1	2.85	0.44
1:L:89:GLU:O	1:L:92:ARG:HB2	2.18	0.44
2:E:106:VAL:O	2:E:106:VAL:HG23	2.17	0.44
1:J:70:GLU:OE2	2:M:61:LYS:HE3	2.18	0.44
2:P:82:PHE:CZ	2:P:158:MET:HE1	2.53	0.44
2:N:170:THR:CB	2:N:171:PRO:CD	2.94	0.44
1:B:70:GLU:OE2	2:E:57:TYR:OH	2.31	0.44
2:M:69:VAL:HB	2:M:106:VAL:HG23	1.99	0.44
2:O:93:TYR:HD1	2:O:93:TYR:N	2.16	0.44
2:N:178:PHE:O	2:N:182:MET:HB2	2.18	0.44
2:G:137:ASN:N	2:G:137:ASN:HD22	2.00	0.43
1:J:89:GLU:O	1:J:92:ARG:HB2	2.19	0.43
1:I:106:PRO:C	1:I:108:TYR:H	2.21	0.43
1:J:70:GLU:OE2	2:M:57:TYR:OH	2.21	0.43
2:F:93:TYR:N	2:F:93:TYR:HD1	2.16	0.43
1:L:17:ILE:H	1:L:17:ILE:HG13	1.64	0.43
2:G:136:ILE:CD1	2:G:146:GLU:HB2	2.38	0.43
1:A:120:PHE:CE1	2:H:61:LYS:HD2	2.53	0.43
2:P:80:GLN:O	2:P:81:PHE:C	2.57	0.43
1:A:79:THR:OG1	1:A:81:GLU:HG2	2.18	0.43
1:C:11:PHE:CD2	2:G:118:LEU:CD2	3.01	0.43
1:J:62:PRO:O	1:J:63:ASP:OD2	2.35	0.43
1:D:59:GLU:O	1:D:62:PRO:HD3	2.18	0.43
2:E:80:GLN:O	2:E:82:PHE:N	2.52	0.43
2:P:72:ASP:N	2:P:72:ASP:OD1	2.51	0.43
1:A:62:PRO:O	1:A:63:ASP:OD2	2.36	0.43
2:F:175:VAL:O	2:F:178:PHE:HB3	2.19	0.43
1:K:108:TYR:CE1	1:K:109:GLU:HG2	2.53	0.43
2:P:215:VAL:O	2:P:216:MET:HB2	2.18	0.43
2:P:178:PHE:O	2:P:182:MET:HB2	2.18	0.43
2:O:178:PHE:O	2:O:182:MET:HB2	2.18	0.43
2:F:86:ASP:OD1	2:F:88:SER:HB3	2.19	0.43
2:P:99:ASP:HB3	2:P:102:GLN:OE1	2.19	0.43
2:P:136:ILE:CD1	2:P:146:GLU:HB2	2.41	0.43
1:C:106:PRO:C	1:C:108:TYR:H	2.22	0.43
1:J:106:PRO:C	1:J:108:TYR:H	2.22	0.43
2:E:93:TYR:HD1	2:E:93:TYR:N	2.17	0.43
2:E:142:ILE:HA	2:E:146:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:10:PRO:HG3	2:N:115:LEU:HD21	2.01	0.43
1:K:62:PRO:O	1:K:63:ASP:OD2	2.37	0.43
2:H:82:PHE:CD1	2:H:157:MET:HG3	2.54	0.43
2:H:164:PRO:HG2	2:H:169:ASP:CB	2.49	0.43
2:O:206:MET:HB3	2:O:206:MET:HE2	1.91	0.43
1:A:11:PHE:HB3	2:E:94:LEU:HD21	2.00	0.43
1:L:21:PRO:HD3	2:P:174:HIS:NE2	2.33	0.43
1:A:18:GLY:O	2:E:178:PHE:HD2	2.02	0.43
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.77	0.42
1:C:38:GLN:HG3	1:C:39:ASP:H	1.76	0.42
2:P:73:THR:O	2:P:77:ILE:CG1	2.67	0.42
2:P:93:TYR:N	2:P:93:TYR:HD1	2.17	0.42
2:H:93:TYR:N	2:H:93:TYR:HD1	2.17	0.42
1:L:15:ALA:HB1	2:P:154:ILE:HD11	2.00	0.42
1:C:9:LEU:N	1:C:10:PRO:CD	2.82	0.42
2:P:57:TYR:HA	2:P:108:PHE:CE1	2.54	0.42
1:K:106:PRO:O	1:K:108:TYR:N	2.46	0.42
2:P:158:MET:H	2:P:158:MET:HG2	1.65	0.42
2:N:80:GLN:O	2:N:81:PHE:C	2.57	0.42
1:D:108:TYR:CE1	1:D:109:GLU:HG2	2.54	0.42
2:M:51:ARG:HG2	2:M:216:MET:CE	2.49	0.42
2:N:57:TYR:HA	2:N:108:PHE:CE1	2.54	0.42
2:F:57:TYR:HA	2:F:108:PHE:CE1	2.54	0.42
1:I:52:GLN:N	1:J:47:SER:O	2.33	0.42
2:F:122:THR:HG23	2:F:125:GLU:HB2	2.01	0.42
1:I:72:GLU:OE2	1:I:72:GLU:HA	2.20	0.42
2:P:155:TYR:OH	2:P:167:ALA:HB2	2.20	0.42
2:F:72:ASP:O	2:F:76:GLN:HG2	2.20	0.42
2:P:142:ILE:HA	2:P:146:GLU:OE1	2.19	0.42
2:H:57:TYR:HA	2:H:108:PHE:CE1	2.54	0.42
1:D:106:PRO:O	1:D:108:TYR:N	2.47	0.42
1:L:70:GLU:OE2	2:O:57:TYR:OH	2.26	0.42
2:M:57:TYR:HA	2:M:108:PHE:CE1	2.55	0.42
1:A:70:GLU:OE2	2:H:57:TYR:OH	2.36	0.42
2:N:93:TYR:N	2:N:93:TYR:HD1	2.17	0.42
1:D:124:LEU:HA	1:D:125:PRO:HD2	1.72	0.42
2:M:73:THR:O	2:M:77:ILE:CG1	2.68	0.42
2:H:167:ALA:C	2:H:169:ASP:H	2.23	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD2	1.90	0.42
2:M:93:TYR:N	2:M:93:TYR:HD1	2.18	0.42
1:J:16:ALA:O	1:J:19:TRP:CD1	2.73	0.42
1:B:78:ASP:C	1:B:80:LYS:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:80:GLN:O	2:O:81:PHE:C	2.59	0.42
1:L:27:MET:C	1:L:29:LEU:N	2.72	0.41
1:J:108:TYR:CE1	1:J:109:GLU:HG2	2.54	0.41
1:D:62:PRO:O	1:D:63:ASP:OD2	2.38	0.41
1:L:124:LEU:HA	1:L:125:PRO:HD2	1.69	0.41
1:C:62:PRO:O	1:C:63:ASP:OD2	2.38	0.41
1:D:89:GLU:OE1	1:D:92:ARG:NH1	2.50	0.41
1:L:21:PRO:O	1:L:26:PRO:HD3	2.20	0.41
1:D:11:PHE:CZ	2:H:115:LEU:HG	2.55	0.41
2:F:209:LEU:HA	2:F:209:LEU:HD23	1.89	0.41
2:N:72:ASP:O	2:N:76:GLN:HG2	2.20	0.41
2:E:73:THR:O	2:E:77:ILE:CG1	2.68	0.41
1:A:106:PRO:C	1:A:108:TYR:H	2.23	0.41
2:E:178:PHE:O	2:E:182:MET:HB2	2.20	0.41
2:M:210:GLN:O	2:M:211:LEU:C	2.58	0.41
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.20	0.41
1:I:11:PHE:O	2:M:90:TYR:OH	2.39	0.41
2:M:80:GLN:O	2:M:81:PHE:C	2.59	0.41
1:B:124:LEU:HD13	1:B:125:PRO:HD2	2.03	0.41
1:C:105:TYR:HA	1:C:106:PRO:HD2	1.85	0.41
2:E:72:ASP:OD1	2:E:72:ASP:N	2.54	0.41
1:J:9:LEU:N	1:J:10:PRO:CD	2.83	0.41
1:A:19:TRP:O	1:A:20:MET:HB2	2.20	0.41
1:D:105:TYR:HA	1:D:106:PRO:HD2	1.85	0.41
1:J:91:PHE:CD2	1:J:91:PHE:O	2.74	0.41
1:B:52:GLN:N	1:C:47:SER:O	2.36	0.41
2:P:137:ASN:N	2:P:137:ASN:HD22	2.00	0.41
2:O:137:ASN:N	2:O:137:ASN:HD22	2.00	0.41
1:L:89:GLU:OE1	1:L:92:ARG:NH1	2.53	0.41
1:C:18:GLY:C	1:C:19:TRP:CD1	2.92	0.41
2:P:64:CYS:SG	2:P:69:VAL:HG22	2.60	0.41
2:E:212:PHE:HE1	2:P:212:PHE:CE1	2.33	0.41
2:N:206:MET:HG3	2:N:210:GLN:NE2	2.36	0.41
2:P:80:GLN:O	2:P:82:PHE:N	2.54	0.41
1:J:59:GLU:O	1:J:62:PRO:HD3	2.21	0.41
1:D:106:PRO:C	1:D:108:TYR:H	2.23	0.41
1:B:91:PHE:O	1:B:91:PHE:CD2	2.74	0.41
1:D:9:LEU:N	1:D:10:PRO:HD2	2.35	0.41
2:N:170:THR:HA	2:N:171:PRO:HD3	1.87	0.41
2:P:122:THR:HG23	2:P:125:GLU:HB2	2.03	0.41
2:P:86:ASP:OD1	2:P:88:SER:HB3	2.21	0.41
2:O:69:VAL:HB	2:O:106:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:19:TRP:CD1	1:J:19:TRP:N	2.89	0.40
1:D:76:ASN:HB3	1:D:79:THR:OG1	2.21	0.40
1:L:106:PRO:C	1:L:108:TYR:H	2.22	0.40
1:D:68:SER:HB2	1:D:69:THR:H	1.75	0.40
1:B:62:PRO:O	1:B:63:ASP:OD2	2.39	0.40
2:H:142:ILE:HA	2:H:146:GLU:OE1	2.21	0.40
2:P:82:PHE:CZ	2:P:158:MET:CE	3.05	0.40
1:D:64:THR:O	1:D:65:LEU:C	2.60	0.40
2:N:93:TYR:CE2	2:N:136:ILE:HD13	2.57	0.40
2:M:106:VAL:O	2:M:106:VAL:HG23	2.21	0.40
2:M:122:THR:HG23	2:M:125:GLU:HB2	2.03	0.40
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.16	0.40
2:H:209:LEU:C	2:H:210:GLN:HG3	2.41	0.40
2:H:152:LYS:HE2	2:H:152:LYS:HB2	1.93	0.40

There are no symmetry-related clashes.

## 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	A	123/144 (85%)	99 (80%)	18 (15%)	6 (5%)	3	30
1	B	120/144 (83%)	98 (82%)	17 (14%)	5 (4%)	4	36
1	C	122/144 (85%)	103 (84%)	16 (13%)	3 (2%)	9	52
1	D	118/144 (82%)	98 (83%)	17 (14%)	3 (2%)	9	52
1	I	129/144 (90%)	102 (79%)	18 (14%)	9 (7%)	2	20
1	J	123/144 (85%)	103 (84%)	16 (13%)	4 (3%)	6	44
1	K	128/144 (89%)	104 (81%)	17 (13%)	7 (6%)	3	26
1	L	136/144 (94%)	104 (76%)	18 (13%)	14 (10%)	1	9
2	E	177/180 (98%)	150 (85%)	14 (8%)	13 (7%)	2	18
2	F	178/180 (99%)	146 (82%)	20 (11%)	12 (7%)	2	21
2	G	170/180 (94%)	148 (87%)	11 (6%)	11 (6%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	172/180 (96%)	146 (85%)	17 (10%)	9 (5%)	3	28
2	M	166/180 (92%)	144 (87%)	13 (8%)	9 (5%)	3	27
2	N	164/180 (91%)	141 (86%)	15 (9%)	8 (5%)	3	30
2	O	164/180 (91%)	141 (86%)	14 (8%)	9 (6%)	3	26
2	P	168/180 (93%)	145 (86%)	13 (8%)	10 (6%)	2	24
All	All	2358/2592 (91%)	1972 (84%)	254 (11%)	132 (6%)	3	26

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	ILE
1	D	17	ILE
2	E	83	PRO
2	E	163	TYR
2	E	164	PRO
2	E	166	LEU
2	F	66	SER
2	F	83	PRO
2	F	163	TYR
2	F	166	LEU
2	G	66	SER
2	G	83	PRO
2	H	66	SER
2	H	83	PRO
2	H	186	LYS
1	I	21	PRO
1	I	38	GLN
1	J	17	ILE
1	K	28	PRO
1	L	22	VAL
1	L	24	ASN
1	L	28	PRO
1	L	30	ALA
1	L	31	PRO
1	L	37	ARG
2	M	83	PRO
2	N	66	SER
2	N	83	PRO
2	N	170	THR
2	N	171	PRO

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Mol	Chain	Res	Type
2	O	66	SER
2	O	83	PRO
2	O	203	ASP
2	O	212	PHE
2	P	66	SER
2	P	83	PRO
1	A	24	ASN
1	A	25	CYS
1	A	65	LEU
1	A	107	ARG
1	B	107	ARG
1	C	17	ILE
1	C	107	ARG
1	D	65	LEU
1	D	107	ARG
2	E	66	SER
2	F	167	ALA
2	G	81	PHE
2	H	81	PHE
2	H	205	ILE
1	I	28	PRO
1	I	107	ARG
1	J	65	LEU
1	J	107	ARG
1	K	107	ARG
1	L	23	ALA
1	L	107	ARG
2	M	66	SER
2	M	212	PHE
2	O	211	LEU
2	P	203	ASP
1	A	17	ILE
1	B	65	LEU
1	C	65	LEU
2	E	81	PHE
2	E	98	PHE
2	E	173	GLN
2	E	211	LEU
2	F	81	PHE
2	F	161	TYR
2	F	162	THR
2	F	173	GLN

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Mol	Chain	Res	Type
2	G	167	ALA
2	G	173	GLN
2	H	173	GLN
1	I	37	ARG
1	I	65	LEU
1	K	65	LEU
1	L	21	PRO
1	L	35	ASN
1	L	65	LEU
2	M	81	PHE
2	M	173	GLN
2	N	81	PHE
2	N	173	GLN
2	O	81	PHE
2	O	173	GLN
2	O	205	ILE
2	P	81	PHE
2	P	98	PHE
2	P	169	ASP
2	F	98	PHE
2	F	211	LEU
2	G	98	PHE
2	G	158	MET
1	K	20	MET
2	M	98	PHE
2	M	169	ASP
2	N	98	PHE
2	P	99	ASP
2	P	173	GLN
1	B	36	LYS
2	E	167	ALA
2	F	209	LEU
2	G	168	GLU
2	G	171	PRO
2	H	98	PHE
2	H	163	TYR
1	I	20	MET
1	I	25	CYS
1	K	17	ILE
1	K	27	MET
1	L	20	MET
2	M	211	LEU

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Mol	Chain	Res	Type
2	O	98	PHE
2	P	171	PRO
2	E	99	ASP
2	E	138	LYS
2	G	138	LYS
2	G	203	ASP
2	H	168	GLU
2	M	138	LYS
2	N	138	LYS
2	P	138	LYS
1	L	125	PRO
1	A	125	PRO
1	I	125	PRO
1	J	125	PRO
1	K	125	PRO
1	B	125	PRO
2	E	159	GLY
1	L	17	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/122 (80%)	84 (87%)	13 (13%)	6	27
1	B	97/122 (80%)	83 (86%)	14 (14%)	5	24
1	C	96/122 (79%)	81 (84%)	15 (16%)	4	20
1	D	96/122 (79%)	84 (88%)	12 (12%)	7	30
1	I	100/122 (82%)	87 (87%)	13 (13%)	6	28
1	J	96/122 (79%)	82 (85%)	14 (15%)	5	23
1	K	100/122 (82%)	86 (86%)	14 (14%)	5	25
1	L	102/122 (84%)	89 (87%)	13 (13%)	6	29
2	E	138/162 (85%)	122 (88%)	16 (12%)	8	35
2	F	139/162 (86%)	121 (87%)	18 (13%)	6	29
2	G	133/162 (82%)	114 (86%)	19 (14%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	137/162 (85%)	115 (84%)	22 (16%)	3	18
2	M	131/162 (81%)	116 (88%)	15 (12%)	8	35
2	N	133/162 (82%)	114 (86%)	19 (14%)	5	24
2	O	134/162 (83%)	115 (86%)	19 (14%)	5	24
2	P	138/162 (85%)	119 (86%)	19 (14%)	5	25
All	All	1867/2272 (82%)	1612 (86%)	255 (14%)	5	26

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TRP
1	A	40	GLU
1	A	41	LEU
1	A	63	ASP
1	A	77	GLU
1	A	78	ASP
1	A	80	LYS
1	A	86	ARG
1	A	110	CYS
1	A	114	TYR
1	A	124	LEU
1	A	130	ASP
1	A	138	ASP
1	B	37	ARG
1	B	40	GLU
1	B	41	LEU
1	B	56	THR
1	B	63	ASP
1	B	77	GLU
1	B	78	ASP
1	B	80	LYS
1	B	86	ARG
1	B	110	CYS
1	B	114	TYR
1	B	124	LEU
1	B	130	ASP
1	B	138	ASP
1	C	19	TRP
1	C	38	GLN
1	C	40	GLU

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Mol	Chain	Res	Type
1	C	41	LEU
1	C	56	THR
1	C	63	ASP
1	C	77	GLU
1	C	78	ASP
1	C	80	LYS
1	C	86	ARG
1	C	110	CYS
1	C	114	TYR
1	C	124	LEU
1	C	130	ASP
1	C	138	ASP
1	D	40	GLU
1	D	41	LEU
1	D	63	ASP
1	D	77	GLU
1	D	78	ASP
1	D	80	LYS
1	D	86	ARG
1	D	110	CYS
1	D	114	TYR
1	D	124	LEU
1	D	130	ASP
1	D	138	ASP
2	E	74	PHE
2	E	84	HIS
2	E	93	TYR
2	E	99	ASP
2	E	109	GLU
2	E	113	THR
2	E	118	LEU
2	E	122	THR
2	E	137	ASN
2	E	138	LYS
2	E	145	GLU
2	E	174	HIS
2	E	182	MET
2	E	184	LYS
2	E	186	LYS
2	E	189	ILE
2	F	74	PHE
2	F	84	HIS

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Mol	Chain	Res	Type
2	F	93	TYR
2	F	99	ASP
2	F	109	GLU
2	F	113	THR
2	F	118	LEU
2	F	122	THR
2	F	137	ASN
2	F	138	LYS
2	F	145	GLU
2	F	158	MET
2	F	174	HIS
2	F	182	MET
2	F	184	LYS
2	F	186	LYS
2	F	189	ILE
2	F	207	ARG
2	G	43	GLU
2	G	74	PHE
2	G	84	HIS
2	G	99	ASP
2	G	109	GLU
2	G	118	LEU
2	G	122	THR
2	G	137	ASN
2	G	138	LYS
2	G	145	GLU
2	G	174	HIS
2	G	182	MET
2	G	184	LYS
2	G	186	LYS
2	G	189	ILE
2	G	197	GLU
2	G	206	MET
2	G	207	ARG
2	G	214	ASN
2	H	43	GLU
2	H	74	PHE
2	H	84	HIS
2	H	93	TYR
2	H	99	ASP
2	H	109	GLU
2	H	113	THR

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Mol	Chain	Res	Type
2	H	115	LEU
2	H	118	LEU
2	H	122	THR
2	H	137	ASN
2	H	138	LYS
2	H	145	GLU
2	H	157	MET
2	H	169	ASP
2	H	174	HIS
2	H	182	MET
2	H	184	LYS
2	H	186	LYS
2	H	189	ILE
2	H	197	GLU
2	H	204	ASN
1	I	19	TRP
1	I	40	GLU
1	I	41	LEU
1	I	56	THR
1	I	63	ASP
1	I	77	GLU
1	I	78	ASP
1	I	86	ARG
1	I	110	CYS
1	I	114	TYR
1	I	124	LEU
1	I	130	ASP
1	I	138	ASP
1	J	20	MET
1	J	40	GLU
1	J	41	LEU
1	J	56	THR
1	J	63	ASP
1	J	77	GLU
1	J	78	ASP
1	J	80	LYS
1	J	86	ARG
1	J	110	CYS
1	J	114	TYR
1	J	124	LEU
1	J	130	ASP
1	J	138	ASP

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Mol	Chain	Res	Type
1	K	38	GLN
1	K	40	GLU
1	K	41	LEU
1	K	56	THR
1	K	63	ASP
1	K	77	GLU
1	K	78	ASP
1	K	80	LYS
1	K	86	ARG
1	K	110	CYS
1	K	114	TYR
1	K	124	LEU
1	K	130	ASP
1	K	138	ASP
1	L	40	GLU
1	L	41	LEU
1	L	56	THR
1	L	63	ASP
1	L	77	GLU
1	L	78	ASP
1	L	80	LYS
1	L	86	ARG
1	L	110	CYS
1	L	114	TYR
1	L	124	LEU
1	L	130	ASP
1	L	138	ASP
2	M	74	PHE
2	M	84	HIS
2	M	99	ASP
2	M	109	GLU
2	M	113	THR
2	M	118	LEU
2	M	122	THR
2	M	137	ASN
2	M	138	LYS
2	M	145	GLU
2	M	174	HIS
2	M	182	MET
2	M	184	LYS
2	M	186	LYS
2	M	189	ILE

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Mol	Chain	Res	Type
2	N	74	PHE
2	N	84	HIS
2	N	99	ASP
2	N	100	THR
2	N	109	GLU
2	N	113	THR
2	N	118	LEU
2	N	122	THR
2	N	137	ASN
2	N	138	LYS
2	N	145	GLU
2	N	157	MET
2	N	174	HIS
2	N	182	MET
2	N	184	LYS
2	N	186	LYS
2	N	189	ILE
2	N	206	MET
2	N	214	ASN
2	O	43	GLU
2	O	74	PHE
2	O	84	HIS
2	O	93	TYR
2	O	99	ASP
2	O	109	GLU
2	O	113	THR
2	O	118	LEU
2	O	122	THR
2	O	137	ASN
2	O	138	LYS
2	O	145	GLU
2	O	152	LYS
2	O	174	HIS
2	O	182	MET
2	O	184	LYS
2	O	186	LYS
2	O	189	ILE
2	O	209	LEU
2	P	74	PHE
2	P	84	HIS
2	P	93	TYR
2	P	99	ASP

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Mol	Chain	Res	Type
2	P	100	THR
2	P	109	GLU
2	P	113	THR
2	P	115	LEU
2	P	122	THR
2	P	137	ASN
2	P	138	LYS
2	P	145	GLU
2	P	158	MET
2	P	174	HIS
2	P	182	MET
2	P	184	LYS
2	P	186	LYS
2	P	189	ILE
2	P	204	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	C	38	GLN
2	E	137	ASN
2	F	76	GLN
2	F	96	ASN
2	F	137	ASN
2	G	76	GLN
2	G	96	ASN
2	G	137	ASN
2	G	214	ASN
2	H	76	GLN
2	H	185	ASN
2	M	76	GLN
2	M	96	ASN
2	M	137	ASN
2	N	76	GLN
2	N	137	ASN
2	N	214	ASN
2	O	137	ASN
2	P	76	GLN
2	P	137	ASN
2	P	204	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	129/144 (89%)	-0.06	0	100	100	122, 128, 135, 142	0
1	B	124/144 (86%)	-0.03	0	100	100	122, 128, 135, 142	0
1	C	126/144 (87%)	0.05	0	100	100	122, 128, 135, 142	0
1	D	122/144 (84%)	0.02	0	100	100	122, 128, 135, 142	0
1	I	133/144 (92%)	0.05	0	100	100	110, 128, 134, 142	0
1	J	129/144 (89%)	0.00	0	100	100	122, 128, 135, 142	0
1	K	132/144 (91%)	-0.00	0	100	100	122, 128, 135, 142	0
1	L	138/144 (95%)	-0.07	1 (0%)	84	50	122, 128, 135, 142	0
2	E	179/180 (99%)	-0.09	0	100	100	31, 128, 138, 142	0
2	F	180/180 (100%)	-0.08	0	100	100	31, 128, 138, 142	0
2	G	174/180 (96%)	-0.01	0	100	100	31, 129, 138, 145	0
2	H	174/180 (96%)	-0.05	0	100	100	31, 128, 137, 142	0
2	M	170/180 (94%)	0.10	2 (1%)	75	37	31, 129, 138, 142	0
2	N	168/180 (93%)	0.19	2 (1%)	75	37	31, 129, 137, 142	0
2	O	168/180 (93%)	0.03	1 (0%)	86	53	31, 129, 137, 143	0
2	P	172/180 (95%)	-0.06	0	100	100	31, 129, 137, 142	0
All	All	2418/2592 (93%)	-0.00	6 (0%)	93	76	31, 128, 137, 145	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	83	PRO	4.1
1	L	108	TYR	2.8
2	N	84	HIS	2.7
2	M	84	HIS	2.4
2	O	87	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	180	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	F	702	1/1	0.38	3.54	105,105,105,105	0
5	NA	H	701	1/1	0.43	2.54	106,106,106,106	0
5	NA	E	703	1/1	0.23	0.19	81,81,81,81	0
4	ZN	I	605	1/1	0.18	-0.17	133,133,133,133	0
3	CA	P	505	1/1	0.20	-0.34	101,101,101,101	0
4	ZN	L	608	1/1	0.16	-0.39	129,129,129,129	0
5	NA	G	704	1/1	0.22	-0.48	106,106,106,106	0
4	ZN	D	604	1/1	0.13	-0.48	139,139,139,139	0
4	ZN	J	606	1/1	0.14	-0.56	144,144,144,144	0
4	ZN	B	602	1/1	0.14	-0.62	130,130,130,130	0
3	CA	H	502	1/1	0.13	-0.68	104,104,104,104	0
3	CA	G	512	1/1	0.14	-0.69	135,135,135,135	0
4	ZN	C	603	1/1	0.14	-0.73	136,136,136,136	0
4	ZN	A	601	1/1	0.12	-0.82	132,132,132,132	0
3	CA	G	504	1/1	0.16	-0.84	123,123,123,123	0
3	CA	N	507	1/1	0.15	-0.90	173,173,173,173	0
3	CA	O	508	1/1	0.16	-0.90	140,140,140,140	0
4	ZN	K	607	1/1	0.11	-0.91	151,151,151,151	0
3	CA	P	513	1/1	0.15	-1.07	123,123,123,123	0
3	CA	E	503	1/1	0.07	-1.24	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	F	501	1/1	0.05	-1.25	111,111,111,111	0
3	CA	E	511	1/1	0.12	-1.45	149,149,149,149	0
3	CA	M	506	1/1	0.08	-1.52	169,169,169,169	0
3	CA	O	516	1/1	0.07	-1.68	206,206,206,206	0
3	CA	F	509	1/1	0.07	-1.73	162,162,162,162	0
3	CA	H	510	1/1	0.08	-2.35	108,108,108,108	0
3	CA	M	514	1/1	0.07	-2.36	156,156,156,156	0
3	CA	N	515	1/1	0.10	-2.80	146,146,146,146	0

## 6.5 Other polymers

There are no such residues in this entry.