Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 09:39 AM EDT

PDB ID	:	6MJ2
EMDB ID	:	EMD-9134
Title	:	Human TRPM2 ion channel in a calcium- and ADPR-bound state
Authors	:	Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on	:	2018-09-20
Resolution	:	6.36 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

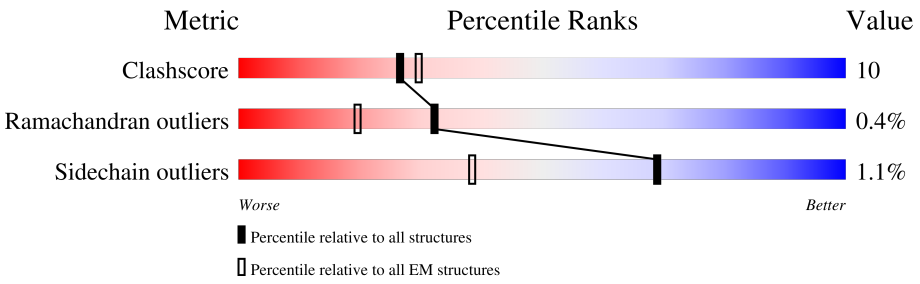
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.36 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1503	65% 23% • 11%
1	B	1503	65% 23% • 11%
1	C	1503	65% 23% • 11%
1	D	1503	65% 23% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 43124 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1337	10780	6942	1865	1919	54	0	0
1	B	1337	10780	6942	1865	1919	54	0	0
1	C	1337	10780	6942	1865	1919	54	0	0
1	D	1337	10780	6942	1865	1919	54	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

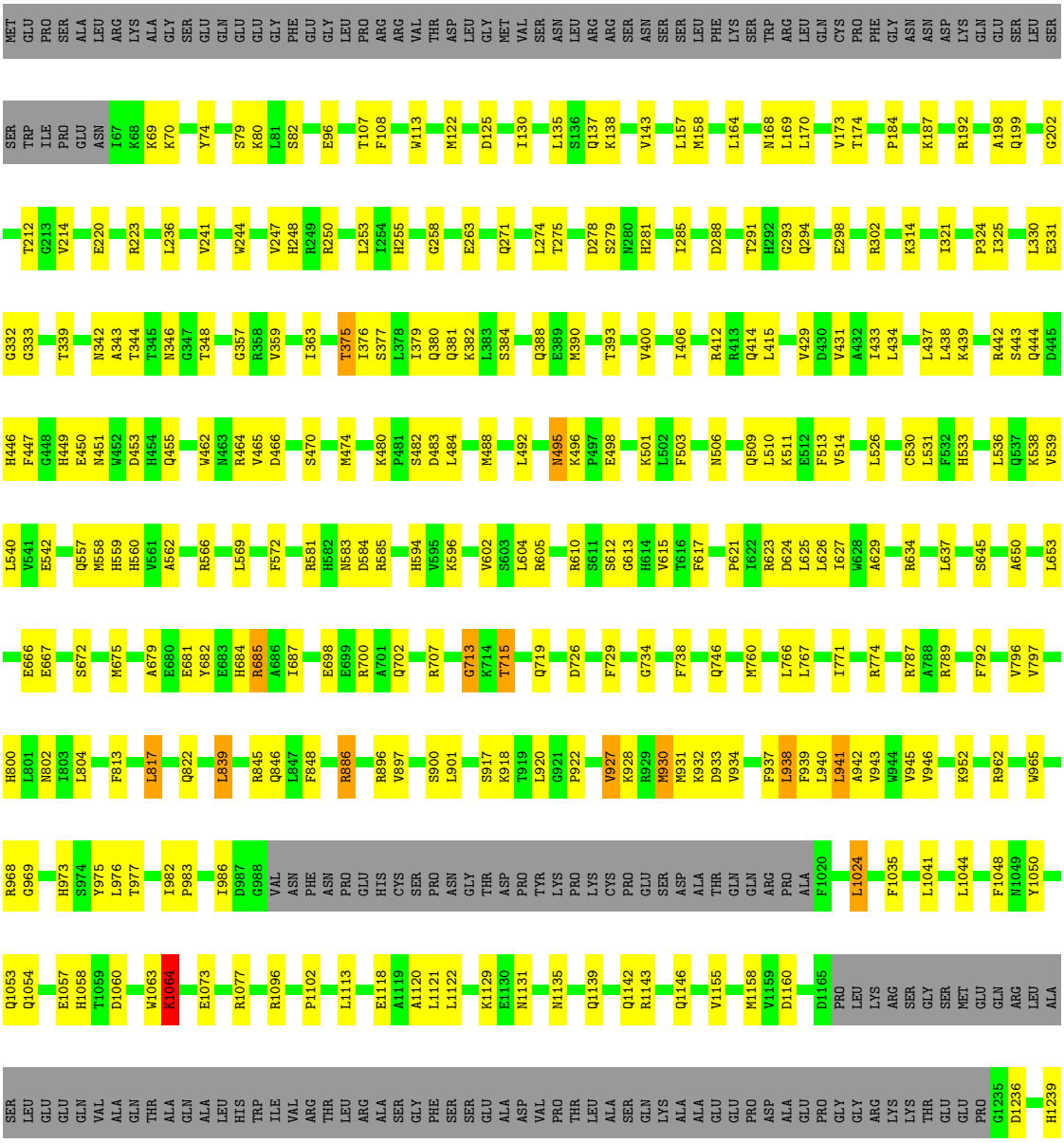
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	1	1	1	0
2	B	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

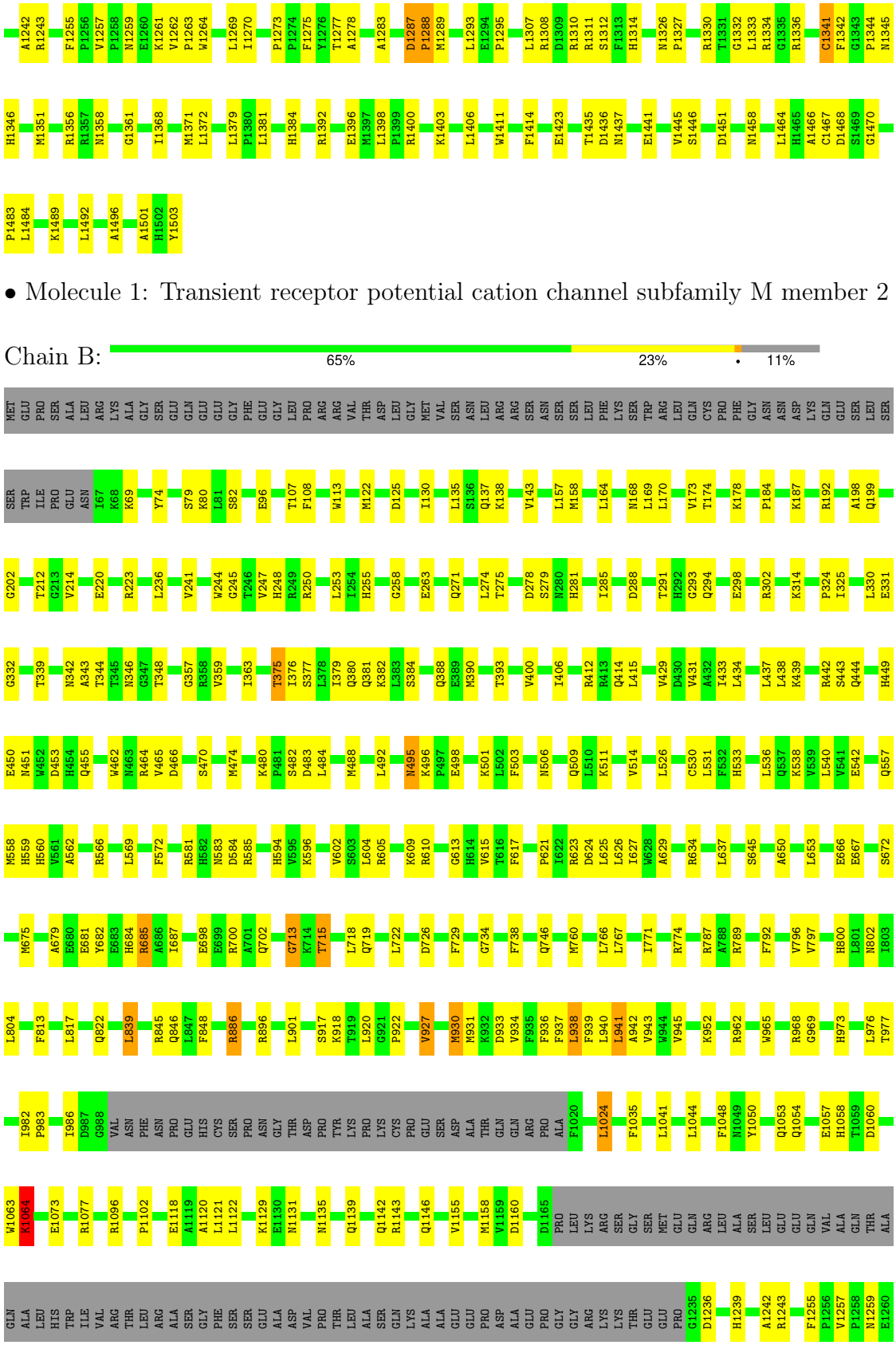
3 Residue-property plots (i)

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. 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. 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: Transient receptor potential cation channel subfamily M member 2

Chain A: 65% 23% • 11%





• Molecule 1: Transient receptor potential cation channel subfamily M member 2

K1261 V1262 P1263 W1264 L1269 I1270 P1273 T1277 A1278 A1283 D1287 P1288 M1289 L1293 E1294 P1295 L1307 R1308 D1309 R1310 R1311 S1312 F1313 H1314 N1326 P1327 R1330 T1331 G1332 L1333 R1334 G1335 R1336 C1341 F1342 G1343 P1344 N1345 H1346 M1351 R1356 R1357 N1358 G1361 I1368

M1371 L1372 K1378 L1379 P1380 L1381 S1382 E1383 H1384 R1392 E1396 M1397 L1398 P1399 R1400 K1403 L1406 W1411 F1414 E1423 T1435 D1436 N1437 E1441 V1445 S1446 D1451 N1458 L1464 H1465 A1466 C1467 D1468 S1469 G1470 P1483 L1484 K1489 L1492 A1496 A1501

H1502 Y1503

• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain C:

MET GLU PRO SER ALA LEU ARG LYS ALA GLY SER GLU GLN GLU GLU GLY PHE GLU GLY LEU PRO ARG ARG VAL THR ASP LEU GLY MET VAL SER ASN LEU ARG ARG SER ASN SER SER LEU PHE LYS SER TRP ARG LEU GLN CYS PRO PHE GLY ASN ASN ASP LYS GLN GLU SER LEU SER

SER TRP ILE PRO GLU ASN I67 K68 K69 Y74 S79 K80 L81 S82 E96 T107 F108 W113 M122 D125 I130 L135 S136 Q137 K138 V143 L157 M158 L164 N168 L169 L170 V173 T174 P184 K187 A198 G202 T212 G213 V214

E220 R223 L236 V241 W244 G245 T246 V247 H248 R249 R250 L253 I254 H255 G258 E263 Q271 G272 N273 L274 T275 D278 S279 N280 H281 I285 D288 T291 H292 G293 Q294 E298 R302 K314 I321 P324 I325 L330 E331 G332 G333

T339 N342 A343 T344 T345 N346 G347 T348 G357 R358 V359 I363 T375 I376 S377 L378 I379 Q380 Q381 K382 L383 S384 V385 Q388 E389 M390 T393 V400 I406 R412 R413 Q414 L415 V429 D430 V431 A432 I433 L434 L437 L438 K439 R442 S443 Q444 D445 H446

F447 G448 H449 E450 N451 W452 D453 H454 Q455 W462 N463 R464 V465 D466 K480 P481 S482 D483 L484 M488 L492 N495 K496 P497 E498 K501 L502 F503 N506 Q509 L510 K511 V514 L526 C530 L531 F532 H533 K538 V539 E542 Q557 M558 H559 H560 V561

A562 R566 L569 F572 R581 H582 N583 D584 R585 H594 V595 K596 V602 S603 L604 R605 K609 R610 G613 H614 V615 T616 F617 P621 I622 R623 D624 L625 L626 T627 W628 A629 R634 L637 A650 L653 K657 E666 E667 S672 M675 A679

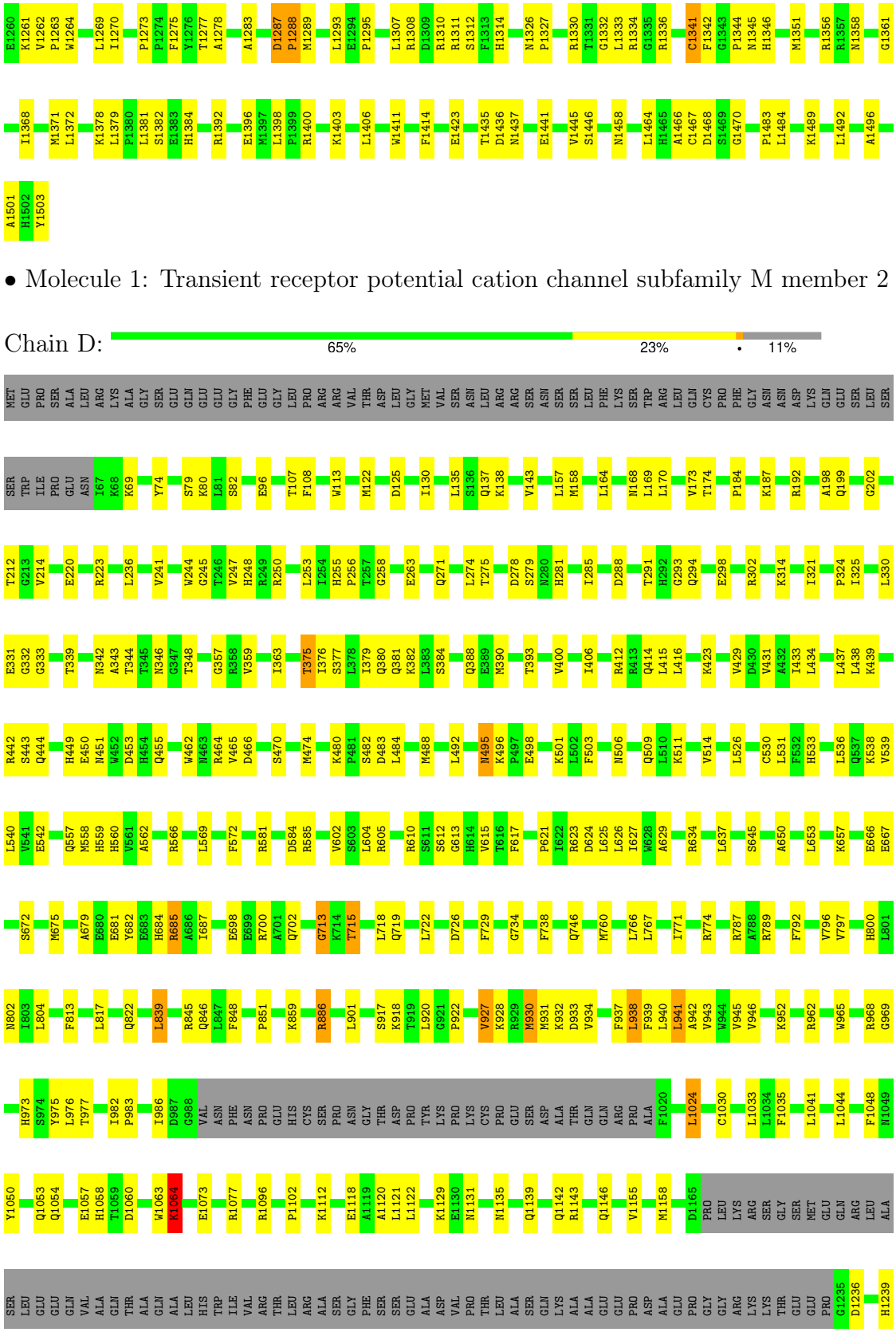
E680 E681 Y682 E683 H684 R685 A686 I687 E698 E699 R700 A701 Q702 R707 G713 K714 T715 Q719 D726 F729 G734 I735 Q736 A737 F738 L739 Q746 L766 L767 I771 R774 R787 A788 R789 F792 V796 H800 L801 N802 I803 L804 F813 L817

Q822 L839 R845 Q846 L847 F848 P851 K859 R886 R896 L901 S917 K918 T919 L920 G921 P922 V927 K928 R929 M930 M931 K932 D933 V934 F937 L938 F939 L940 L941 A942 V943 W944 V945 K952 R962 W965 R968 G969 H973 L976 T977

I982 P983 I986 D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 L1024 F1035 L1041 L1044 F1048 N1049 Y1050 Q1053 Q1054 E1057 H1058 T1059 D1060 W1063

K1064 E1073 R1077 R1096 P1102 L1113 E1114 K1115 E1118 A1119 A1120 L1121 L1122 N1131 N1135 Q1139 Q1142 R1143 Q1146 V1155 M1158 V1159 D1160 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR

ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 H1239 A1242 R1243 F1255 P1256 V1257 P1258 N1259



Chain D: 65% 23% • 11%

• Molecule 1: Transient receptor potential cation channel subfamily M member 2

A1242
R1243
F1255
P1256
V1257
P1258
N1259
E1260
K1261
V1262
P1263
W1264
L1269
I1270
P1273
T1277
A1278
A1283
D1287
P1288
M1289
L1293
E1294
P1295
L1307
R1308
D1309
R1310
R1311
S1312
F1313
H1314
N1326
P1327
R1330
T1331
G1332
L1333
R1334
G1335
R1336
C1341
F1342
G1343
P1344
N1345
H1346
M1351
R1356
R1357
N1358
G1361
I1368
M1371
L1372
K1378
L1379
P1380
L1381
S1382
E1383
H1384
R1392
E1396
M1397
L1398
P1399
R1400
K1403
L1406
W1411
F1414
E1423
T1435
D1436
N1437
E1441
V1445
S1446
D1451
N1458
L1464
H1465
A1466
C1467
D1468
S1469
G1470
P1483
L1484
K1489
L1492
A1496
A1501
H1502
Y1503

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70.072	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/11050	0.67	19/14990 (0.1%)
1	B	0.30	0/11050	0.67	19/14990 (0.1%)
1	C	0.30	0/11050	0.67	19/14990 (0.1%)
1	D	0.30	0/11050	0.67	19/14990 (0.1%)
All	All	0.30	0/44200	0.67	76/59960 (0.1%)

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	13
1	B	0	13
1	C	0	13
1	D	0	13
All	All	0	52

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	933	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	D	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	C	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	933	ASP	CB-CG-OD2	-8.74	110.44	118.30
1	C	933	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	933	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	933	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	933	ASP	CB-CG-OD1	8.49	125.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	B	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	D	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	C	685	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	B	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	D	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	C	1048	PHE	CB-CG-CD2	-7.31	115.68	120.80
1	B	938	LEU	CB-CG-CD1	6.62	122.26	111.00
1	A	938	LEU	CB-CG-CD1	6.60	122.22	111.00
1	D	938	LEU	CB-CG-CD1	6.60	122.22	111.00
1	C	938	LEU	CB-CG-CD1	6.59	122.20	111.00
1	A	1064	LYS	CA-CB-CG	6.48	127.65	113.40
1	B	1064	LYS	CA-CB-CG	6.46	127.62	113.40
1	C	1064	LYS	CA-CB-CG	6.46	127.62	113.40
1	D	1064	LYS	CA-CB-CG	6.45	127.59	113.40
1	A	685	ARG	CG-CD-NE	6.23	124.89	111.80
1	B	685	ARG	CG-CD-NE	6.20	124.83	111.80
1	C	685	ARG	CG-CD-NE	6.20	124.82	111.80
1	D	685	ARG	CG-CD-NE	6.20	124.82	111.80
1	A	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	B	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	C	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	D	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	C	938	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	938	LEU	CA-CB-CG	5.99	129.07	115.30
1	D	938	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	938	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	941	LEU	CB-CG-CD1	5.84	120.94	111.00
1	C	941	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	941	LEU	CB-CG-CD1	5.83	120.91	111.00
1	D	941	LEU	CB-CG-CD1	5.82	120.89	111.00
1	B	1048	PHE	CB-CG-CD1	5.73	124.81	120.80
1	C	976	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	A	976	LEU	CB-CG-CD1	-5.71	101.28	111.00
1	D	976	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	B	976	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	A	1048	PHE	CB-CG-CD1	5.65	124.76	120.80
1	D	1048	PHE	CB-CG-CD1	5.65	124.76	120.80
1	C	1048	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	839	LEU	CB-CG-CD2	5.61	120.53	111.00
1	B	839	LEU	CB-CG-CD2	5.61	120.53	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	839	LEU	CB-CG-CD2	5.59	120.50	111.00
1	D	839	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	813	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	B	813	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	C	813	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	C	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	B	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	D	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	A	804	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	C	839	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	D	813	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	A	839	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	839	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	D	839	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	817	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	D	817	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	817	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	817	LEU	CB-CG-CD1	-5.23	102.10	111.00
1	B	976	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	976	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	976	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	976	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	945	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	B	945	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	C	945	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	D	945	VAL	CG1-CB-CG2	-5.06	102.81	110.90

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	PHE	Peptide
1	A	1050	TYR	Sidechain
1	A	1287	ASP	Peptide
1	A	1341	CYS	Peptide
1	A	1368	ILE	Peptide
1	A	375	THR	Peptide
1	A	388	GLN	Peptide
1	A	495	ASN	Peptide
1	A	615	VAL	Peptide
1	A	617	PHE	Peptide
1	A	713	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	82	SER	Peptide
1	A	927	VAL	Peptide
1	B	1035	PHE	Peptide
1	B	1050	TYR	Sidechain
1	B	1287	ASP	Peptide
1	B	1341	CYS	Peptide
1	B	1368	ILE	Peptide
1	B	375	THR	Peptide
1	B	388	GLN	Peptide
1	B	495	ASN	Peptide
1	B	615	VAL	Peptide
1	B	617	PHE	Peptide
1	B	713	GLY	Peptide
1	B	82	SER	Peptide
1	B	927	VAL	Peptide
1	C	1035	PHE	Peptide
1	C	1050	TYR	Sidechain
1	C	1287	ASP	Peptide
1	C	1341	CYS	Peptide
1	C	1368	ILE	Peptide
1	C	375	THR	Peptide
1	C	388	GLN	Peptide
1	C	495	ASN	Peptide
1	C	615	VAL	Peptide
1	C	617	PHE	Peptide
1	C	713	GLY	Peptide
1	C	82	SER	Peptide
1	C	927	VAL	Peptide
1	D	1035	PHE	Peptide
1	D	1050	TYR	Sidechain
1	D	1287	ASP	Peptide
1	D	1341	CYS	Peptide
1	D	1368	ILE	Peptide
1	D	375	THR	Peptide
1	D	388	GLN	Peptide
1	D	495	ASN	Peptide
1	D	615	VAL	Peptide
1	D	617	PHE	Peptide
1	D	713	GLY	Peptide
1	D	82	SER	Peptide
1	D	927	VAL	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	10780	0	10822	212	0
1	B	10780	0	10822	209	0
1	C	10780	0	10822	215	0
1	D	10780	0	10822	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	43124	0	43288	843	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 10.

All (843) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HD13	1:A:572:PHE:HB2	1.76	0.68
1:D:569:LEU:HD13	1:D:572:PHE:HB2	1.77	0.67
1:B:569:LEU:HD13	1:B:572:PHE:HB2	1.76	0.67
1:C:569:LEU:HD13	1:C:572:PHE:HB2	1.76	0.66
1:B:962:ARG:H	1:B:965:TRP:HB2	1.60	0.66
1:D:962:ARG:H	1:D:965:TRP:HB2	1.60	0.66
1:A:962:ARG:H	1:A:965:TRP:HB2	1.60	0.66
1:D:602:VAL:HG23	1:D:604:LEU:H	1.61	0.66
1:C:1356:ARG:NH1	1:C:1371:MET:SD	2.69	0.65
1:C:962:ARG:H	1:C:965:TRP:HB2	1.60	0.65
1:D:1356:ARG:NH1	1:D:1371:MET:SD	2.69	0.65
1:A:602:VAL:HG23	1:A:604:LEU:H	1.61	0.65
1:A:1356:ARG:NH1	1:A:1371:MET:SD	2.69	0.65
1:B:1356:ARG:NH1	1:B:1371:MET:SD	2.69	0.65
1:C:602:VAL:HG23	1:C:604:LEU:H	1.61	0.65
1:C:713:GLY:O	1:C:715:THR:OG1	2.16	0.64
1:B:602:VAL:HG23	1:B:604:LEU:H	1.61	0.64
1:D:713:GLY:O	1:D:715:THR:OG1	2.16	0.63
1:A:746:GLN:HE22	1:A:774:ARG:HH11	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HB2	1:B:113:TRP:HB2	1.82	0.61
1:A:713:GLY:O	1:A:715:THR:OG1	2.16	0.61
1:D:746:GLN:HE22	1:D:774:ARG:HH11	1.48	0.61
1:A:79:SER:HB2	1:A:113:TRP:HB2	1.82	0.61
1:A:174:THR:HG21	1:A:339:THR:HG21	1.83	0.61
1:A:1288:PRO:HA	1:A:1308:ARG:HH21	1.66	0.61
1:C:79:SER:HB2	1:C:113:TRP:HB2	1.82	0.61
1:B:713:GLY:O	1:B:715:THR:OG1	2.16	0.60
1:D:79:SER:HB2	1:D:113:TRP:HB2	1.82	0.60
1:D:174:THR:HG21	1:D:339:THR:HG21	1.83	0.60
1:D:1288:PRO:HA	1:D:1308:ARG:HH21	1.66	0.60
1:B:581:ARG:HA	1:B:584:ASP:HB2	1.84	0.60
1:C:581:ARG:HA	1:C:584:ASP:HB2	1.84	0.60
1:B:174:THR:HG21	1:B:339:THR:HG21	1.83	0.60
1:B:1288:PRO:HA	1:B:1308:ARG:HH21	1.66	0.60
1:C:174:THR:HG21	1:C:339:THR:HG21	1.83	0.60
1:A:581:ARG:HA	1:A:584:ASP:HB2	1.84	0.59
1:B:480:LYS:HB3	1:B:482:SER:H	1.67	0.59
1:D:480:LYS:HB3	1:D:482:SER:H	1.68	0.59
1:B:746:GLN:HE22	1:B:774:ARG:HH11	1.48	0.59
1:C:746:GLN:HE22	1:C:774:ARG:HH11	1.48	0.59
1:B:624:ASP:HA	1:B:627:ILE:HD12	1.85	0.59
1:C:624:ASP:HA	1:C:627:ILE:HD12	1.85	0.59
1:C:1288:PRO:HA	1:C:1308:ARG:HH21	1.66	0.59
1:A:480:LYS:HB3	1:A:482:SER:H	1.68	0.59
1:B:434:LEU:HD12	1:B:462:TRP:HZ2	1.68	0.59
1:C:845:ARG:HH12	1:C:1077:ARG:HG2	1.68	0.59
1:D:581:ARG:HA	1:D:584:ASP:HB2	1.84	0.59
1:D:434:LEU:HD12	1:D:462:TRP:HZ2	1.67	0.59
1:D:845:ARG:HH12	1:D:1077:ARG:HG2	1.68	0.59
1:A:449:HIS:CE1	1:A:453:ASP:HB2	2.38	0.59
1:C:509:GLN:HE21	1:C:511:LYS:H	1.51	0.59
1:D:511:LYS:HZ2	1:D:621:PRO:HD2	1.66	0.59
1:A:624:ASP:HA	1:A:627:ILE:HD12	1.85	0.59
1:A:845:ARG:HH12	1:A:1077:ARG:HG2	1.68	0.59
1:C:449:HIS:CE1	1:C:453:ASP:HB2	2.38	0.59
1:C:480:LYS:HB3	1:C:482:SER:H	1.68	0.59
1:B:449:HIS:CE1	1:B:453:ASP:HB2	2.38	0.58
1:C:434:LEU:HD12	1:C:462:TRP:HZ2	1.68	0.58
1:D:624:ASP:HA	1:D:627:ILE:HD12	1.85	0.58
1:A:434:LEU:HD12	1:A:462:TRP:HZ2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ARG:HH12	1:B:1077:ARG:HG2	1.68	0.58
1:B:509:GLN:HE21	1:B:511:LYS:H	1.51	0.58
1:D:509:GLN:HE21	1:D:511:LYS:H	1.51	0.58
1:A:511:LYS:HZ2	1:A:621:PRO:HD2	1.68	0.58
1:C:1139:GLN:HA	1:C:1142:GLN:HB2	1.86	0.58
1:D:1139:GLN:HA	1:D:1142:GLN:HB2	1.86	0.58
1:D:449:HIS:CE1	1:D:453:ASP:HB2	2.38	0.58
1:A:1139:GLN:HA	1:A:1142:GLN:HB2	1.86	0.58
1:B:1139:GLN:HA	1:B:1142:GLN:HB2	1.86	0.58
1:B:125:ASP:O	1:B:255:HIS:N	2.34	0.57
1:A:125:ASP:O	1:A:255:HIS:N	2.34	0.57
1:D:952:LYS:HZ2	1:D:982:ILE:HG23	1.69	0.57
1:C:1063:TRP:HE3	1:C:1064:LYS:HD2	1.69	0.57
1:A:509:GLN:HE21	1:A:511:LYS:H	1.51	0.57
1:D:1458:ASN:ND2	1:D:1464:LEU:O	2.38	0.57
1:C:846:GLN:NE2	1:C:1073:GLU:OE2	2.38	0.57
1:B:952:LYS:HZ2	1:B:982:ILE:HG23	1.70	0.57
1:C:137:GLN:HE21	1:C:138:LYS:NZ	2.02	0.57
1:C:511:LYS:HZ2	1:C:621:PRO:HD2	1.70	0.57
1:A:1063:TRP:HE3	1:A:1064:LYS:HD2	1.70	0.57
1:C:143:VAL:HG21	1:C:157:LEU:HD11	1.87	0.57
1:D:137:GLN:HE21	1:D:138:LYS:NZ	2.02	0.57
1:A:1458:ASN:ND2	1:A:1464:LEU:O	2.38	0.56
1:A:137:GLN:HE21	1:A:138:LYS:NZ	2.02	0.56
1:A:143:VAL:HG21	1:A:157:LEU:HD11	1.87	0.56
1:A:342:ASN:O	1:A:346:ASN:ND2	2.39	0.56
1:A:952:LYS:HZ2	1:A:982:ILE:HG23	1.71	0.56
1:B:137:GLN:HE21	1:B:138:LYS:NZ	2.02	0.56
1:D:846:GLN:NE2	1:D:1073:GLU:OE2	2.38	0.56
1:D:1255:PHE:HD2	1:D:1332:GLY:HA2	1.70	0.56
1:B:143:VAL:HG21	1:B:157:LEU:HD11	1.87	0.56
1:B:846:GLN:NE2	1:B:1073:GLU:OE2	2.38	0.56
1:C:1255:PHE:HD2	1:C:1332:GLY:HA2	1.70	0.56
1:B:342:ASN:O	1:B:346:ASN:ND2	2.39	0.56
1:B:1458:ASN:ND2	1:B:1464:LEU:O	2.38	0.56
1:C:342:ASN:O	1:C:346:ASN:ND2	2.39	0.56
1:A:846:GLN:NE2	1:A:1073:GLU:OE2	2.38	0.56
1:B:74:TYR:OH	1:B:125:ASP:OD1	2.24	0.56
1:C:952:LYS:HZ2	1:C:982:ILE:HG23	1.71	0.56
1:C:1458:ASN:ND2	1:C:1464:LEU:O	2.38	0.56
1:B:1063:TRP:HE3	1:B:1064:LYS:HD2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:O	1:D:346:ASN:ND2	2.39	0.56
1:D:700:ARG:HE	1:D:1121:LEU:HD23	1.71	0.56
1:B:380:GLN:HG3	1:B:381:GLN:HE21	1.71	0.55
1:B:1239:HIS:O	1:B:1243:ARG:NE	2.39	0.55
1:D:143:VAL:HG21	1:D:157:LEU:HD11	1.87	0.55
1:D:1063:TRP:HE3	1:D:1064:LYS:HD2	1.69	0.55
1:C:380:GLN:HG3	1:C:381:GLN:HE21	1.71	0.55
1:B:1379:LEU:HD23	1:B:1381:LEU:H	1.70	0.55
1:C:1379:LEU:HD23	1:C:1381:LEU:H	1.70	0.55
1:A:1239:HIS:O	1:A:1243:ARG:NE	2.39	0.55
1:D:1392:ARG:HB2	1:D:1398:LEU:HD23	1.88	0.55
1:A:74:TYR:OH	1:A:125:ASP:OD1	2.24	0.55
1:B:1255:PHE:HD2	1:B:1332:GLY:HA2	1.70	0.55
1:C:700:ARG:HE	1:C:1121:LEU:HD23	1.71	0.55
1:D:1314:HIS:HB3	1:D:1327:PRO:HG2	1.89	0.55
1:A:1379:LEU:HD23	1:A:1381:LEU:H	1.70	0.55
1:D:1379:LEU:HD23	1:D:1381:LEU:H	1.70	0.55
1:A:700:ARG:HE	1:A:1121:LEU:HD23	1.71	0.55
1:B:700:ARG:HE	1:B:1121:LEU:HD23	1.71	0.55
1:C:1314:HIS:HB3	1:C:1327:PRO:HG2	1.89	0.55
1:A:1392:ARG:HB2	1:A:1398:LEU:HD23	1.88	0.55
1:B:1396:GLU:HB3	1:B:1400:ARG:HD2	1.89	0.55
1:C:444:GLN:O	1:C:451:ASN:ND2	2.40	0.55
1:D:241:VAL:HA	1:D:285:ILE:HB	1.89	0.55
1:B:1400:ARG:HA	1:B:1403:LYS:HB2	1.89	0.55
1:C:74:TYR:OH	1:C:125:ASP:OD1	2.24	0.55
1:A:1314:HIS:HB3	1:A:1327:PRO:HG2	1.89	0.54
1:B:511:LYS:HZ2	1:B:621:PRO:HD2	1.71	0.54
1:C:241:VAL:HA	1:C:285:ILE:HB	1.89	0.54
1:D:969:GLY:HA2	1:D:973:HIS:HD2	1.71	0.54
1:C:125:ASP:O	1:C:255:HIS:N	2.34	0.54
1:C:503:PHE:HA	1:C:506:ASN:HD22	1.72	0.54
1:B:503:PHE:HA	1:B:506:ASN:HD22	1.72	0.54
1:C:715:THR:HG22	1:C:719:GLN:HB3	1.89	0.54
1:C:969:GLY:HA2	1:C:973:HIS:HD2	1.71	0.54
1:A:514:VAL:HB	1:A:621:PRO:HB3	1.90	0.54
1:A:1255:PHE:HD2	1:A:1332:GLY:HA2	1.70	0.54
1:B:969:GLY:HA2	1:B:973:HIS:HD2	1.71	0.54
1:B:1060:ASP:OD2	1:B:1064:LYS:NZ	2.41	0.54
1:B:1063:TRP:CE3	1:B:1064:LYS:HD2	2.42	0.54
1:B:1314:HIS:HB3	1:B:1327:PRO:HG2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1392:ARG:HB2	1:C:1398:LEU:HD23	1.88	0.54
1:D:380:GLN:HG3	1:D:381:GLN:HE21	1.71	0.54
1:A:241:VAL:HA	1:A:285:ILE:HB	1.89	0.54
1:A:969:GLY:HA2	1:A:973:HIS:HD2	1.71	0.54
1:A:1400:ARG:HA	1:A:1403:LYS:HB2	1.89	0.54
1:D:1239:HIS:O	1:D:1243:ARG:NE	2.39	0.54
1:A:715:THR:HG22	1:A:719:GLN:HB3	1.89	0.54
1:B:241:VAL:HA	1:B:285:ILE:HB	1.89	0.54
1:B:449:HIS:CE1	1:B:483:ASP:HB2	2.43	0.54
1:C:1400:ARG:HA	1:C:1403:LYS:HB2	1.89	0.54
1:D:444:GLN:O	1:D:451:ASN:ND2	2.40	0.54
1:D:514:VAL:HB	1:D:621:PRO:HB3	1.90	0.54
1:A:380:GLN:HG3	1:A:381:GLN:HE21	1.71	0.54
1:D:125:ASP:O	1:D:255:HIS:N	2.34	0.54
1:D:1396:GLU:HB3	1:D:1400:ARG:HD2	1.89	0.54
1:A:444:GLN:O	1:A:451:ASN:ND2	2.40	0.54
1:A:1396:GLU:HB3	1:A:1400:ARG:HD2	1.89	0.54
1:B:168:ASN:OD1	1:B:314:LYS:NZ	2.38	0.54
1:B:444:GLN:O	1:B:451:ASN:ND2	2.40	0.54
1:B:1392:ARG:HB2	1:B:1398:LEU:HD23	1.88	0.54
1:C:244:TRP:HB3	1:C:288:ASP:HA	1.90	0.54
1:C:1396:GLU:HB3	1:C:1400:ARG:HD2	1.89	0.54
1:D:1063:TRP:CE3	1:D:1064:LYS:HD2	2.42	0.54
1:A:503:PHE:HA	1:A:506:ASN:HD22	1.72	0.54
1:D:169:LEU:HD22	1:D:434:LEU:HD13	1.90	0.54
1:D:244:TRP:HB3	1:D:288:ASP:HA	1.90	0.54
1:D:1060:ASP:OD2	1:D:1064:LYS:NZ	2.41	0.54
1:A:414:GLN:HG3	1:A:443:SER:HB3	1.91	0.53
1:B:414:GLN:HG3	1:B:443:SER:HB3	1.91	0.53
1:C:1257:VAL:HG13	1:C:1261:LYS:HG3	1.90	0.53
1:C:1239:HIS:O	1:C:1243:ARG:NE	2.39	0.53
1:D:503:PHE:HA	1:D:506:ASN:HD22	1.72	0.53
1:D:715:THR:HG22	1:D:719:GLN:HB3	1.89	0.53
1:D:1257:VAL:HG13	1:D:1261:LYS:HG3	1.90	0.53
1:A:1060:ASP:OD2	1:A:1064:LYS:NZ	2.41	0.53
1:A:1063:TRP:CE3	1:A:1064:LYS:HD2	2.42	0.53
1:B:130:ILE:HG23	1:B:263:GLU:HA	1.90	0.53
1:C:1060:ASP:OD2	1:C:1064:LYS:NZ	2.41	0.53
1:D:168:ASN:OD1	1:D:314:LYS:NZ	2.38	0.53
1:D:449:HIS:CE1	1:D:483:ASP:HB2	2.43	0.53
1:A:343:ALA:HB1	1:A:348:THR:HB	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:HIS:CE1	1:A:483:ASP:HB2	2.43	0.53
1:A:1257:VAL:HG13	1:A:1261:LYS:HG3	1.90	0.53
1:A:1264:TRP:NE1	1:A:1326:ASN:O	2.42	0.53
1:B:1257:VAL:HG13	1:B:1261:LYS:HG3	1.90	0.53
1:B:1264:TRP:NE1	1:B:1326:ASN:O	2.42	0.53
1:D:414:GLN:HG3	1:D:443:SER:HB3	1.91	0.53
1:D:1400:ARG:HA	1:D:1403:LYS:HB2	1.89	0.53
1:A:379:ILE:HG23	1:A:382:LYS:HD2	1.90	0.53
1:C:169:LEU:HD22	1:C:434:LEU:HD13	1.89	0.53
1:C:449:HIS:CE1	1:C:483:ASP:HB2	2.43	0.53
1:B:169:LEU:HD22	1:B:434:LEU:HD13	1.89	0.53
1:B:1358:ASN:OD1	1:B:1361:GLY:N	2.42	0.53
1:C:414:GLN:HG3	1:C:443:SER:HB3	1.91	0.53
1:C:514:VAL:HB	1:C:621:PRO:HB3	1.90	0.53
1:C:1063:TRP:CE3	1:C:1064:LYS:HD2	2.42	0.53
1:C:1264:TRP:NE1	1:C:1326:ASN:O	2.42	0.53
1:C:400:VAL:HG11	1:C:1269:LEU:HD13	1.90	0.53
1:D:400:VAL:HG11	1:D:1269:LEU:HD13	1.90	0.53
1:A:605:ARG:HE	1:A:613:GLY:HA3	1.74	0.53
1:D:74:TYR:OH	1:D:125:ASP:OD1	2.24	0.53
1:D:1264:TRP:NE1	1:D:1326:ASN:O	2.42	0.53
1:B:715:THR:HG22	1:B:719:GLN:HB3	1.89	0.53
1:C:214:VAL:HG13	1:C:330:LEU:HD12	1.91	0.53
1:C:343:ALA:HB1	1:C:348:THR:HB	1.91	0.53
1:D:379:ILE:HG23	1:D:382:LYS:HD2	1.90	0.53
1:A:244:TRP:HB3	1:A:288:ASP:HA	1.90	0.53
1:B:796:VAL:O	1:B:800:HIS:N	2.37	0.53
1:C:130:ILE:HG23	1:C:263:GLU:HA	1.90	0.53
1:C:379:ILE:HG23	1:C:382:LYS:HD2	1.90	0.53
1:B:379:ILE:HG23	1:B:382:LYS:HD2	1.90	0.52
1:D:214:VAL:HG13	1:D:330:LEU:HD12	1.91	0.52
1:B:244:TRP:HB3	1:B:288:ASP:HA	1.90	0.52
1:C:605:ARG:HE	1:C:613:GLY:HA3	1.74	0.52
1:A:169:LEU:HD22	1:A:434:LEU:HD13	1.89	0.52
1:D:681:GLU:HA	1:D:684:HIS:HB3	1.91	0.52
1:A:324:PRO:HB2	1:A:437:LEU:HD13	1.91	0.52
1:A:400:VAL:HG11	1:A:1269:LEU:HD13	1.90	0.52
1:B:324:PRO:HB2	1:B:437:LEU:HD13	1.91	0.52
1:B:605:ARG:HE	1:B:613:GLY:HA3	1.74	0.52
1:C:324:PRO:HB2	1:C:437:LEU:HD13	1.91	0.52
1:A:681:GLU:HA	1:A:684:HIS:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:HG23	1:D:263:GLU:HA	1.91	0.52
1:D:343:ALA:HB1	1:D:348:THR:HB	1.91	0.52
1:D:605:ARG:HE	1:D:613:GLY:HA3	1.74	0.52
1:A:538:LYS:O	1:A:542:GLU:N	2.43	0.52
1:A:1384:HIS:HA	1:A:1483:PRO:HG2	1.92	0.52
1:B:214:VAL:HG13	1:B:330:LEU:HD12	1.91	0.52
1:B:514:VAL:HB	1:B:621:PRO:HB3	1.90	0.52
1:B:538:LYS:O	1:B:542:GLU:N	2.43	0.52
1:A:130:ILE:HG23	1:A:263:GLU:HA	1.90	0.52
1:A:1358:ASN:OD1	1:A:1361:GLY:N	2.42	0.52
1:D:324:PRO:HB2	1:D:437:LEU:HD13	1.91	0.52
1:D:538:LYS:O	1:D:542:GLU:N	2.43	0.52
1:A:244:TRP:HA	1:A:247:VAL:HG23	1.92	0.52
1:B:244:TRP:HA	1:B:247:VAL:HG23	1.92	0.52
1:B:400:VAL:HG11	1:B:1269:LEU:HD13	1.91	0.52
1:A:1131:ASN:O	1:A:1135:ASN:ND2	2.43	0.51
1:A:1341:CYS:HB3	1:A:1344:PRO:HG3	1.92	0.51
1:B:1131:ASN:O	1:B:1135:ASN:ND2	2.43	0.51
1:C:244:TRP:HA	1:C:247:VAL:HG23	1.92	0.51
1:C:1131:ASN:O	1:C:1135:ASN:ND2	2.43	0.51
1:D:244:TRP:HA	1:D:247:VAL:HG23	1.92	0.51
1:D:917:SER:HB3	1:D:920:LEU:HG	1.93	0.51
1:A:1334:ARG:O	1:A:1435:THR:OG1	2.29	0.51
1:B:1341:CYS:HB3	1:B:1344:PRO:HG3	1.93	0.51
1:C:538:LYS:O	1:C:542:GLU:N	2.43	0.51
1:A:917:SER:HB3	1:A:920:LEU:HG	1.93	0.51
1:D:1131:ASN:O	1:D:1135:ASN:ND2	2.43	0.51
1:A:214:VAL:HG13	1:A:330:LEU:HD12	1.91	0.51
1:A:331:GLU:HA	1:A:357:GLY:HA2	1.93	0.51
1:A:726:ASP:HB3	1:A:729:PHE:HB3	1.92	0.51
1:A:212:THR:HB	1:A:275:THR:HG21	1.93	0.51
1:D:1341:CYS:HB3	1:D:1344:PRO:HG3	1.92	0.51
1:A:291:THR:OG1	1:A:294:GLN:OE1	2.29	0.51
1:B:331:GLU:HA	1:B:357:GLY:HA2	1.93	0.51
1:D:331:GLU:HA	1:D:357:GLY:HA2	1.93	0.51
1:B:343:ALA:HB1	1:B:348:THR:HB	1.91	0.51
1:B:726:ASP:HB3	1:B:729:PHE:HB3	1.92	0.51
1:C:291:THR:OG1	1:C:294:GLN:OE1	2.29	0.51
1:C:1155:VAL:HA	1:C:1158:MET:HG2	1.93	0.51
1:A:822:GLN:H	1:A:886:ARG:HH22	1.59	0.51
1:D:1334:ARG:O	1:D:1435:THR:OG1	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1384:HIS:HA	1:D:1483:PRO:HG2	1.92	0.51
1:B:291:THR:OG1	1:B:294:GLN:OE1	2.29	0.51
1:B:681:GLU:HA	1:B:684:HIS:HB3	1.91	0.51
1:B:1384:HIS:HA	1:B:1483:PRO:HG2	1.92	0.51
1:C:331:GLU:HA	1:C:357:GLY:HA2	1.93	0.51
1:C:917:SER:HB3	1:C:920:LEU:HG	1.93	0.51
1:C:1384:HIS:HA	1:C:1483:PRO:HG2	1.92	0.51
1:C:1492:LEU:HB3	1:C:1503:TYR:HE2	1.76	0.51
1:D:212:THR:HB	1:D:275:THR:HG21	1.93	0.51
1:D:1155:VAL:HA	1:D:1158:MET:HG2	1.93	0.51
1:A:531:LEU:HD22	1:A:666:GLU:HB3	1.93	0.50
1:A:796:VAL:O	1:A:800:HIS:N	2.37	0.50
1:A:1096:ARG:HH22	1:A:1102:PRO:HG3	1.77	0.50
1:B:1334:ARG:O	1:B:1435:THR:OG1	2.29	0.50
1:A:1239:HIS:HB3	1:A:1242:ALA:HB3	1.93	0.50
1:B:822:GLN:H	1:B:886:ARG:HH22	1.59	0.50
1:C:1341:CYS:HB3	1:C:1344:PRO:HG3	1.92	0.50
1:C:1358:ASN:OD1	1:C:1361:GLY:N	2.42	0.50
1:D:158:MET:HB3	1:D:164:LEU:HD12	1.93	0.50
1:B:917:SER:HB3	1:B:920:LEU:HG	1.93	0.50
1:C:531:LEU:HD22	1:C:666:GLU:HB3	1.94	0.50
1:C:1336:ARG:H	1:C:1435:THR:HG21	1.76	0.50
1:D:1358:ASN:OD1	1:D:1361:GLY:N	2.42	0.50
1:A:414:GLN:HA	1:A:439:LYS:HE2	1.93	0.50
1:B:531:LEU:HD22	1:B:666:GLU:HB3	1.94	0.50
1:C:681:GLU:HA	1:C:684:HIS:HB3	1.92	0.50
1:C:726:ASP:HB3	1:C:729:PHE:HB3	1.92	0.50
1:C:1334:ARG:O	1:C:1435:THR:OG1	2.29	0.50
1:D:291:THR:OG1	1:D:294:GLN:OE1	2.29	0.50
1:D:726:ASP:HB3	1:D:729:PHE:HB3	1.92	0.50
1:D:1096:ARG:HH22	1:D:1102:PRO:HG3	1.77	0.50
1:C:414:GLN:HA	1:C:439:LYS:HE2	1.93	0.50
1:D:822:GLN:H	1:D:886:ARG:HH22	1.59	0.50
1:A:1484:LEU:HD23	1:A:1489:LYS:HB2	1.93	0.50
1:B:158:MET:HB3	1:B:164:LEU:HD12	1.93	0.50
1:B:414:GLN:HA	1:B:439:LYS:HE2	1.93	0.50
1:B:1492:LEU:HB3	1:B:1503:TYR:HE2	1.76	0.50
1:C:1261:LYS:HE3	1:C:1269:LEU:HB2	1.94	0.50
1:B:1239:HIS:HB3	1:B:1242:ALA:HB3	1.93	0.50
1:D:414:GLN:HA	1:D:439:LYS:HE2	1.93	0.50
1:D:531:LEU:HD22	1:D:666:GLU:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:GLU:HB2	1:D:672:SER:HB3	1.94	0.50
1:D:1484:LEU:HD23	1:D:1489:LYS:HB2	1.93	0.50
1:D:1492:LEU:HB3	1:D:1503:TYR:HE2	1.76	0.50
1:B:1096:ARG:HH22	1:B:1102:PRO:HG3	1.77	0.50
1:B:1336:ARG:H	1:B:1435:THR:HG21	1.76	0.50
1:B:1155:VAL:HA	1:B:1158:MET:HG2	1.93	0.49
1:C:158:MET:HB3	1:C:164:LEU:HD12	1.93	0.49
1:D:796:VAL:O	1:D:800:HIS:N	2.37	0.49
1:A:158:MET:HB3	1:A:164:LEU:HD12	1.93	0.49
1:C:466:ASP:OD1	1:C:466:ASP:N	2.45	0.49
1:C:822:GLN:H	1:C:886:ARG:HH22	1.59	0.49
1:C:1096:ARG:HH22	1:C:1102:PRO:HG3	1.77	0.49
1:C:1239:HIS:HB3	1:C:1242:ALA:HB3	1.93	0.49
1:B:466:ASP:N	1:B:466:ASP:OD1	2.45	0.49
1:B:684:HIS:HA	1:B:687:ILE:HD12	1.95	0.49
1:D:375:THR:O	1:D:377:SER:N	2.46	0.49
1:A:375:THR:O	1:A:377:SER:N	2.46	0.49
1:C:212:THR:HB	1:C:275:THR:HG21	1.93	0.49
1:A:137:GLN:NE2	1:A:138:LYS:NZ	2.60	0.49
1:A:684:HIS:HA	1:A:687:ILE:HD12	1.95	0.49
1:A:1155:VAL:HA	1:A:1158:MET:HG2	1.93	0.49
1:B:137:GLN:NE2	1:B:138:LYS:NZ	2.60	0.49
1:B:1261:LYS:HE3	1:B:1269:LEU:HB2	1.94	0.49
1:C:375:THR:O	1:C:377:SER:N	2.46	0.49
1:A:667:GLU:HB2	1:A:672:SER:HB3	1.94	0.49
1:B:667:GLU:HB2	1:B:672:SER:HB3	1.94	0.49
1:B:1118:GLU:HB3	1:B:1122:LEU:HD23	1.94	0.49
1:D:137:GLN:NE2	1:D:138:LYS:NZ	2.60	0.49
1:D:684:HIS:HA	1:D:687:ILE:HD12	1.95	0.49
1:D:1261:LYS:HE3	1:D:1269:LEU:HB2	1.93	0.49
1:B:69:LYS:HD2	1:B:258:GLY:HA3	1.95	0.49
1:B:931:MET:HA	1:B:934:VAL:HB	1.95	0.49
1:B:1484:LEU:HD23	1:B:1489:LYS:HB2	1.93	0.49
1:C:684:HIS:HA	1:C:687:ILE:HD12	1.95	0.49
1:D:1118:GLU:HB3	1:D:1122:LEU:HD23	1.94	0.49
1:D:1239:HIS:HB3	1:D:1242:ALA:HB3	1.93	0.49
1:A:931:MET:HA	1:A:934:VAL:HB	1.95	0.49
1:C:137:GLN:NE2	1:C:138:LYS:NZ	2.60	0.49
1:C:1262:VAL:HG23	1:C:1263:PRO:HD3	1.95	0.49
1:A:1261:LYS:HE3	1:A:1269:LEU:HB2	1.93	0.49
1:B:212:THR:HB	1:B:275:THR:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASP:OD1	1:B:288:ASP:N	2.45	0.49
1:D:1336:ARG:H	1:D:1435:THR:HG21	1.76	0.49
1:A:466:ASP:OD1	1:A:466:ASP:N	2.45	0.48
1:B:344:THR:HB	1:B:415:LEU:HD13	1.95	0.48
1:D:1054:GLN:HB2	1:D:1058:HIS:HB2	1.95	0.48
1:D:1262:VAL:HG23	1:D:1263:PRO:HD3	1.95	0.48
1:A:1492:LEU:HB3	1:A:1503:TYR:HE2	1.76	0.48
1:C:667:GLU:HB2	1:C:672:SER:HB3	1.94	0.48
1:C:931:MET:HA	1:C:934:VAL:HB	1.95	0.48
1:A:69:LYS:HD2	1:A:258:GLY:HA3	1.95	0.48
1:C:1484:LEU:HD23	1:C:1489:LYS:HB2	1.93	0.48
1:D:344:THR:HB	1:D:415:LEU:HD13	1.95	0.48
1:D:466:ASP:N	1:D:466:ASP:OD1	2.45	0.48
1:D:931:MET:HA	1:D:934:VAL:HB	1.95	0.48
1:A:1336:ARG:H	1:A:1435:THR:HG21	1.76	0.48
1:A:484:LEU:O	1:A:488:MET:N	2.40	0.48
1:B:433:ILE:HG23	1:B:434:LEU:HG	1.96	0.48
1:B:484:LEU:O	1:B:488:MET:N	2.40	0.48
1:C:344:THR:HB	1:C:415:LEU:HD13	1.95	0.48
1:C:1054:GLN:HB2	1:C:1058:HIS:HB2	1.96	0.48
1:A:1118:GLU:HB3	1:A:1122:LEU:HD23	1.94	0.48
1:B:1351:MET:HB2	1:B:1446:SER:HA	1.96	0.48
1:C:69:LYS:HD2	1:C:258:GLY:HA3	1.95	0.48
1:A:135:LEU:HD21	1:A:279:SER:HA	1.96	0.48
1:A:168:ASN:OD1	1:A:314:LYS:NZ	2.38	0.48
1:A:344:THR:HB	1:A:415:LEU:HD13	1.95	0.48
1:A:977:THR:HB	1:A:982:ILE:HD13	1.96	0.48
1:A:1054:GLN:HB2	1:A:1058:HIS:HB2	1.96	0.48
1:B:137:GLN:NE2	1:B:138:LYS:HZ2	2.10	0.48
1:C:1118:GLU:HB3	1:C:1122:LEU:HD23	1.94	0.48
1:C:1243:ARG:NH1	1:C:1259:ASN:OD1	2.44	0.48
1:A:1262:VAL:HG23	1:A:1263:PRO:HD3	1.95	0.48
1:A:433:ILE:HG23	1:A:434:LEU:HG	1.96	0.48
1:C:796:VAL:O	1:C:800:HIS:N	2.37	0.48
1:D:137:GLN:NE2	1:D:138:LYS:HZ2	2.12	0.48
1:B:1054:GLN:HB2	1:B:1058:HIS:HB2	1.96	0.47
1:B:1143:ARG:HG2	1:B:1146:GLN:H	1.79	0.47
1:B:1262:VAL:HG23	1:B:1263:PRO:HD3	1.95	0.47
1:B:1310:ARG:NH1	1:B:1342:PHE:O	2.47	0.47
1:B:1403:LYS:HA	1:B:1406:LEU:HB2	1.96	0.47
1:B:363:ILE:HG23	1:B:406:ILE:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:THR:HB	1:B:982:ILE:HD13	1.96	0.47
1:D:1351:MET:HB2	1:D:1446:SER:HA	1.96	0.47
1:C:168:ASN:OD1	1:C:314:LYS:NZ	2.38	0.47
1:C:1236:ASP:O	1:C:1243:ARG:NH2	2.46	0.47
1:D:69:LYS:HD2	1:D:258:GLY:HA3	1.95	0.47
1:D:135:LEU:HD21	1:D:279:SER:HA	1.96	0.47
1:A:1403:LYS:HA	1:A:1406:LEU:HB2	1.97	0.47
1:B:375:THR:O	1:B:377:SER:N	2.46	0.47
1:D:1310:ARG:NH1	1:D:1342:PHE:O	2.47	0.47
1:A:558:MET:HB3	1:A:585:ARG:HG2	1.96	0.47
1:A:1310:ARG:NH1	1:A:1342:PHE:O	2.47	0.47
1:A:1351:MET:HB2	1:A:1446:SER:HA	1.96	0.47
1:B:135:LEU:HD21	1:B:279:SER:HA	1.96	0.47
1:B:170:LEU:HB2	1:B:325:ILE:HG13	1.97	0.47
1:C:135:LEU:HD21	1:C:279:SER:HA	1.96	0.47
1:C:433:ILE:HG23	1:C:434:LEU:HG	1.96	0.47
1:C:558:MET:HB3	1:C:585:ARG:HG2	1.96	0.47
1:C:1143:ARG:HG2	1:C:1146:GLN:H	1.79	0.47
1:C:1351:MET:HB2	1:C:1446:SER:HA	1.96	0.47
1:D:170:LEU:HB2	1:D:325:ILE:HG13	1.96	0.47
1:D:433:ILE:HG23	1:D:434:LEU:HG	1.96	0.47
1:A:170:LEU:HB2	1:A:325:ILE:HG13	1.97	0.47
1:B:927:VAL:HA	1:B:930:MET:HB2	1.97	0.47
1:C:977:THR:HB	1:C:982:ILE:HD13	1.96	0.47
1:C:1311:ARG:O	1:C:1346:HIS:ND1	2.48	0.47
1:B:558:MET:HB3	1:B:585:ARG:HG2	1.96	0.47
1:C:802:ASN:OD1	1:C:1077:ARG:NH1	2.48	0.47
1:D:558:MET:HB3	1:D:585:ARG:HG2	1.96	0.47
1:A:623:ARG:HA	1:A:626:LEU:HD12	1.97	0.47
1:A:1053:GLN:NE2	1:B:1057:GLU:OE2	2.48	0.47
1:C:363:ILE:HG23	1:C:406:ILE:HG23	1.97	0.47
1:D:977:THR:HB	1:D:982:ILE:HD13	1.96	0.47
1:A:802:ASN:OD1	1:A:1077:ARG:NH1	2.48	0.46
1:B:623:ARG:HA	1:B:626:LEU:HD12	1.97	0.46
1:B:802:ASN:OD1	1:B:1077:ARG:NH1	2.48	0.46
1:C:1310:ARG:NH1	1:C:1342:PHE:O	2.47	0.46
1:A:1057:GLU:OE2	1:D:1053:GLN:NE2	2.48	0.46
1:B:645:SER:O	1:B:1129:LYS:NZ	2.40	0.46
1:C:623:ARG:HA	1:C:626:LEU:HD12	1.97	0.46
1:D:623:ARG:HA	1:D:626:LEU:HD12	1.97	0.46
1:C:1053:GLN:NE2	1:D:1057:GLU:OE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1403:LYS:HA	1:C:1406:LEU:HB2	1.97	0.46
1:C:170:LEU:HB2	1:C:325:ILE:HG13	1.96	0.46
1:C:634:ARG:HB3	1:C:637:LEU:HD13	1.97	0.46
1:D:734:GLY:O	1:D:738:PHE:N	2.49	0.46
1:D:802:ASN:OD1	1:D:1077:ARG:NH1	2.48	0.46
1:D:1143:ARG:HG2	1:D:1146:GLN:H	1.79	0.46
1:A:332:GLY:HA2	1:A:333:GLY:HA3	1.72	0.46
1:B:917:SER:H	1:B:920:LEU:HD12	1.80	0.46
1:C:917:SER:H	1:C:920:LEU:HD12	1.80	0.46
1:C:927:VAL:HA	1:C:930:MET:HB2	1.97	0.46
1:A:137:GLN:NE2	1:A:138:LYS:HZ2	2.13	0.46
1:A:927:VAL:HA	1:A:930:MET:HB2	1.97	0.46
1:D:173:VAL:O	1:D:302:ARG:NH2	2.46	0.46
1:D:934:VAL:HG12	1:D:938:LEU:HD12	1.98	0.46
1:B:1243:ARG:NH1	1:B:1259:ASN:OD1	2.44	0.46
1:D:484:LEU:O	1:D:488:MET:N	2.40	0.46
1:A:1143:ARG:HG2	1:A:1146:GLN:H	1.79	0.46
1:C:274:LEU:HD21	1:C:293:GLY:HA2	1.98	0.46
1:C:734:GLY:O	1:C:738:PHE:N	2.49	0.46
1:D:363:ILE:HG23	1:D:406:ILE:HG23	1.97	0.46
1:D:1236:ASP:O	1:D:1243:ARG:NH2	2.46	0.46
1:B:634:ARG:HB3	1:B:637:LEU:HD13	1.97	0.46
1:B:934:VAL:HG12	1:B:938:LEU:HD12	1.98	0.46
1:D:1403:LYS:HA	1:D:1406:LEU:HB2	1.96	0.46
1:A:734:GLY:O	1:A:738:PHE:N	2.49	0.45
1:B:557:GLN:HB2	1:B:560:HIS:HD2	1.81	0.45
1:C:1024:LEU:HD21	1:D:901:LEU:HD11	1.98	0.45
1:A:198:ALA:HA	1:A:202:GLY:H	1.81	0.45
1:C:332:GLY:HA3	1:C:359:VAL:HB	1.99	0.45
1:C:939:PHE:HA	1:C:942:ALA:HB3	1.98	0.45
1:D:332:GLY:HA2	1:D:333:GLY:HA3	1.72	0.45
1:A:557:GLN:HB2	1:A:560:HIS:HD2	1.81	0.45
1:A:789:ARG:HA	1:A:792:PHE:HD2	1.82	0.45
1:C:291:THR:HG1	1:C:292:HIS:H	1.65	0.45
1:D:274:LEU:HD21	1:D:293:GLY:HA2	1.98	0.45
1:D:927:VAL:HA	1:D:930:MET:HB2	1.97	0.45
1:D:1330:ARG:HG3	1:D:1436:ASP:HB3	1.98	0.45
1:A:634:ARG:HB3	1:A:637:LEU:HD13	1.97	0.45
1:A:917:SER:H	1:A:920:LEU:HD12	1.80	0.45
1:B:734:GLY:O	1:B:738:PHE:N	2.49	0.45
1:B:1435:THR:HG23	1:B:1437:ASN:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:PRO:HA	1:D:187:LYS:HD2	1.99	0.45
1:D:332:GLY:HA3	1:D:359:VAL:HB	1.99	0.45
1:D:917:SER:H	1:D:920:LEU:HD12	1.80	0.45
1:A:332:GLY:HA3	1:A:359:VAL:HB	1.99	0.45
1:A:363:ILE:HG23	1:A:406:ILE:HG23	1.96	0.45
1:A:934:VAL:HG12	1:A:938:LEU:HD12	1.98	0.45
1:A:1236:ASP:O	1:A:1243:ARG:NH2	2.46	0.45
1:A:1435:THR:HG23	1:A:1437:ASN:H	1.82	0.45
1:B:184:PRO:HA	1:B:187:LYS:HD2	1.99	0.45
1:B:332:GLY:HA3	1:B:359:VAL:HB	1.99	0.45
1:C:80:LYS:HD3	1:C:96:GLU:HG3	1.99	0.45
1:C:198:ALA:HA	1:C:202:GLY:H	1.81	0.45
1:C:1435:THR:HG23	1:C:1437:ASN:H	1.82	0.45
1:A:438:LEU:O	1:A:442:ARG:NH1	2.50	0.45
1:A:901:LEU:HD11	1:D:1024:LEU:HD21	1.97	0.45
1:A:939:PHE:HA	1:A:942:ALA:HB3	1.98	0.45
1:B:939:PHE:HA	1:B:942:ALA:HB3	1.98	0.45
1:C:438:LEU:O	1:C:442:ARG:NH1	2.50	0.45
1:D:80:LYS:HD3	1:D:96:GLU:HG3	1.99	0.45
1:D:634:ARG:HB3	1:D:637:LEU:HD13	1.97	0.45
1:B:526:LEU:HB3	1:B:533:HIS:HB2	1.99	0.45
1:B:1311:ARG:O	1:B:1346:HIS:ND1	2.48	0.45
1:C:509:GLN:HG3	1:C:511:LYS:HB2	1.99	0.45
1:D:198:ALA:HA	1:D:202:GLY:H	1.81	0.45
1:D:946:VAL:O	1:D:975:TYR:OH	2.29	0.45
1:A:946:VAL:O	1:A:975:TYR:OH	2.29	0.45
1:C:184:PRO:HA	1:C:187:LYS:HD2	1.99	0.45
1:A:1243:ARG:NH1	1:A:1259:ASN:OD1	2.44	0.45
1:A:1278:ALA:HB2	1:A:1283:ALA:HA	1.99	0.45
1:B:278:ASP:HB3	1:B:281:HIS:CD2	2.52	0.45
1:C:557:GLN:HB2	1:C:560:HIS:HD2	1.81	0.45
1:D:939:PHE:HA	1:D:942:ALA:HB3	1.98	0.45
1:A:1311:ARG:O	1:A:1346:HIS:ND1	2.48	0.44
1:C:789:ARG:HA	1:C:792:PHE:HD2	1.82	0.44
1:C:1293:LEU:HG	1:C:1295:PRO:HD2	2.00	0.44
1:D:698:GLU:O	1:D:702:GLN:N	2.49	0.44
1:A:1345:ASN:HB2	1:A:1441:GLU:H	1.83	0.44
1:C:1330:ARG:HG3	1:C:1436:ASP:HB3	1.98	0.44
1:D:438:LEU:O	1:D:442:ARG:NH1	2.50	0.44
1:A:278:ASP:HB3	1:A:281:HIS:CD2	2.52	0.44
1:B:274:LEU:HD21	1:B:293:GLY:HA2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1278:ALA:HB2	1:B:1283:ALA:HA	1.99	0.44
1:B:1372:LEU:HG	1:B:1501:ALA:HB2	1.99	0.44
1:C:1345:ASN:HB2	1:C:1441:GLU:H	1.83	0.44
1:D:536:LEU:O	1:D:540:LEU:N	2.46	0.44
1:D:557:GLN:HB2	1:D:560:HIS:HD2	1.81	0.44
1:D:789:ARG:HA	1:D:792:PHE:HD2	1.82	0.44
1:D:1293:LEU:HG	1:D:1295:PRO:HD2	2.00	0.44
1:D:1435:THR:HG23	1:D:1437:ASN:H	1.82	0.44
1:A:74:TYR:HB2	1:A:122:MET:H	1.83	0.44
1:B:74:TYR:HB2	1:B:122:MET:H	1.83	0.44
1:B:1053:GLN:NE2	1:C:1057:GLU:OE2	2.50	0.44
1:B:1345:ASN:HB2	1:B:1441:GLU:H	1.83	0.44
1:C:698:GLU:O	1:C:702:GLN:N	2.49	0.44
1:C:928:LYS:HD2	1:C:928:LYS:HA	1.83	0.44
1:C:932:LYS:HA	1:C:932:LYS:HD2	1.84	0.44
1:C:934:VAL:HG12	1:C:938:LEU:HD12	1.98	0.44
1:D:278:ASP:HB3	1:D:281:HIS:CD2	2.52	0.44
1:D:1278:ALA:HB2	1:D:1283:ALA:HA	1.99	0.44
1:D:1372:LEU:HG	1:D:1501:ALA:HB2	1.99	0.44
1:A:449:HIS:NE2	1:A:483:ASP:HB2	2.33	0.44
1:A:698:GLU:O	1:A:702:GLN:N	2.49	0.44
1:B:198:ALA:HA	1:B:202:GLY:H	1.81	0.44
1:B:789:ARG:HA	1:B:792:PHE:HD2	1.82	0.44
1:C:449:HIS:NE2	1:C:483:ASP:HB2	2.33	0.44
1:C:1160:ASP:OD1	1:C:1160:ASP:N	2.50	0.44
1:D:509:GLN:HG3	1:D:511:LYS:HB2	1.99	0.44
1:A:184:PRO:HA	1:A:187:LYS:HD2	1.99	0.44
1:A:274:LEU:HD21	1:A:293:GLY:HA2	1.98	0.44
1:B:449:HIS:NE2	1:B:483:ASP:HB2	2.33	0.44
1:B:1330:ARG:HG3	1:B:1436:ASP:HB3	1.98	0.44
1:D:1273:PRO:HD2	1:D:1333:LEU:HB2	2.00	0.44
1:A:450:GLU:HA	1:A:453:ASP:HB3	2.00	0.44
1:B:438:LEU:O	1:B:442:ARG:NH1	2.50	0.44
1:C:1411:TRP:NE1	1:C:1414:PHE:O	2.51	0.44
1:D:449:HIS:NE2	1:D:483:ASP:HB2	2.33	0.44
1:A:1273:PRO:HD2	1:A:1333:LEU:HB2	2.00	0.44
1:B:450:GLU:HA	1:B:453:ASP:HB3	2.00	0.44
1:B:1423:GLU:HA	1:B:1445:VAL:HA	2.00	0.44
1:C:450:GLU:HA	1:C:453:ASP:HB3	2.00	0.44
1:D:450:GLU:HA	1:D:453:ASP:HB3	2.00	0.44
1:D:1243:ARG:NH1	1:D:1259:ASN:OD1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1311:ARG:O	1:D:1346:HIS:ND1	2.48	0.44
1:D:1345:ASN:HB2	1:D:1441:GLU:H	1.83	0.44
1:A:363:ILE:HG12	1:A:406:ILE:HG12	2.00	0.44
1:B:509:GLN:HG3	1:B:511:LYS:HB2	1.99	0.44
1:C:220:GLU:HG3	1:C:223:ARG:HH21	1.83	0.44
1:C:278:ASP:HB3	1:C:281:HIS:CD2	2.52	0.44
1:C:332:GLY:HA2	1:C:333:GLY:HA3	1.72	0.44
1:C:609:LYS:HA	1:C:609:LYS:HD3	1.75	0.44
1:C:1273:PRO:HD2	1:C:1333:LEU:HB2	2.00	0.44
1:D:248:HIS:HB2	1:D:271:GLN:HB2	2.00	0.44
1:D:1041:LEU:HG	1:D:1044:LEU:HD22	2.00	0.44
1:A:1160:ASP:OD1	1:A:1160:ASP:N	2.50	0.43
1:B:609:LYS:HA	1:B:609:LYS:HD3	1.75	0.43
1:B:698:GLU:O	1:B:702:GLN:N	2.49	0.43
1:B:1293:LEU:HG	1:B:1295:PRO:HD2	2.00	0.43
1:A:465:VAL:HG21	1:A:498:GLU:HB2	2.01	0.43
1:A:1330:ARG:HG3	1:A:1436:ASP:HB3	1.98	0.43
1:A:1372:LEU:HG	1:A:1501:ALA:HB2	1.99	0.43
1:B:80:LYS:HD3	1:B:96:GLU:HG3	1.99	0.43
1:B:530:CYS:SG	1:B:531:LEU:N	2.91	0.43
1:B:766:LEU:O	1:B:787:ARG:NH2	2.51	0.43
1:B:1273:PRO:HD2	1:B:1333:LEU:HB2	2.00	0.43
1:C:922:PRO:HG3	1:C:1063:TRP:HB2	1.99	0.43
1:C:1278:ALA:HB2	1:C:1283:ALA:HA	1.99	0.43
1:C:1423:GLU:HA	1:C:1445:VAL:HA	2.00	0.43
1:D:922:PRO:HG3	1:D:1063:TRP:HB2	1.99	0.43
1:A:173:VAL:O	1:A:302:ARG:NH2	2.46	0.43
1:A:431:VAL:HG11	1:A:464:ARG:HH11	1.84	0.43
1:A:1411:TRP:NE1	1:A:1414:PHE:O	2.51	0.43
1:B:363:ILE:HG12	1:B:406:ILE:HG12	2.00	0.43
1:C:526:LEU:HB3	1:C:533:HIS:HB2	1.99	0.43
1:C:766:LEU:O	1:C:787:ARG:NH2	2.51	0.43
1:D:526:LEU:HB3	1:D:533:HIS:HB2	1.99	0.43
1:D:766:LEU:O	1:D:787:ARG:NH2	2.51	0.43
1:A:526:LEU:HB3	1:A:533:HIS:HB2	1.99	0.43
1:B:198:ALA:HB3	1:B:236:LEU:HD22	2.01	0.43
1:B:437:LEU:O	1:B:455:GLN:NE2	2.49	0.43
1:B:936:PHE:O	1:B:940:LEU:N	2.40	0.43
1:C:107:THR:HG22	1:C:108:PHE:H	1.84	0.43
1:C:288:ASP:OD1	1:C:288:ASP:N	2.45	0.43
1:C:1372:LEU:HG	1:C:1501:ALA:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ASP:OD1	1:D:288:ASP:N	2.45	0.43
1:D:1411:TRP:NE1	1:D:1414:PHE:O	2.51	0.43
1:D:1423:GLU:HA	1:D:1445:VAL:HA	2.00	0.43
1:A:80:LYS:HD3	1:A:96:GLU:HG3	1.99	0.43
1:A:107:THR:HG22	1:A:108:PHE:H	1.84	0.43
1:A:650:ALA:HA	1:A:653:LEU:HD13	2.01	0.43
1:A:1311:ARG:NH1	1:A:1312:SER:O	2.52	0.43
1:A:1423:GLU:HA	1:A:1445:VAL:HA	2.00	0.43
1:B:650:ALA:HA	1:B:653:LEU:HD13	2.01	0.43
1:B:922:PRO:HG3	1:B:1063:TRP:HB2	1.99	0.43
1:B:1041:LEU:HG	1:B:1044:LEU:HD22	2.00	0.43
1:C:530:CYS:SG	1:C:531:LEU:N	2.91	0.43
1:C:1236:ASP:OD1	1:C:1236:ASP:N	2.52	0.43
1:A:509:GLN:HG3	1:A:511:LYS:HB2	1.99	0.43
1:A:629:ALA:HB1	1:A:634:ARG:HB2	2.01	0.43
1:A:672:SER:HA	1:A:675:MET:HG2	2.01	0.43
1:A:932:LYS:HA	1:A:932:LYS:HD2	1.84	0.43
1:A:1293:LEU:HG	1:A:1295:PRO:HD2	2.00	0.43
1:B:1467:CYS:SG	1:B:1468:ASP:N	2.92	0.43
1:C:363:ILE:HG12	1:C:406:ILE:HG12	2.00	0.43
1:D:672:SER:HA	1:D:675:MET:HG2	2.01	0.43
1:A:220:GLU:HG3	1:A:223:ARG:HH21	1.83	0.43
1:A:1024:LEU:HD21	1:B:901:LEU:HD11	2.00	0.43
1:A:1467:CYS:SG	1:A:1468:ASP:N	2.92	0.43
1:B:107:THR:HG22	1:B:108:PHE:H	1.84	0.43
1:C:74:TYR:HB2	1:C:122:MET:H	1.83	0.43
1:C:1311:ARG:NH1	1:C:1312:SER:O	2.52	0.43
1:D:74:TYR:HB2	1:D:122:MET:H	1.83	0.43
1:D:845:ARG:HA	1:D:848:PHE:HD2	1.84	0.43
1:D:1311:ARG:NH1	1:D:1312:SER:O	2.52	0.43
1:A:70:LYS:HE3	1:A:70:LYS:HB2	1.89	0.43
1:B:220:GLU:HG3	1:B:223:ARG:HH21	1.83	0.43
1:C:248:HIS:HB2	1:C:271:GLN:HB2	2.00	0.43
1:D:932:LYS:HA	1:D:932:LYS:HD2	1.84	0.43
1:A:248:HIS:HB2	1:A:271:GLN:HB2	2.00	0.43
1:B:1236:ASP:OD1	1:B:1236:ASP:N	2.52	0.43
1:C:983:PRO:HB2	1:C:986:ILE:HG12	2.01	0.43
1:C:1467:CYS:SG	1:C:1468:ASP:N	2.92	0.43
1:A:766:LEU:O	1:A:787:ARG:NH2	2.51	0.43
1:A:922:PRO:HG3	1:A:1063:TRP:HB2	1.99	0.43
1:A:1287:ASP:O	1:A:1289:MET:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1411:TRP:NE1	1:B:1414:PHE:O	2.51	0.43
1:C:845:ARG:HA	1:C:848:PHE:HD2	1.84	0.43
1:C:1378:LYS:NZ	1:C:1382:SER:O	2.51	0.43
1:D:363:ILE:HG12	1:D:406:ILE:HG12	2.00	0.43
1:D:629:ALA:HB1	1:D:634:ARG:HB2	2.01	0.43
1:D:928:LYS:HA	1:D:928:LYS:HD2	1.83	0.43
1:A:530:CYS:SG	1:A:531:LEU:N	2.91	0.42
1:B:390:MET:HB2	1:B:393:THR:HG22	2.01	0.42
1:B:431:VAL:HG11	1:B:464:ARG:HH11	1.84	0.42
1:B:1378:LYS:NZ	1:B:1382:SER:O	2.51	0.42
1:D:245:GLY:O	1:D:250:ARG:NH2	2.52	0.42
1:D:431:VAL:HG11	1:D:464:ARG:HH11	1.84	0.42
1:D:983:PRO:HB2	1:D:986:ILE:HG12	2.01	0.42
1:A:390:MET:HB2	1:A:393:THR:HG22	2.01	0.42
1:A:612:SER:O	1:A:612:SER:OG	2.37	0.42
1:A:845:ARG:HA	1:A:848:PHE:HD2	1.84	0.42
1:B:245:GLY:O	1:B:250:ARG:NH2	2.52	0.42
1:C:245:GLY:O	1:C:250:ARG:NH2	2.52	0.42
1:C:412:ARG:HE	1:C:415:LEU:HD12	1.84	0.42
1:C:629:ALA:HB1	1:C:634:ARG:HB2	2.01	0.42
1:D:198:ALA:HB3	1:D:236:LEU:HD22	2.00	0.42
1:D:220:GLU:HG3	1:D:223:ARG:HH21	1.83	0.42
1:B:173:VAL:O	1:B:302:ARG:NH2	2.46	0.42
1:B:629:ALA:HB1	1:B:634:ARG:HB2	2.01	0.42
1:B:1024:LEU:HD21	1:C:901:LEU:HD11	2.01	0.42
1:B:1239:HIS:HB2	1:B:1243:ARG:HG3	2.01	0.42
1:C:390:MET:HB2	1:C:393:THR:HG22	2.01	0.42
1:C:1041:LEU:HG	1:C:1044:LEU:HD22	2.00	0.42
1:D:107:THR:HG22	1:D:108:PHE:H	1.84	0.42
1:D:498:GLU:HA	1:D:501:LYS:HB3	2.01	0.42
1:D:530:CYS:SG	1:D:531:LEU:N	2.91	0.42
1:D:650:ALA:HA	1:D:653:LEU:HD13	2.01	0.42
1:D:937:PHE:HA	1:D:940:LEU:HB3	2.01	0.42
1:D:1287:ASP:O	1:D:1289:MET:N	2.52	0.42
1:A:498:GLU:HA	1:A:501:LYS:HB3	2.01	0.42
1:A:1041:LEU:HG	1:A:1044:LEU:HD22	2.00	0.42
1:B:412:ARG:HE	1:B:415:LEU:HD12	1.84	0.42
1:B:965:TRP:HA	1:B:968:ARG:HB3	2.02	0.42
1:B:1236:ASP:O	1:B:1243:ARG:NH2	2.46	0.42
1:B:1451:ASP:OD1	1:B:1451:ASP:N	2.52	0.42
1:C:484:LEU:O	1:C:488:MET:N	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:MET:HB2	1:D:393:THR:HG22	2.01	0.42
1:D:718:LEU:O	1:D:722:LEU:N	2.48	0.42
1:D:1143:ARG:NH2	1:D:1146:GLN:OE1	2.53	0.42
1:D:1307:LEU:O	1:D:1392:ARG:NH2	2.53	0.42
1:D:1467:CYS:SG	1:D:1468:ASP:N	2.92	0.42
1:D:1496:ALA:HB1	1:D:1501:ALA:HB3	2.02	0.42
1:A:198:ALA:HB3	1:A:236:LEU:HD22	2.01	0.42
1:A:1496:ALA:HB1	1:A:1501:ALA:HB3	2.02	0.42
1:B:248:HIS:HB2	1:B:271:GLN:HB2	2.00	0.42
1:B:679:ALA:HA	1:B:682:TYR:HB2	2.02	0.42
1:B:1311:ARG:NH1	1:B:1312:SER:O	2.52	0.42
1:C:650:ALA:HA	1:C:653:LEU:HD13	2.01	0.42
1:C:679:ALA:HA	1:C:682:TYR:HB2	2.02	0.42
1:C:1143:ARG:NH2	1:C:1146:GLN:OE1	2.53	0.42
1:D:465:VAL:HG21	1:D:498:GLU:HB2	2.01	0.42
1:D:1239:HIS:HB2	1:D:1243:ARG:HG3	2.01	0.42
1:A:817:LEU:O	1:A:896:ARG:NH1	2.52	0.42
1:B:250:ARG:HE	1:B:250:ARG:HB2	1.65	0.42
1:B:1143:ARG:NH2	1:B:1146:GLN:OE1	2.53	0.42
1:C:173:VAL:O	1:C:302:ARG:NH2	2.46	0.42
1:C:672:SER:HA	1:C:675:MET:HG2	2.01	0.42
1:C:934:VAL:HA	1:C:937:PHE:HB3	2.02	0.42
1:D:1489:LYS:O	1:D:1503:TYR:OH	2.35	0.42
1:A:412:ARG:HE	1:A:415:LEU:HD12	1.85	0.42
1:C:559:HIS:HA	1:C:562:ALA:HB3	2.02	0.42
1:D:1451:ASP:N	1:D:1451:ASP:OD1	2.53	0.42
1:A:679:ALA:HA	1:A:682:TYR:HB2	2.02	0.42
1:A:1239:HIS:HB2	1:A:1243:ARG:HG3	2.01	0.42
1:B:1287:ASP:O	1:B:1289:MET:N	2.52	0.42
1:C:465:VAL:HG21	1:C:498:GLU:HB2	2.01	0.42
1:C:817:LEU:O	1:C:896:ARG:NH1	2.52	0.42
1:C:1496:ALA:HB1	1:C:1501:ALA:HB3	2.02	0.42
1:A:437:LEU:O	1:A:455:GLN:NE2	2.49	0.42
1:A:934:VAL:HA	1:A:937:PHE:HB3	2.02	0.42
1:A:937:PHE:HA	1:A:940:LEU:HB3	2.02	0.42
1:C:1239:HIS:HB2	1:C:1243:ARG:HG3	2.00	0.42
1:D:1466:ALA:HB1	1:D:1470:GLY:HA3	2.02	0.42
1:A:514:VAL:HG21	1:A:625:LEU:HD11	2.01	0.42
1:A:1466:ALA:HB1	1:A:1470:GLY:HA3	2.02	0.42
1:B:465:VAL:HG21	1:B:498:GLU:HB2	2.01	0.42
1:B:845:ARG:HA	1:B:848:PHE:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:ALA:HA	1:D:682:TYR:HB2	2.02	0.42
1:D:939:PHE:O	1:D:943:VAL:N	2.53	0.42
1:B:583:ASN:HD22	1:B:602:VAL:HG12	1.85	0.41
1:B:672:SER:HA	1:B:675:MET:HG2	2.01	0.41
1:B:1307:LEU:O	1:B:1392:ARG:NH2	2.53	0.41
1:B:1326:ASN:OD1	1:B:1326:ASN:N	2.49	0.41
1:B:1496:ALA:HB1	1:B:1501:ALA:HB3	2.02	0.41
1:C:137:GLN:NE2	1:C:138:LYS:HZ2	2.17	0.41
1:C:514:VAL:HG21	1:C:625:LEU:HD11	2.01	0.41
1:C:965:TRP:HA	1:C:968:ARG:HB3	2.01	0.41
1:A:192:ARG:NH2	1:A:199:GLN:OE1	2.54	0.41
1:A:1143:ARG:NH2	1:A:1146:GLN:OE1	2.53	0.41
1:A:1261:LYS:HD2	1:A:1269:LEU:HD12	2.02	0.41
1:C:198:ALA:HB3	1:C:236:LEU:HD22	2.00	0.41
1:C:937:PHE:HA	1:C:940:LEU:HB3	2.02	0.41
1:D:559:HIS:HA	1:D:562:ALA:HB3	2.02	0.41
1:A:583:ASN:HD22	1:A:602:VAL:HG12	1.85	0.41
1:B:983:PRO:HB2	1:B:986:ILE:HG12	2.01	0.41
1:C:1287:ASP:O	1:C:1289:MET:N	2.52	0.41
1:D:255:HIS:HA	1:D:256:PRO:HD3	1.89	0.41
1:D:412:ARG:HE	1:D:415:LEU:HD12	1.85	0.41
1:A:771:ILE:O	1:A:787:ARG:NH2	2.54	0.41
1:A:939:PHE:O	1:A:943:VAL:N	2.53	0.41
1:B:192:ARG:NH2	1:B:199:GLN:OE1	2.54	0.41
1:B:492:LEU:O	1:B:495:ASN:ND2	2.54	0.41
1:B:700:ARG:NH2	1:B:1120:ALA:O	2.53	0.41
1:B:718:LEU:O	1:B:722:LEU:N	2.48	0.41
1:C:431:VAL:HG11	1:C:464:ARG:HH11	1.84	0.41
1:C:1466:ALA:HB1	1:C:1470:GLY:HA3	2.02	0.41
1:D:437:LEU:O	1:D:455:GLN:NE2	2.49	0.41
1:D:492:LEU:O	1:D:495:ASN:ND2	2.54	0.41
1:A:250:ARG:HE	1:A:250:ARG:HB2	1.65	0.41
1:A:965:TRP:HA	1:A:968:ARG:HB3	2.01	0.41
1:B:498:GLU:HA	1:B:501:LYS:HB3	2.01	0.41
1:C:498:GLU:HA	1:C:501:LYS:HB3	2.01	0.41
1:C:1277:THR:HA	1:C:1336:ARG:HA	2.03	0.41
1:D:250:ARG:HE	1:D:250:ARG:HB2	1.65	0.41
1:D:612:SER:O	1:D:612:SER:OG	2.37	0.41
1:B:514:VAL:HG21	1:B:625:LEU:HD11	2.01	0.41
1:B:934:VAL:HA	1:B:937:PHE:HB3	2.02	0.41
1:C:437:LEU:O	1:C:455:GLN:NE2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1307:LEU:O	1:C:1392:ARG:NH2	2.53	0.41
1:D:416:LEU:O	1:D:439:LYS:NZ	2.45	0.41
1:D:771:ILE:O	1:D:787:ARG:NH2	2.54	0.41
1:B:771:ILE:O	1:B:787:ARG:NH2	2.54	0.41
1:B:1466:ALA:HB1	1:B:1470:GLY:HA3	2.02	0.41
1:C:594:HIS:CE1	1:C:596:LYS:HG2	2.56	0.41
1:C:1261:LYS:HD2	1:C:1269:LEU:HD12	2.02	0.41
1:D:514:VAL:HG21	1:D:625:LEU:HD11	2.01	0.41
1:D:645:SER:O	1:D:1129:LYS:NZ	2.40	0.41
1:D:700:ARG:NH2	1:D:1120:ALA:O	2.53	0.41
1:A:983:PRO:HB2	1:A:986:ILE:HG12	2.01	0.41
1:B:559:HIS:HA	1:B:562:ALA:HB3	2.02	0.41
1:B:937:PHE:HA	1:B:940:LEU:HB3	2.01	0.41
1:B:1277:THR:HA	1:B:1336:ARG:HA	2.03	0.41
1:C:539:VAL:HA	1:C:542:GLU:HB2	2.03	0.41
1:C:771:ILE:O	1:C:787:ARG:NH2	2.54	0.41
1:D:965:TRP:HA	1:D:968:ARG:HB3	2.01	0.41
1:A:700:ARG:NH2	1:A:1120:ALA:O	2.53	0.41
1:A:707:ARG:HG3	1:A:1113:LEU:HD21	2.03	0.41
1:A:760:MET:HE3	1:A:797:VAL:HA	2.03	0.41
1:A:1451:ASP:OD1	1:A:1451:ASP:N	2.52	0.41
1:B:178:LYS:HD2	1:B:178:LYS:HA	1.89	0.41
1:B:1261:LYS:HD2	1:B:1269:LEU:HD12	2.02	0.41
1:C:385:VAL:H	1:C:385:VAL:HG23	1.60	0.41
1:C:583:ASN:HD22	1:C:602:VAL:HG12	1.86	0.41
1:C:707:ARG:HG3	1:C:1113:LEU:HD21	2.03	0.41
1:C:939:PHE:O	1:C:943:VAL:N	2.53	0.41
1:C:1489:LYS:HB2	1:C:1489:LYS:HE2	1.93	0.41
1:D:137:GLN:HE21	1:D:138:LYS:HZ2	1.67	0.41
1:D:423:LYS:HA	1:D:423:LYS:HD3	1.90	0.41
1:D:470:SER:HA	1:D:474:MET:HG2	2.03	0.41
1:D:569:LEU:HA	1:D:657:LYS:HZ3	1.85	0.41
1:D:934:VAL:HA	1:D:937:PHE:HB3	2.02	0.41
1:A:645:SER:O	1:A:1129:LYS:NZ	2.40	0.41
1:A:1277:THR:HA	1:A:1336:ARG:HA	2.03	0.41
1:B:470:SER:HA	1:B:474:MET:HG2	2.03	0.41
1:B:760:MET:HE1	1:B:797:VAL:HA	2.02	0.41
1:C:492:LEU:O	1:C:495:ASN:ND2	2.54	0.41
1:D:314:LYS:HD3	1:D:321:ILE:HD11	2.03	0.41
1:D:539:VAL:HA	1:D:542:GLU:HB2	2.03	0.41
1:D:851:PRO:HA	1:D:859:LYS:HE3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LYS:HD3	1:A:321:ILE:HD11	2.04	0.40
1:A:492:LEU:O	1:A:495:ASN:ND2	2.54	0.40
1:A:559:HIS:HA	1:A:562:ALA:HB3	2.02	0.40
1:B:536:LEU:O	1:B:540:LEU:N	2.46	0.40
1:B:594:HIS:CE1	1:B:596:LYS:HG2	2.56	0.40
1:B:939:PHE:O	1:B:943:VAL:N	2.53	0.40
1:D:1261:LYS:HD2	1:D:1269:LEU:HD12	2.02	0.40
1:D:1277:THR:HA	1:D:1336:ARG:HA	2.03	0.40
1:A:241:VAL:HG12	1:A:298:GLU:HG2	2.04	0.40
1:A:510:LEU:HA	1:A:513:PHE:HB3	2.03	0.40
1:A:536:LEU:O	1:A:540:LEU:N	2.46	0.40
1:A:928:LYS:HD2	1:A:928:LYS:HA	1.83	0.40
1:A:1275:PHE:HE1	1:A:1333:LEU:HB3	1.86	0.40
1:C:137:GLN:HE21	1:C:138:LYS:HZ1	1.67	0.40
1:C:314:LYS:HD3	1:C:321:ILE:HD11	2.04	0.40
1:C:700:ARG:NH2	1:C:1120:ALA:O	2.53	0.40
1:C:1275:PHE:HE1	1:C:1333:LEU:HB3	1.86	0.40
1:C:1344:PRO:O	1:C:1346:HIS:ND1	2.54	0.40
1:D:760:MET:HE3	1:D:797:VAL:HA	2.03	0.40
1:A:594:HIS:CE1	1:A:596:LYS:HG2	2.56	0.40
1:B:241:VAL:HG12	1:B:298:GLU:HG2	2.03	0.40
1:B:1344:PRO:O	1:B:1346:HIS:ND1	2.54	0.40
1:D:192:ARG:NH2	1:D:199:GLN:OE1	2.54	0.40
1:D:241:VAL:HG12	1:D:298:GLU:HG2	2.04	0.40
1:D:1030:CYS:HA	1:D:1033:LEU:HB3	2.03	0.40
1:D:1344:PRO:O	1:D:1346:HIS:ND1	2.54	0.40
1:D:1378:LYS:NZ	1:D:1382:SER:O	2.51	0.40
1:A:446:HIS:HB3	1:A:447:PHE:H	1.73	0.40
1:A:539:VAL:HA	1:A:542:GLU:HB2	2.03	0.40
1:A:1307:LEU:O	1:A:1392:ARG:NH2	2.53	0.40
1:A:1344:PRO:O	1:A:1346:HIS:ND1	2.54	0.40
1:B:1160:ASP:N	1:B:1160:ASP:OD1	2.50	0.40
1:C:241:VAL:HG12	1:C:298:GLU:HG2	2.03	0.40
1:C:377:SER:HA	1:C:380:GLN:HB2	2.03	0.40
1:C:446:HIS:HB3	1:C:447:PHE:H	1.73	0.40
1:C:736:GLN:HA	1:C:739:LEU:HG	2.04	0.40
1:C:1115:LYS:HA	1:C:1115:LYS:HD3	1.98	0.40
1:A:470:SER:HA	1:A:474:MET:HG2	2.03	0.40
1:A:897:VAL:O	1:A:900:SER:OG	2.31	0.40
1:B:377:SER:HA	1:B:380:GLN:HB2	2.04	0.40
1:B:896:ARG:HH11	1:B:896:ARG:HD2	1.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASN:OD1	1:C:273:ASN:N	2.55	0.40
1:C:569:LEU:HA	1:C:657:LYS:HZ3	1.87	0.40
1:C:851:PRO:HA	1:C:859:LYS:HE3	2.03	0.40
1:D:1112:LYS:HA	1:D:1112:LYS:HD2	1.98	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 PDB entries followed by that with respect to all EM entries.

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	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
1	B	1331/1503 (89%)	1133 (85%)	193 (14%)	5 (0%)	30	68
1	C	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
1	D	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
All	All	5324/6012 (89%)	4526 (85%)	778 (15%)	20 (0%)	32	68

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE
1	B	376	ILE
1	C	376	ILE
1	D	376	ILE
1	A	384	SER
1	B	384	SER
1	C	384	SER
1	D	384	SER
1	A	1288	PRO
1	B	1288	PRO
1	C	1288	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1288	PRO
1	A	429	VAL
1	A	1270	ILE
1	B	429	VAL
1	B	1270	ILE
1	C	429	VAL
1	C	1270	ILE
1	D	429	VAL
1	D	1270	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	B	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	C	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	D	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
All	All	4704/5272 (89%)	4652 (99%)	52 (1%)	69	80

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	LEU
1	A	496	LYS
1	A	566	ARG
1	A	610	ARG
1	A	685	ARG
1	A	715	THR
1	A	839	LEU
1	A	886	ARG
1	A	918	LYS
1	A	930	MET
1	A	941	LEU
1	A	1024	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1064	LYS
1	B	253	LEU
1	B	496	LYS
1	B	566	ARG
1	B	610	ARG
1	B	685	ARG
1	B	715	THR
1	B	839	LEU
1	B	886	ARG
1	B	918	LYS
1	B	930	MET
1	B	941	LEU
1	B	1024	LEU
1	B	1064	LYS
1	C	253	LEU
1	C	496	LYS
1	C	566	ARG
1	C	610	ARG
1	C	685	ARG
1	C	715	THR
1	C	839	LEU
1	C	886	ARG
1	C	918	LYS
1	C	930	MET
1	C	941	LEU
1	C	1024	LEU
1	C	1064	LYS
1	D	253	LEU
1	D	496	LYS
1	D	566	ARG
1	D	610	ARG
1	D	685	ARG
1	D	715	THR
1	D	839	LEU
1	D	886	ARG
1	D	918	LYS
1	D	930	MET
1	D	941	LEU
1	D	1024	LEU
1	D	1064	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	338	HIS
1	A	381	GLN
1	A	446	HIS
1	A	451	ASN
1	A	454	HIS
1	A	506	ASN
1	A	509	GLN
1	A	525	ASN
1	A	560	HIS
1	A	594	HIS
1	A	646	GLN
1	A	684	HIS
1	A	800	HIS
1	A	973	HIS
1	A	1135	ASN
1	A	1461	ASN
1	A	1502	HIS
1	B	137	GLN
1	B	338	HIS
1	B	381	GLN
1	B	446	HIS
1	B	451	ASN
1	B	454	HIS
1	B	506	ASN
1	B	509	GLN
1	B	525	ASN
1	B	560	HIS
1	B	594	HIS
1	B	646	GLN
1	B	684	HIS
1	B	800	HIS
1	B	973	HIS
1	B	1135	ASN
1	B	1461	ASN
1	B	1502	HIS
1	C	137	GLN
1	C	338	HIS
1	C	381	GLN
1	C	446	HIS
1	C	451	ASN
1	C	454	HIS
1	C	506	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	509	GLN
1	C	525	ASN
1	C	560	HIS
1	C	594	HIS
1	C	646	GLN
1	C	684	HIS
1	C	800	HIS
1	C	973	HIS
1	C	1135	ASN
1	C	1461	ASN
1	C	1502	HIS
1	D	137	GLN
1	D	338	HIS
1	D	381	GLN
1	D	446	HIS
1	D	454	HIS
1	D	506	ASN
1	D	509	GLN
1	D	525	ASN
1	D	560	HIS
1	D	594	HIS
1	D	646	GLN
1	D	684	HIS
1	D	973	HIS
1	D	1135	ASN
1	D	1461	ASN
1	D	1502	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9134. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.