



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 03:24 PM EDT

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 X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

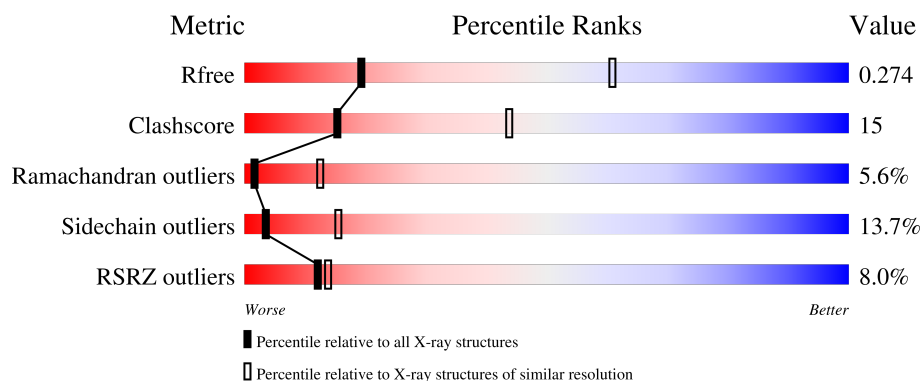
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	144	<div> <div>4%</div> <div> <div>55%</div> <div>31%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	144	<div> <div>5%</div> <div> <div>53%</div> <div>28%</div> <div>5%</div> <div>14%</div> </div> </div>
1	C	144	<div> <div>8%</div> <div> <div>58%</div> <div>27%</div> <div>••</div> <div>12%</div> </div> </div>
1	D	144	<div> <div>6%</div> <div> <div>53%</div> <div>28%</div> <div>•</div> <div>15%</div> </div> </div>
1	I	144	<div> <div>8%</div> <div> <div>54%</div> <div>34%</div> <div>•</div> <div>8%</div> </div> </div>

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18970 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 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 mutation	UNP Q9NZI2
E	167	ALA	LYS	engineered mutation	UNP Q9NZI2
F	160	ALA	LYS	engineered mutation	UNP Q9NZI2
F	167	ALA	LYS	engineered mutation	UNP Q9NZI2
G	160	ALA	LYS	engineered mutation	UNP Q9NZI2
G	167	ALA	LYS	engineered mutation	UNP Q9NZI2
H	160	ALA	LYS	engineered mutation	UNP Q9NZI2
H	167	ALA	LYS	engineered mutation	UNP Q9NZI2
M	160	ALA	LYS	engineered mutation	UNP Q9NZI2
M	167	ALA	LYS	engineered mutation	UNP Q9NZI2
N	160	ALA	LYS	engineered mutation	UNP Q9NZI2
N	167	ALA	LYS	engineered mutation	UNP Q9NZI2
O	160	ALA	LYS	engineered mutation	UNP Q9NZI2
O	167	ALA	LYS	engineered mutation	UNP Q9NZI2
P	160	ALA	LYS	engineered mutation	UNP Q9NZI2

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

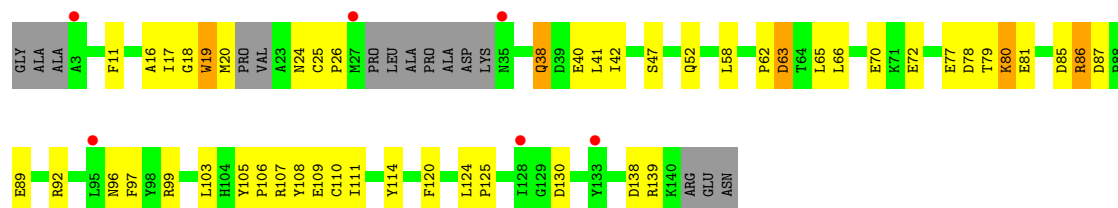
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Na 1	0	0
5	F	1	Total 1	Na 1	0	0
5	G	1	Total 1	Na 1	0	0
5	H	1	Total 1	Na 1	0	0

### 3 Residue-property plots [i](#)

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

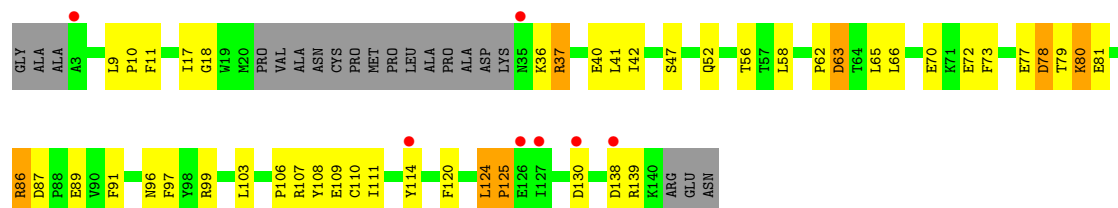
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain A: 



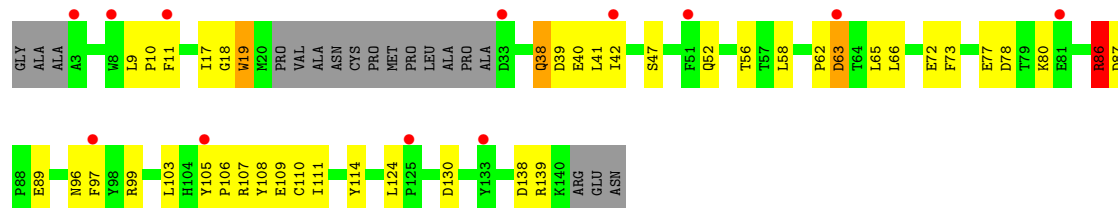
- Molecule 1: Potassium voltage-gated channel subfamily D member 3

Chain B: 



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

Chain C: 

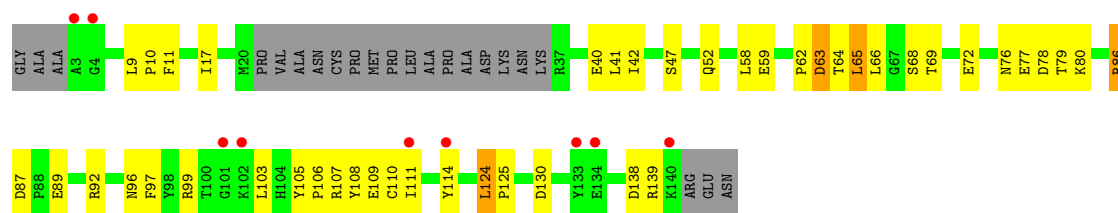


- Molecule 1: Potassium voltage-gated channel subfamily D member 3

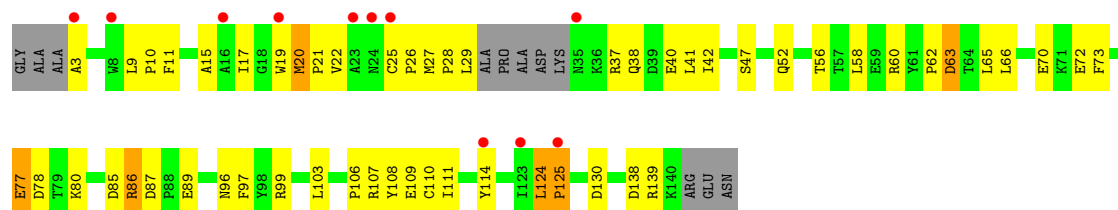
Chain D: 



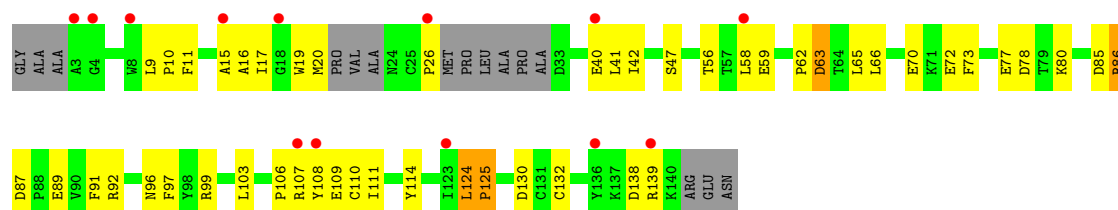




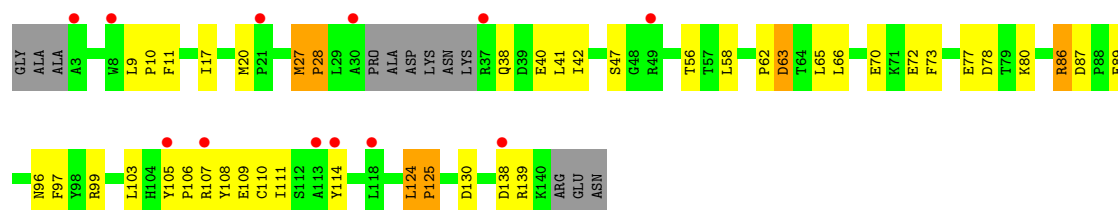
- Molecule 1: Potassium voltage-gated channel subfamily D member 3



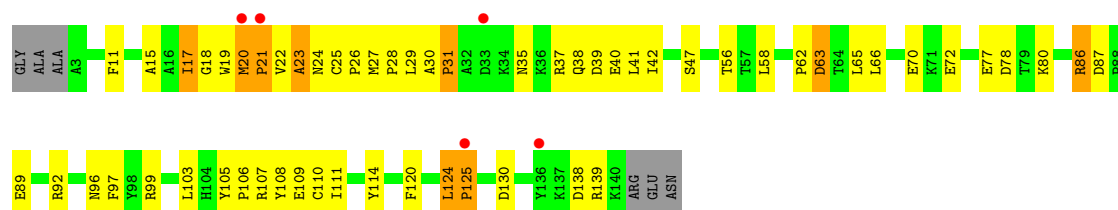
- Molecule 1: Potassium voltage-gated channel subfamily D member 3



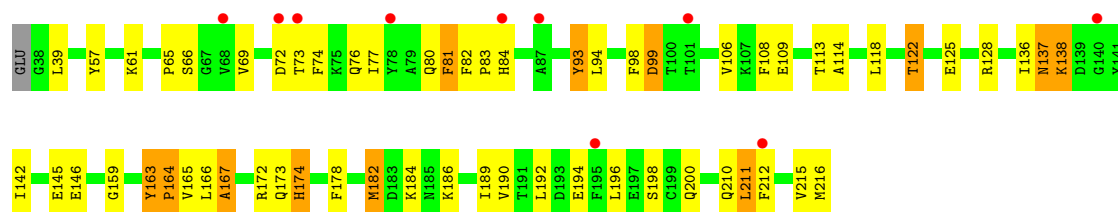
- Molecule 1: Potassium voltage-gated channel subfamily D member 3



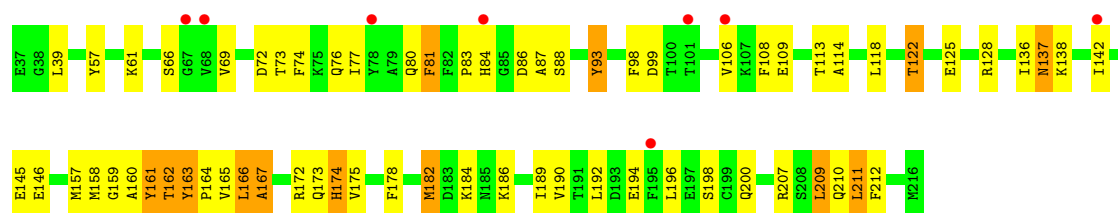
- Molecule 1: Potassium voltage-gated channel subfamily D member 3



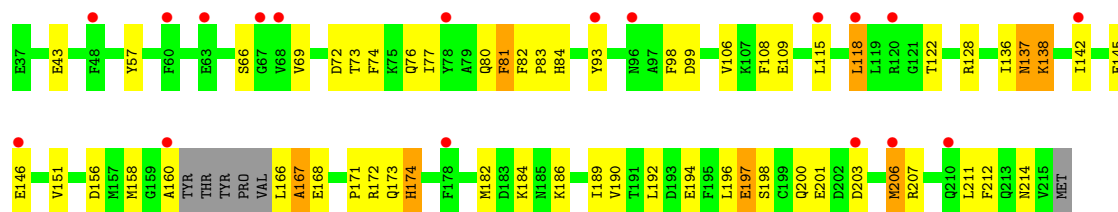
- Molecule 2: Kv channel-interacting protein 1



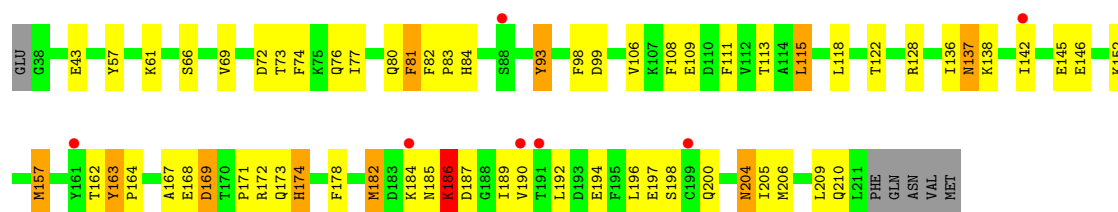
- Molecule 2: Kv channel-interacting protein 1



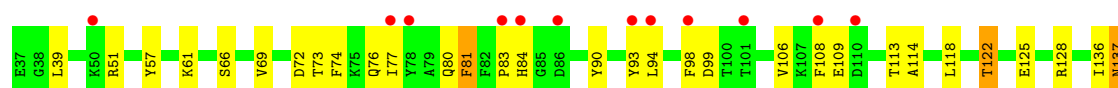
- Molecule 2: Kv channel-interacting protein 1



- Molecule 2: Kv channel-interacting protein 1

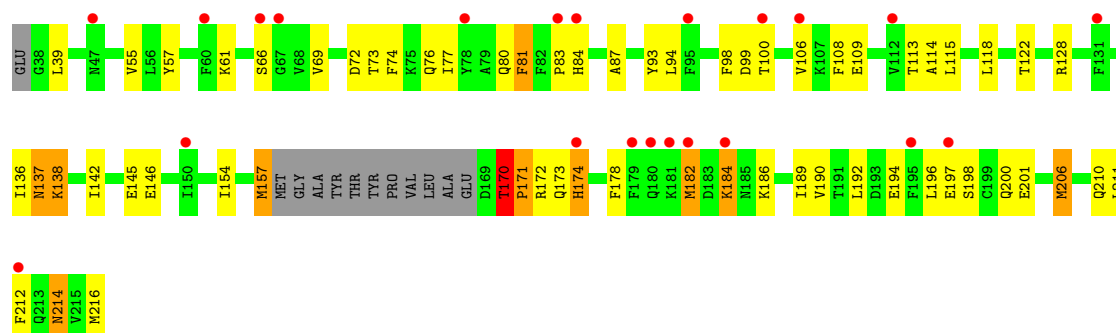


- Molecule 2: Kv channel-interacting protein 1

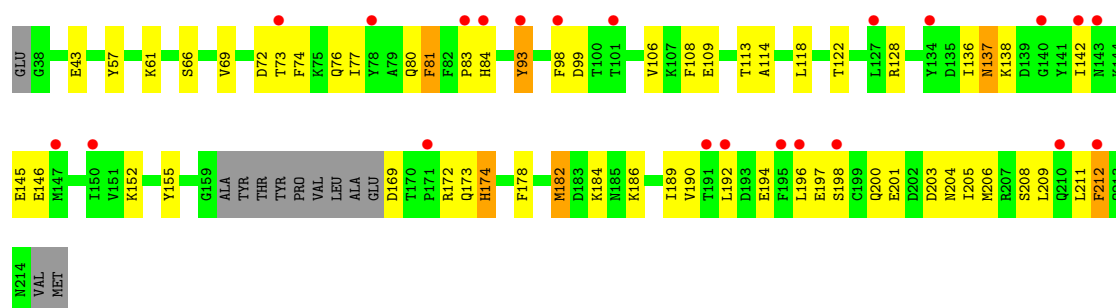




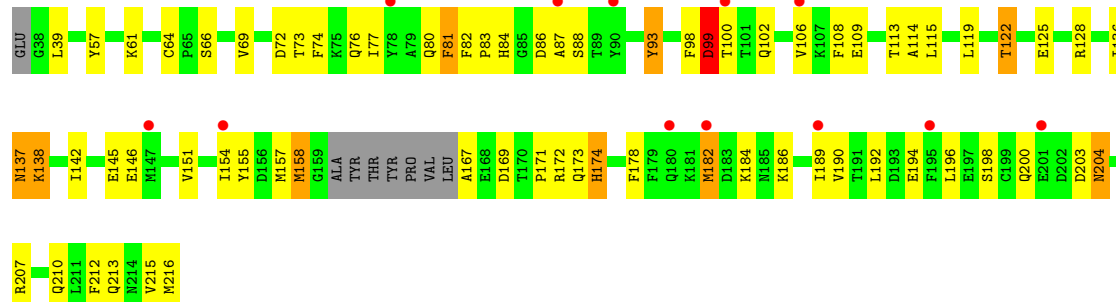
• Molecule 2: Kv channel-interacting protein 1



• Molecule 2: Kv channel-interacting protein 1



• Molecule 2: Kv channel-interacting protein 1



## 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 , 0.274	Depositor DCC
$R_{free}$ test set	2038 reflections (5.02%)	wwPDB-VP
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 , 163.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	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.

<sup>2</sup>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

### 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 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	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	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	1	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (534) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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	Interatomic distance (Å)	Clash overlap (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:H	2:G:137:ASN:HD22	1.19	0.91
1:A:86:ARG:HG3	1:A:86:ARG:HH11	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:HD22	2:M:137:ASN:H	1.19	0.88
1:K:86:ARG:HH11	1:K:86:ARG:HG3	1.38	0.88
2:F:137:ASN:HD22	2:F:137:ASN:H	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:HG3	1:B:86:ARG:HH11	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:E:163:TYR:H	2:E:164:PRO:CD	1.92	0.83
2:P:119:LEU:HD22	2:P:213:GLN:HG3	1.60	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	3:J:606:ZN:ZN	0.99	0.75
1:L:38:GLN:HG2	1:L:39:ASP:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:ARG:HH22	1:K:47:SER:HB2	1.48	0.75
1:C:11:PHE:CZ	2:G:115:LEU:HG	2.24	0.73
1:I:89:GLU:HA	1:I:89:GLU:OE2	1.88	0.73
1:C:86:ARG:HG3	1:C:86:ARG:HH11	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:OE2	1:J:89:GLU:HA	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
1:C:89:GLU:OE2	1:C:89:GLU:HA	1.95	0.67
2:M:202:ASP:CG	2:M:205:ILE:HG12	2.15	0.67
1:B:42:ILE:HD11	1:B:58:LEU:HD12	1.76	0.67
1:J:111:ILE:HG13	1:J:139:ARG:O	1.93	0.67
1:C:42:ILE:HD11	1:C:58:LEU:HD12	1.75	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: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:HH11	1:J:86:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:196:LEU:O	2:G:200:GLN:HG2	1.97	0.65
1:B:111:ILE:HG13	1:B:139:ARG:O	1.97	0.65
2:H:196:LEU:O	2:H:200:GLN:HG2	1.96	0.65
1:D:86:ARG:HH11	1:D:86:ARG:CG	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
1:K:97:PHE:CD2	1:K:103:LEU:HB2	2.34	0.61
2:N:87:ALA:HB2	2:N:157:MET:CG	2.14	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:G:69:VAL:HB	2:G:106:VAL:CG2	2.33	0.59
2:P:73:THR:O	2:P:77:ILE:HG13	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:97:PHE:CD2	1:D:103:LEU:HB2	2.38	0.59
2:F:159:GLY:C	2:F:161:TYR:H	2.07	0.59
1:L:42:ILE:HD11	1:L:58:LEU:CD1	2.32	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:HH11	1:A:86:ARG:CG	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:58:LEU:HD13	1:J:66:LEU:HB3	1.87	0.57
1:J:73:PHE:HE1	2:M:39:LEU:HD13	1.70	0.57
1:A:97:PHE:CD2	1:A:103:LEU:HB2	2.39	0.57
1:D:86:ARG:HG3	1:D:86:ARG:NH1	2.09	0.57
2:H:194:GLU:O	2:H:198:SER:HB2	2.05	0.57
1:L:86:ARG:HH11	1:L:86:ARG:CG	2.16	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
1:J:9:LEU:N	1:J:10:PRO:HD2	2.20	0.56
2:N:137:ASN:H	2:N:137:ASN:ND2	1.98	0.56
2:P:142:ILE:HB	2:P:190:VAL:HG12	1.87	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
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
2:P:137:ASN:H	2:P:137:ASN:ND2	1.98	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:SER:O	1:D:52:GLN:N	2.30	0.55
1:A:87:ASP:HB2	1:D:96:ASN:OD1	2.07	0.55
1:I:87:ASP:HB2	1:L:96:ASN:OD1	2.06	0.55
2:O:137:ASN:H	2:O:137:ASN:ND2	1.98	0.54
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
2:H:80:GLN:O	2:H:81:PHE:C	2.46	0.54
1:K:42:ILE:HD11	1:K:58:LEU:CD1	2.38	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
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:137:ASN:H	2:H:137:ASN:ND2	1.98	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:H	2:M:137:ASN:ND2	1.98	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:P:87:ALA:HB2	2:P:157:MET:CG	2.30	0.52
2:G:156:ASP:HA	2:G:160:ALA:HB2	1.92	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:HG23	2:P:106:VAL:O	2.09	0.52
2:H:163:TYR:N	2:H:164:PRO:HD3	2.25	0.51
1:I:47:SER:CB	1:L:99:ARG:NH2	2.60	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:TYR:CE2	2:F:61:LYS:HG3	2.46	0.51
1:B:106:PRO:O	1:B:108:TYR:N	2.39	0.51
2:O:142:ILE:HB	2:O:190:VAL:HG12	1.92	0.51
2:E:137:ASN:HD22	2:E:137:ASN:N	2.00	0.51
2:H:73:THR:O	2:H:77:ILE:HG13	2.11	0.51
1:J:11:PHE:HE2	2:N:114:ALA:HB1	1.76	0.51
1:K:70:GLU:OE2	2:N:57:TYR:OH	2.24	0.51
1:K:73:PHE:CE1	2:N:39:LEU:HD13	2.45	0.51
2:G:106:VAL:HG23	2:G:106:VAL:O	2.11	0.51
2:G:137:ASN:H	2:G:137:ASN:ND2	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
1:J:96:ASN:OD1	1:K:87:ASP:HB2	2.11	0.50
2:N:69:VAL:HB	2:N:106:VAL:HG22	1.94	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
1:B:79:THR:OG1	1:B:81:GLU:HG2	2.12	0.50
1:I:106:PRO:O	1:I:108:TYR:N	2.41	0.50
1:J:11:PHE:HB3	2:N:94:LEU:HD21	1.94	0.50
2:N:57:TYR:CE2	2:N:61:LYS:HG3	2.46	0.50
2:O:155:TYR:HE2	2:O:169:ASP:HA	1.77	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:3:ALA:HB2	1:I:60:ARG:NH2	2.27	0.49
1:I:96:ASN:OD1	1:J:87:ASP:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:142:ILE:HB	2:G:190:VAL:CG1	2.43	0.49
2:H:136:ILE:CD1	2:H:146:GLU:HB2	2.36	0.49
1:C:18:GLY:C	1:C:19:TRP:HD1	2.17	0.48
2:F:142:ILE:HB	2:F:190:VAL:CG1	2.43	0.48
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
2:O:106:VAL:O	2:O:106:VAL:HG23	2.11	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:H:172:ARG:C	2:H:174:HIS:H	2.16	0.48
2:M:136:ILE:CD1	2:M:146:GLU:HB2	2.37	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:B:9:LEU:N	1:B:10:PRO:HD2	2.28	0.48
1:D:89:GLU:O	1:D:92:ARG:HB2	2.14	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:B:11:PHE:HE2	2:F:114:ALA:HB1	1.79	0.47
1:C:106:PRO:O	1:C:108:TYR:N	2.45	0.47
2:F:212:PHE:HE1	2:O:212:PHE:HE1	1.62	0.47
1:K:72:GLU:OE2	1:K:72:GLU:HA	2.14	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:18:GLY:O	2:F:178:PHE:HD2	1.98	0.47
2:E:128:ARG:HG3	2:E:192:LEU:HD21	1.95	0.47
2:F:142:ILE:HB	2:F:190:VAL:HG12	1.96	0.47
2:G:80:GLN:O	2:G:82:PHE:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:GLU:OE2	1:L:72:GLU:HA	2.15	0.47
1:A:38:GLN:HE22	1:I:77:GLU:HG2	1.80	0.47
1:A:72:GLU:OE2	1:A:72:GLU:HA	2.15	0.47
1:A:80:LYS:HG2	1:I:80:LYS:HG2	1.96	0.47
1:A:108:TYR:CE1	1:A:109:GLU:HG2	2.49	0.47
2:G:69:VAL:HB	2:G:106:VAL:HG22	1.97	0.47
2:G:172:ARG:C	2:G:174:HIS:H	2.18	0.47
2:H:57:TYR:CE2	2:H:61:LYS:HG3	2.49	0.47
2:N:55:VAL:HG21	2:N:216:MET:HE3	1.95	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
2:F:178:PHE:O	2:F:182:MET:HB2	2.15	0.47
2:G:200:GLN:HA	2:G:206:MET:SD	2.55	0.47
1:K:99:ARG:NH2	1:L:47:SER:CB	2.62	0.47
1:C:73:PHE:CE1	2:F:39:LEU:HD13	2.50	0.46
2:F:93:TYR:CD1	2:F:93:TYR:N	2.84	0.46
2:H:209:LEU:O	2:H:210:GLN:CG	2.62	0.46
1:I:124:LEU:HA	1:I:125:PRO:HD2	1.71	0.46
1:B:106:PRO:C	1:B:108:TYR:H	2.18	0.46
2:F:69:VAL:HB	2:F:106:VAL:HG22	1.97	0.46
2:H:69:VAL:HB	2:H:106:VAL:CG2	2.45	0.46
1:I:70:GLU:OE2	2:P:61:LYS:HE3	2.16	0.46
1:L:38:GLN:HG2	1:L:39:ASP:N	2.24	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:B:73:PHE:CE1	2:E:39:LEU:HD13	2.51	0.46
2:E:93:TYR:CD1	2:E:93:TYR:N	2.84	0.46
1:J:72:GLU:OE2	1:J:72:GLU:HA	2.15	0.46
2:H:142:ILE:HB	2:H:190:VAL:CG1	2.45	0.46
1:L:106:PRO:O	1:L:108:TYR:N	2.48	0.46
2:P:72:ASP:O	2:P:76:GLN:HG2	2.16	0.46
2:P:93:TYR:CD1	2:P:93:TYR:N	2.84	0.46
1:A:96:ASN:OD1	1:B:87:ASP:HB2	2.16	0.46
1:J:124:LEU:HA	1:J:125:PRO:HD2	1.71	0.46
2:M:172:ARG:C	2:M:174:HIS:H	2.19	0.46
2:N:93:TYR:CD1	2:N:93:TYR:N	2.84	0.46
2:O:57:TYR:HA	2:O:108:PHE:CE1	2.50	0.46
1:B:11:PHE:CE2	2:F:114:ALA:HB1	2.51	0.46
2:E:172:ARG:C	2:E:174:HIS:H	2.18	0.46
2:F:161:TYR:O	2:F:162:THR:C	2.54	0.46
2:O:172:ARG:C	2:O:174:HIS:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:ASN:H	2:F:137:ASN:ND2	1.98	0.46
1:L:20:MET:CG	1:L:25:CYS:HA	2.46	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
2:F:172:ARG:C	2:F:174:HIS:H	2.18	0.46
1:I:62:PRO:O	1:I:63:ASP:OD2	2.33	0.46
2:E:137:ASN:H	2:E:137:ASN:ND2	1.98	0.45
1:I:58:LEU:HD13	1:I:66:LEU:HB3	1.97	0.45
2:N:87:ALA:HB2	2:N:157:MET:CE	2.47	0.45
2:F:80:GLN:O	2:F:81:PHE:C	2.54	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
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:I:73:PHE:CE1	2:P:39:LEU:HD13	2.52	0.45
1:K:124:LEU:HA	1:K:125:PRO:HD2	1.71	0.45
2:E:57:TYR:HA	2:E:108:PHE:CE1	2.52	0.45
2:G:128:ARG:HG3	2:G:192:LEU:HD21	1.99	0.45
2:P:69:VAL:HB	2:P:106:VAL:HG22	1.98	0.45
2:G:93:TYR:CD1	2:G:93:TYR:N	2.85	0.45
1:L:105:TYR:HA	1:L:106:PRO:HD2	1.84	0.45
1:B:37:ARG:CA	1:B:37:ARG:HE	2.30	0.45
1:C:72:GLU:OE2	1:C:72:GLU:HA	2.17	0.45
2:G:72:ASP:O	2:G:76:GLN:HG2	2.17	0.45
1:I:15:ALA:HB1	2:M:154:ILE:HD11	1.98	0.45
2:N:136:ILE:CD1	2:N:146:GLU:HB2	2.40	0.45
2:G:57:TYR:HA	2:G:108:PHE:CE1	2.52	0.44
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:H:108:PHE:O	2:H:111:PHE:HB3	2.18	0.44
2:M:93:TYR:CD1	2:M:93:TYR:N	2.84	0.44
2:O:69:VAL:HB	2:O:106:VAL:HG22	1.98	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:N:137:ASN:HD22	2:N:137:ASN:N	2.00	0.44
2:P:172:ARG:C	2:P:174:HIS:H	2.21	0.44
1:A:66:LEU:H	1:A:66:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:VAL:O	2:E:167:ALA:N	2.50	0.44
2:F:128:ARG:HG3	2:F:192:LEU:HD21	2.00	0.44
1:I:99:ARG:HD3	1:J:85:ASP:O	2.17	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:OE2	1:K:89:GLU:CA	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
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
2:E:106:VAL:HG23	2:E:106:VAL:O	2.17	0.44
1:J:70:GLU:OE2	2:M:61:LYS:HE3	2.18	0.44
1:L:89:GLU:O	1:L:92:ARG:HB2	2.18	0.44
2:N:170:THR:CB	2:N:171:PRO:CD	2.94	0.44
2:P:82:PHE:CZ	2:P:158:MET:HE1	2.53	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:N:178:PHE:O	2:N:182:MET:HB2	2.18	0.44
2:O:93:TYR:N	2:O:93:TYR:HD1	2.16	0.44
2:F:93:TYR:N	2:F:93:TYR:HD1	2.16	0.43
2:G:137:ASN:HD22	2:G:137:ASN:N	2.00	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
1:J:89:GLU:O	1:J:92:ARG:HB2	2.19	0.43
1:L:17:ILE:H	1:L:17:ILE:HG13	1.64	0.43
1:A:79:THR:OG1	1:A:81:GLU:HG2	2.18	0.43
1:A:120:PHE:CE1	2:H:61:LYS:HD2	2.53	0.43
2:G:136:ILE:CD1	2:G:146:GLU:HB2	2.38	0.43
2:P:80:GLN:O	2:P:81:PHE:C	2.57	0.43
1:C:11:PHE:CD2	2:G:118:LEU:CD2	3.01	0.43
1:D:59:GLU:O	1:D:62:PRO:HD3	2.18	0.43
1:J:62:PRO:O	1:J:63:ASP:OD2	2.35	0.43
1:A:62:PRO:O	1:A:63:ASP:OD2	2.36	0.43
2:E:80:GLN:O	2:E:82:PHE:N	2.52	0.43
2:P:72:ASP:OD1	2:P:72:ASP:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:86:ASP:OD1	2:F:88:SER:HB3	2.19	0.43
2:O:178:PHE:O	2:O:182:MET:HB2	2.18	0.43
2:P:99:ASP:HB3	2:P:102:GLN:OE1	2.19	0.43
1:C:106:PRO:C	1:C:108:TYR:H	2.22	0.43
2:E:93:TYR:N	2:E:93:TYR:HD1	2.17	0.43
1:J:106:PRO:C	1:J:108:TYR:H	2.22	0.43
2:P:136:ILE:CD1	2:P:146:GLU:HB2	2.41	0.43
2:E:142:ILE:HA	2:E:146:GLU:OE1	2.19	0.43
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
1:A:11:PHE:HB3	2:E:94:LEU:HD21	2.00	0.43
1:A:18:GLY:O	2:E:178:PHE:HD2	2.02	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
1:L:21:PRO:HD3	2:P:174:HIS:NE2	2.33	0.43
2:O:206:MET:HB3	2:O:206:MET:HE2	1.91	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: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
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
1:C:9:LEU:N	1:C:10:PRO:CD	2.82	0.42
1:D:108:TYR:CE1	1:D:109:GLU:HG2	2.54	0.42
1:K:106:PRO:O	1:K:108:TYR:N	2.46	0.42
2:N:80:GLN:O	2:N:81:PHE:C	2.57	0.42
2:P:57:TYR:HA	2:P:108:PHE:CE1	2.54	0.42
2:P:158:MET:H	2:P:158:MET:HG2	1.65	0.42
2:F:57:TYR:HA	2:F:108:PHE:CE1	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:122:THR:HG23	2:F:125:GLU:HB2	2.01	0.42
1:I:52:GLN:N	1:J:47:SER:O	2.33	0.42
1:I:72:GLU:HA	1:I:72:GLU:OE2	2.20	0.42
2:F:72:ASP:O	2:F:76:GLN:HG2	2.20	0.42
2:P:155:TYR:OH	2:P:167:ALA:HB2	2.20	0.42
1:D:106:PRO:O	1:D:108:TYR:N	2.47	0.42
2:H:57:TYR:HA	2:H:108:PHE:CE1	2.54	0.42
2:P:142:ILE:HA	2:P:146:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE2	2:H:57:TYR:OH	2.36	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:D:124:LEU:HA	1:D:125:PRO:HD2	1.72	0.42
2:N:93:TYR:N	2:N:93:TYR:HD1	2.17	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD2	1.90	0.42
1:B:78:ASP:C	1:B:80:LYS:N	2.73	0.42
2:H:167:ALA:C	2:H:169:ASP:H	2.23	0.42
1:J:16:ALA:O	1:J:19:TRP:CD1	2.73	0.42
2:M:73:THR:O	2:M:77:ILE:CG1	2.68	0.42
2:M:93:TYR:N	2:M:93:TYR:HD1	2.18	0.42
2:O:80:GLN:O	2:O:81:PHE:C	2.59	0.42
1:C:62:PRO:O	1:C:63:ASP:OD2	2.38	0.41
1:D:62:PRO:O	1:D:63:ASP:OD2	2.38	0.41
1:J:108:TYR:CE1	1:J:109:GLU:HG2	2.54	0.41
1:L:27:MET:C	1:L:29:LEU:N	2.72	0.41
1:L:124:LEU:HA	1:L:125:PRO:HD2	1.69	0.41
1:D:11:PHE:CZ	2:H:115:LEU:HG	2.55	0.41
1:D:89:GLU:OE1	1:D:92:ARG:NH1	2.50	0.41
2:F:209:LEU:HA	2:F:209:LEU:HD23	1.89	0.41
1:L:21:PRO:O	1:L:26:PRO:HD3	2.20	0.41
2:N:72:ASP:O	2:N:76:GLN:HG2	2.20	0.41
1:A:106:PRO:C	1:A:108:TYR:H	2.23	0.41
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.20	0.41
2:E:73:THR:O	2:E:77:ILE:CG1	2.68	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:124:LEU:HD13	1:B:125:PRO:HD2	2.03	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: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
1:B:91:PHE:O	1:B:91:PHE:CD2	2.74	0.41
1:C:18:GLY:C	1:C:19:TRP:CD1	2.92	0.41
1:D:9:LEU:N	1:D:10:PRO:HD2	2.35	0.41
1:D:106:PRO:C	1:D:108:TYR:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:PHE:HE1	2:P:212:PHE:CE1	2.33	0.41
1:J:59:GLU:O	1:J:62:PRO:HD3	2.21	0.41
1:L:89:GLU:OE1	1:L:92:ARG:NH1	2.53	0.41
2:N:206:MET:HG3	2:N:210:GLN:NE2	2.36	0.41
2:O:137:ASN:HD22	2:O:137:ASN:N	2.00	0.41
2:P:64:CYS:SG	2:P:69:VAL:HG22	2.60	0.41
2:P:80:GLN:O	2:P:82:PHE:N	2.54	0.41
2:P:137:ASN:HD22	2:P:137:ASN:N	2.00	0.41
2:N:170:THR:HA	2:N:171:PRO:HD3	1.87	0.41
2:P:86:ASP:OD1	2:P:88:SER:HB3	2.21	0.41
2:P:122:THR:HG23	2:P:125:GLU:HB2	2.03	0.41
1:D:76:ASN:HB3	1:D:79:THR:OG1	2.21	0.40
1:J:19:TRP:CD1	1:J:19:TRP:N	2.89	0.40
2:O:69:VAL:HB	2:O:106:VAL:HG23	2.02	0.40
1:B:62:PRO:O	1:B:63:ASP:OD2	2.39	0.40
1:D:68:SER:HB2	1:D:69:THR:H	1.75	0.40
1:L:106:PRO:C	1:L:108:TYR:H	2.22	0.40
1:D:64:THR:O	1:D:65:LEU:C	2.60	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
2:M:106:VAL:HG23	2:M:106:VAL:O	2.21	0.40
2:M:122:THR:HG23	2:M:125:GLU:HB2	2.03	0.40
2:N:93:TYR:CE2	2:N:136:ILE:HD13	2.57	0.40
1:A:86:ARG:HG3	1:A:86:ARG:NH1	2.16	0.40
2:H:152:LYS:HB2	2:H:152:LYS:HE2	1.93	0.40
2:H:209:LEU:C	2:H:210:GLN:HG3	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/144 (85%)	99 (80%)	18 (15%)	6 (5%)	2	15
1	B	120/144 (83%)	98 (82%)	17 (14%)	5 (4%)	3	19
1	C	122/144 (85%)	103 (84%)	16 (13%)	3 (2%)	5	29
1	D	118/144 (82%)	98 (83%)	17 (14%)	3 (2%)	5	29
1	I	129/144 (90%)	102 (79%)	18 (14%)	9 (7%)	1	8
1	J	123/144 (85%)	103 (84%)	16 (13%)	4 (3%)	4	24
1	K	128/144 (89%)	104 (81%)	17 (13%)	7 (6%)	2	13
1	L	136/144 (94%)	104 (76%)	18 (13%)	14 (10%)	0	3
2	E	177/180 (98%)	150 (85%)	14 (8%)	13 (7%)	1	7
2	F	178/180 (99%)	146 (82%)	20 (11%)	12 (7%)	1	9
2	G	170/180 (94%)	148 (87%)	11 (6%)	11 (6%)	1	10
2	H	172/180 (96%)	146 (85%)	17 (10%)	9 (5%)	2	14
2	M	166/180 (92%)	144 (87%)	13 (8%)	9 (5%)	2	13
2	N	164/180 (91%)	141 (86%)	15 (9%)	8 (5%)	2	15
2	O	164/180 (91%)	141 (86%)	14 (8%)	9 (6%)	2	13
2	P	168/180 (93%)	145 (86%)	13 (8%)	10 (6%)	1	11
All	All	2358/2592 (91%)	1972 (84%)	254 (11%)	132 (6%)	2	12

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	4	16
1	B	97/122 (80%)	83 (86%)	14 (14%)	3	14
1	C	96/122 (79%)	81 (84%)	15 (16%)	2	11
1	D	96/122 (79%)	84 (88%)	12 (12%)	4	18
1	I	100/122 (82%)	87 (87%)	13 (13%)	4	17
1	J	96/122 (79%)	82 (85%)	14 (15%)	3	13
1	K	100/122 (82%)	86 (86%)	14 (14%)	3	15
1	L	102/122 (84%)	89 (87%)	13 (13%)	4	18
2	E	138/162 (85%)	122 (88%)	16 (12%)	5	21
2	F	139/162 (86%)	121 (87%)	18 (13%)	4	17
2	G	133/162 (82%)	114 (86%)	19 (14%)	3	14
2	H	137/162 (85%)	115 (84%)	22 (16%)	2	10
2	M	131/162 (81%)	116 (88%)	15 (12%)	5	22
2	N	133/162 (82%)	114 (86%)	19 (14%)	3	14
2	O	134/162 (83%)	115 (86%)	19 (14%)	3	14
2	P	138/162 (85%)	119 (86%)	19 (14%)	3	15
All	All	1867/2272 (82%)	1612 (86%)	255 (14%)	3	15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
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 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 monosaccharides 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.

No monomer is involved in short contacts.



## 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, 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%)	0.38	6 (4%) 31 34	122, 128, 135, 142	0
1	B	124/144 (86%)	0.49	7 (5%) 24 26	122, 128, 134, 142	0
1	C	126/144 (87%)	0.68	12 (9%) 8 10	122, 128, 135, 142	0
1	D	122/144 (84%)	0.57	9 (7%) 14 17	122, 128, 134, 142	0
1	I	133/144 (92%)	0.56	11 (8%) 11 13	110, 128, 134, 142	0
1	J	129/144 (89%)	0.64	13 (10%) 7 8	122, 128, 135, 142	0
1	K	132/144 (91%)	0.51	12 (9%) 9 11	122, 128, 134, 142	0
1	L	138/144 (95%)	0.40	5 (3%) 42 45	122, 128, 135, 142	0
2	E	179/180 (99%)	0.29	10 (5%) 24 26	31, 128, 138, 142	0
2	F	180/180 (100%)	0.28	8 (4%) 34 37	31, 128, 138, 142	0
2	G	174/180 (96%)	0.59	18 (10%) 6 7	31, 129, 138, 145	0
2	H	174/180 (96%)	0.40	7 (4%) 38 40	31, 128, 137, 142	0
2	M	170/180 (94%)	0.57	20 (11%) 4 5	31, 129, 138, 142	0
2	N	168/180 (93%)	0.85	22 (13%) 3 4	31, 129, 137, 142	0
2	O	168/180 (93%)	0.61	22 (13%) 3 4	31, 129, 137, 143	0
2	P	172/180 (95%)	0.48	12 (6%) 16 18	31, 129, 137, 142	0
All	All	2418/2592 (93%)	0.52	194 (8%) 12 14	31, 128, 137, 145	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	84	HIS	8.3
1	L	21	PRO	8.1
2	G	160	ALA	8.0
2	N	78	TYR	6.4
2	N	83	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	3	ALA	5.5
1	A	35	ASN	5.4
2	F	142	ILE	5.2
2	E	84	HIS	5.2
1	B	35	ASN	5.1
2	G	68	VAL	5.1
1	C	8	TRP	4.9
1	J	8	TRP	4.9
1	C	11	PHE	4.9
1	A	3	ALA	4.7
1	J	18	GLY	4.6
1	D	3	ALA	4.6
2	P	189	ILE	4.5
2	H	199	CYS	4.5
2	M	83	PRO	4.5
2	O	83	PRO	4.4
2	M	84	HIS	4.3
1	J	15	ALA	4.3
2	O	84	HIS	4.2
1	D	114	TYR	4.2
1	I	19	TRP	4.1
1	C	125	PRO	4.1
1	B	3	ALA	4.1
2	E	140	GLY	4.0
2	M	155	TYR	3.9
1	J	3	ALA	3.9
2	O	140	GLY	3.9
2	N	100	THR	3.9
1	K	37	ARG	3.9
2	O	212	PHE	3.8
2	N	180	GLN	3.8
1	I	125	PRO	3.7
2	E	212	PHE	3.7
2	H	161	TYR	3.7
2	M	195	PHE	3.6
1	I	23	ALA	3.6
2	O	143	ASN	3.6
2	H	142	ILE	3.5
2	G	93	TYR	3.5
2	E	72	ASP	3.5
2	O	134	TYR	3.4
1	K	30	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	M	156	ASP	3.4
2	O	150	ILE	3.3
1	K	118	LEU	3.3
1	K	8	TRP	3.3
2	O	73	THR	3.3
1	I	8	TRP	3.3
1	K	113	ALA	3.3
1	L	125	PRO	3.3
1	D	140	LYS	3.3
1	I	35	ASN	3.2
2	N	106	VAL	3.2
2	P	195	PHE	3.2
1	A	27	MET	3.2
2	H	191	THR	3.2
1	B	138	ASP	3.0
2	M	78	TYR	3.0
2	M	93	TYR	3.0
2	E	68	VAL	3.0
2	O	78	TYR	3.0
2	G	78	TYR	3.0
1	B	127	ILE	3.0
1	D	102	LYS	3.0
2	N	182	MET	3.0
2	O	171	PRO	2.9
2	P	201	GLU	2.9
2	G	120	ARG	2.9
2	M	216	MET	2.9
1	K	3	ALA	2.9
2	H	88	SER	2.9
2	G	203	ASP	2.9
2	N	197	GLU	2.9
2	G	178	PHE	2.9
1	I	24	ASN	2.8
2	O	191	THR	2.8
2	O	198	SER	2.8
1	I	3	ALA	2.8
2	O	210	GLN	2.8
2	P	90	TYR	2.8
2	N	60	PHE	2.8
1	J	40	GLU	2.8
2	F	68	VAL	2.8
2	N	95	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	190	VAL	2.8
2	F	106	VAL	2.7
1	L	33	ASP	2.7
2	G	115	LEU	2.7
1	B	114	TYR	2.7
1	I	114	TYR	2.7
2	N	150	ILE	2.7
2	N	184	LYS	2.7
2	E	73	THR	2.7
2	O	195	PHE	2.7
2	G	210	GLN	2.7
1	J	123	ILE	2.7
1	D	133	TYR	2.6
2	O	142	ILE	2.6
2	M	185	ASN	2.6
1	A	133	TYR	2.6
2	P	87	ALA	2.6
2	F	84	HIS	2.6
2	P	106	VAL	2.6
2	M	77	ILE	2.6
1	L	136	TYR	2.6
2	O	196	LEU	2.6
2	N	195	PHE	2.6
2	O	192	LEU	2.6
2	N	66	SER	2.6
2	G	67	GLY	2.5
2	M	108	PHE	2.5
2	N	179	PHE	2.5
2	M	179	PHE	2.5
1	J	4	GLY	2.5
2	O	127	LEU	2.5
2	P	78	TYR	2.5
1	I	25	CYS	2.5
2	G	63	GLU	2.5
2	M	199	CYS	2.4
1	I	16	ALA	2.4
2	F	67	GLY	2.4
2	G	96	ASN	2.4
1	C	51	PHE	2.4
1	C	97	PHE	2.4
2	N	212	PHE	2.4
2	G	60	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	2.4
1	J	108	TYR	2.4
2	P	154	ILE	2.4
1	C	105	TYR	2.4
1	D	111	ILE	2.3
1	J	139	ARG	2.3
1	D	101	GLY	2.3
2	O	101	THR	2.3
2	P	180	GLN	2.3
1	J	136	TYR	2.3
1	J	26	PRO	2.3
2	N	47	ASN	2.3
1	C	133	TYR	2.3
1	K	114	TYR	2.3
2	M	98	PHE	2.3
2	P	100	THR	2.3
2	F	195	PHE	2.3
2	N	181	LYS	2.3
2	O	147	MET	2.3
2	M	194	GLU	2.3
2	M	101	THR	2.3
2	E	101	THR	2.3
1	C	33	ASP	2.2
1	D	134	GLU	2.2
1	J	58	LEU	2.2
2	F	101	THR	2.2
2	G	48	PHE	2.2
2	O	93	TYR	2.2
1	L	20	MET	2.2
1	A	128	ILE	2.2
2	F	78	TYR	2.2
2	N	131	PHE	2.2
2	P	182	MET	2.2
2	M	50	LYS	2.2
2	P	147	MET	2.2
1	K	107	ARG	2.2
2	G	142	ILE	2.2
1	B	130	ASP	2.1
1	D	4	GLY	2.1
2	G	118	LEU	2.1
1	K	105	TYR	2.1
2	H	184	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	81	GLU	2.1
1	I	123	ILE	2.1
1	C	63	ASP	2.1
2	G	146	GLU	2.1
2	N	112	VAL	2.1
2	M	94	LEU	2.1
1	K	49	ARG	2.1
2	E	87	ALA	2.1
1	A	95	LEU	2.1
2	N	67	GLY	2.1
2	E	195	PHE	2.0
2	G	206	MET	2.0
2	M	86	ASP	2.0
2	N	174	HIS	2.0
1	J	107	ARG	2.0
1	K	138	ASP	2.0
2	M	110	ASP	2.0
1	K	21	PRO	2.0
2	O	98	PHE	2.0
1	C	42	ILE	2.0
2	E	78	TYR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	H	701	1/1	0.38	0.16	106,106,106,106	0
4	CA	E	511	1/1	0.82	0.06	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	O	516	1/1	0.84	0.11	206,206,206,206	0
4	CA	N	507	1/1	0.85	0.06	173,173,173,173	0
4	CA	F	509	1/1	0.87	0.10	162,162,162,162	0
4	CA	H	502	1/1	0.87	0.09	104,104,104,104	0
4	CA	M	514	1/1	0.87	0.08	156,156,156,156	0
4	CA	G	512	1/1	0.88	0.08	135,135,135,135	0
5	NA	E	703	1/1	0.90	0.12	81,81,81,81	0
5	NA	G	704	1/1	0.91	0.09	106,106,106,106	0
5	NA	F	702	1/1	0.91	0.09	105,105,105,105	0
4	CA	H	510	1/1	0.92	0.09	108,108,108,108	0
4	CA	F	501	1/1	0.92	0.12	111,111,111,111	0
4	CA	N	515	1/1	0.93	0.03	146,146,146,146	0
3	ZN	I	605	1/1	0.93	0.05	133,133,133,133	0
4	CA	P	505	1/1	0.94	0.09	101,101,101,101	0
3	ZN	J	606	1/1	0.95	0.15	144,144,144,144	0
3	ZN	A	601	1/1	0.96	0.11	132,132,132,132	0
4	CA	P	513	1/1	0.96	0.13	123,123,123,123	0
3	ZN	D	604	1/1	0.96	0.09	139,139,139,139	0
3	ZN	K	607	1/1	0.96	0.08	151,151,151,151	0
4	CA	O	508	1/1	0.96	0.04	140,140,140,140	0
4	CA	M	506	1/1	0.96	0.08	169,169,169,169	0
3	ZN	L	608	1/1	0.97	0.07	129,129,129,129	0
4	CA	E	503	1/1	0.97	0.06	112,112,112,112	0
3	ZN	C	603	1/1	0.98	0.08	136,136,136,136	0
3	ZN	B	602	1/1	0.98	0.10	130,130,130,130	0
4	CA	G	504	1/1	0.98	0.16	123,123,123,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.