Full wwPDB EM Validation Report

Dec 10, 2022 – 11:55 pm GMT

PDB ID	:	6R7F
EMDB ID	:	EMD-4739
Title	:	Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors	:	Faull, S.V.; Lau, A.M.C.; Martens, C.; Ahdash, Z.; Yebenes, H.; Schmidt, C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.
Deposited on	:	2019-03-28
Resolution	:	8.20 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:

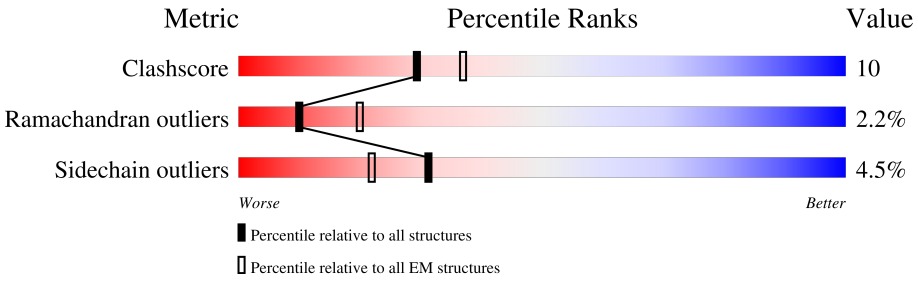
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 8.20 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.



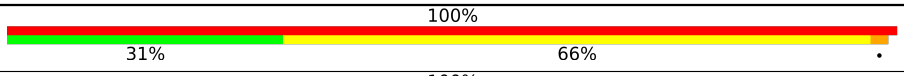
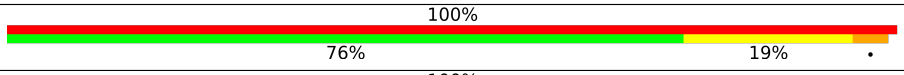
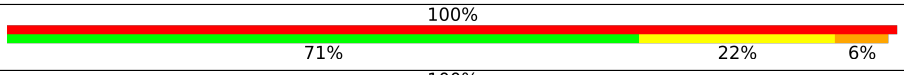
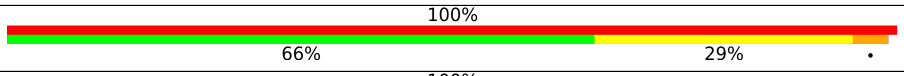
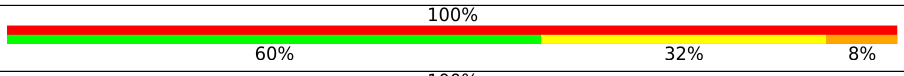
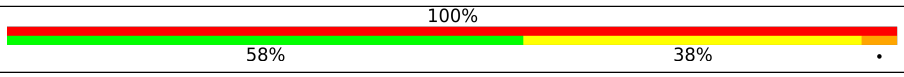
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	100% 76% 21% ·
2	B	443	93% 63% 24% 6% 7%
3	C	403	100% 73% 23% ·
4	D	406	100% 78% 18% · ·
5	E	311	100% 71% 21% 7% ·
6	F	288	100% 74% 21% · ·
7	H	209	80% 60% 17% · 20%
8	G	208	100% 80% 15% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	V	160	
10	P	118	
11	Q	112	
12	O	745	
13	R	90	
14	N	76	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31558 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3450	2174	605	649	22	0	0

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	414	3386	2149	579	643	15	0	0

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	403	3205	2040	537	601	27	0	0

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	406	3251	2047	566	622	16	0	0

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	311	2472	1575	412	471	14	0	0

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	288	2280	1452	379	434	15	0	0

- Molecule 7 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	168	Total	C	N	O	S	0	0
			1340	859	232	245	4		

- Molecule 8 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	208	Total	C	N	O	S	0	0
			1645	1039	279	321	6		

- Molecule 9 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	160	Total	C	N	O	S	0	0
			1308	824	245	235	4		

- Molecule 10 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	118	Total	C	N	O	S	0	0
			921	575	156	185	5		

- Molecule 11 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	112	Total	C	N	O	S	0	0
			873	553	139	173	8		

- Molecule 12 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	744	Total	C	N	O	S	0	0
			6090	3869	1029	1146	46		

- Molecule 13 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	90	Total	C	N	O	S	0	0
			746	472	137	128	9		

- Molecule 14 is a protein called NEDD8.

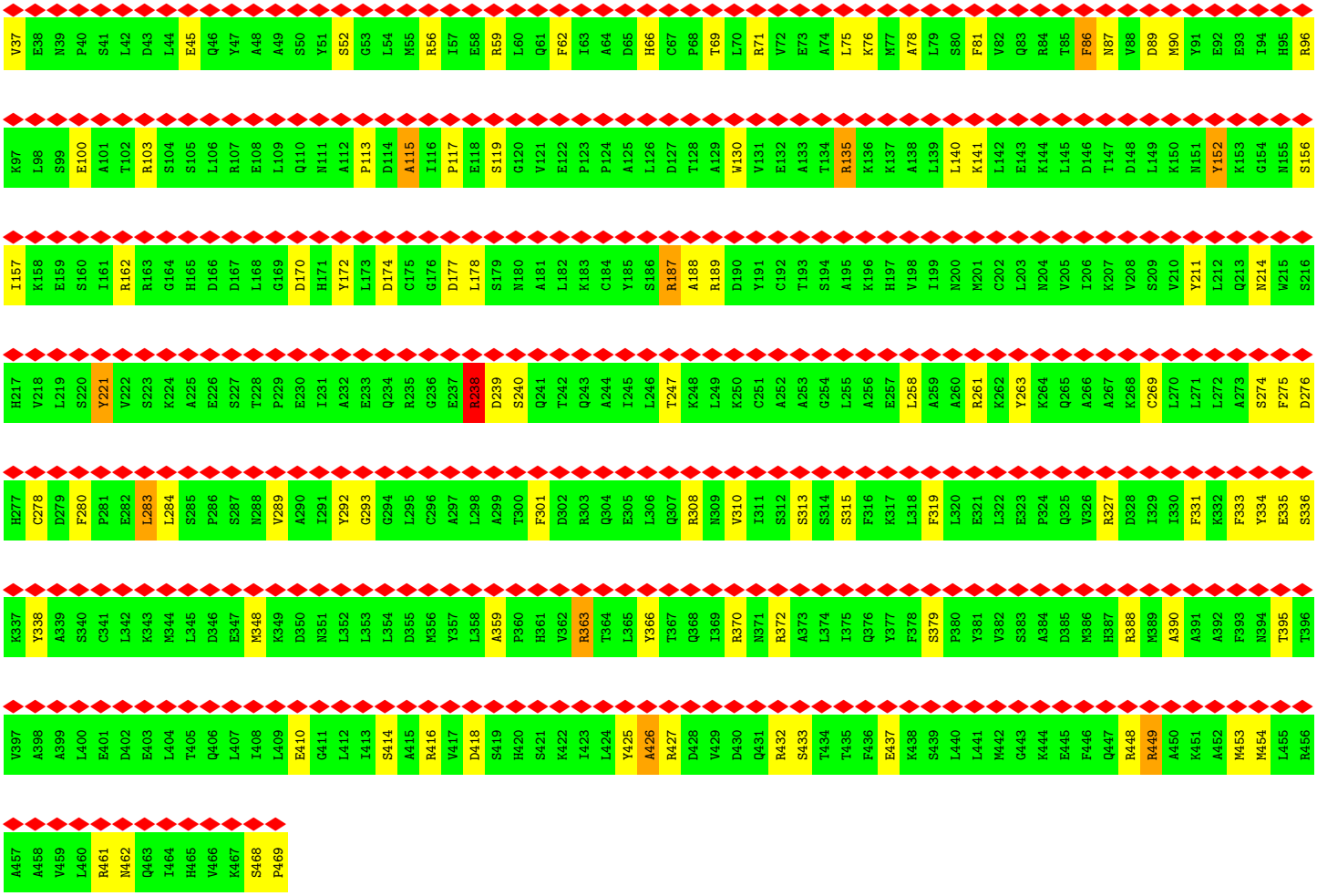
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	76	Total	C	N	O	S	0	0
			591	372	102	115	2		

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

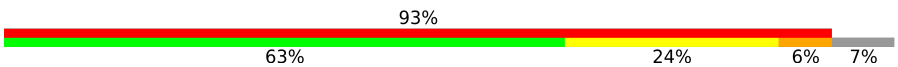
• Molecule 1: COP9 signalosome complex subunit 1

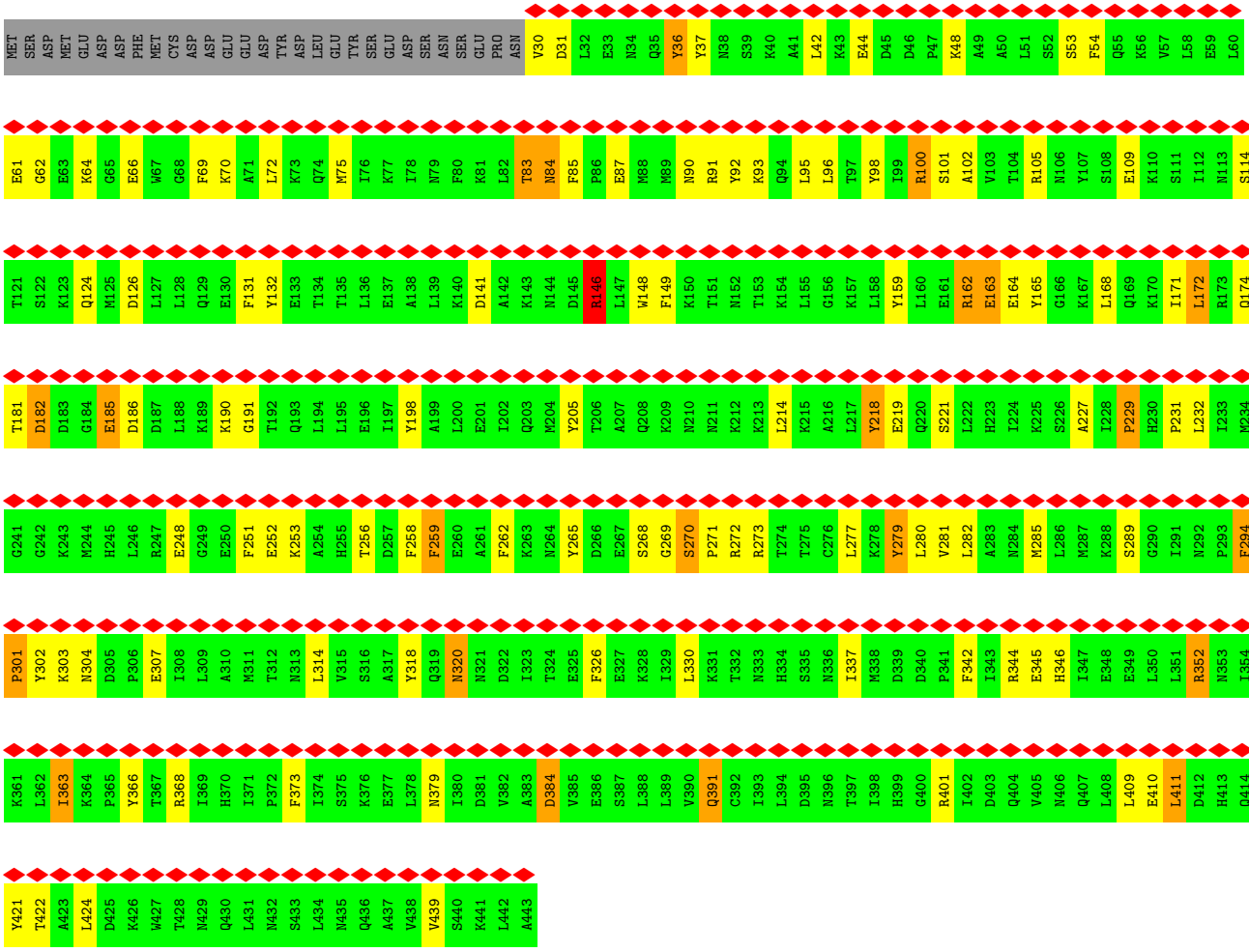
Chain A:



• Molecule 2: COP9 signalosome complex subunit 2

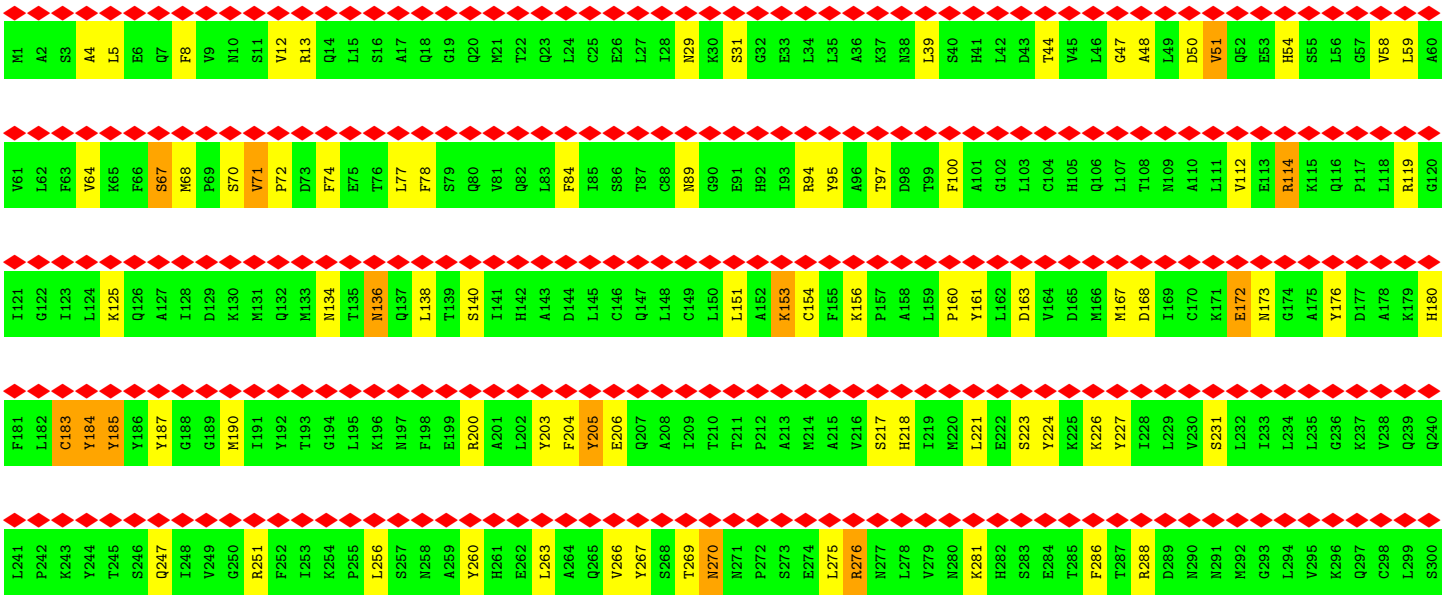
Chain B:

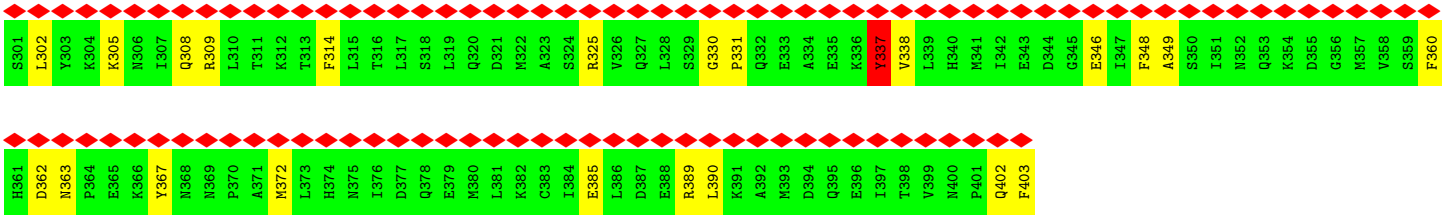




• Molecule 3: COP9 signalosome complex subunit 3

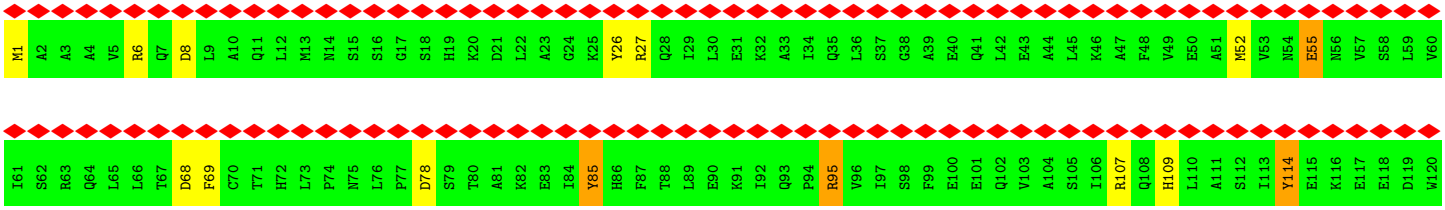
Chain C:





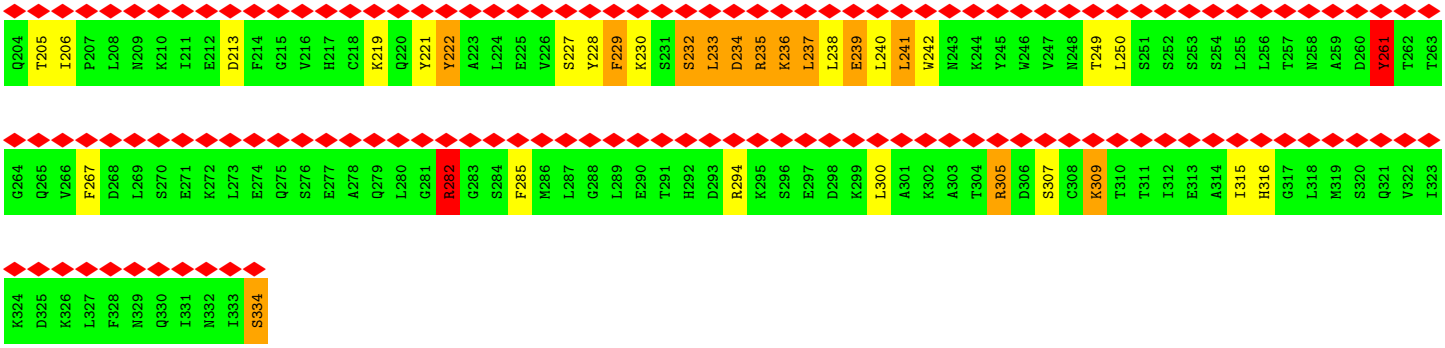
• Molecule 4: COP9 signalosome complex subunit 4

Chain D:



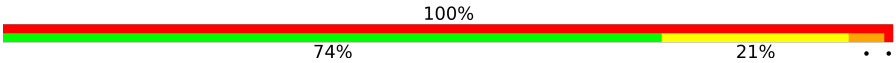
• Molecule 5: COP9 signalosome complex subunit 5

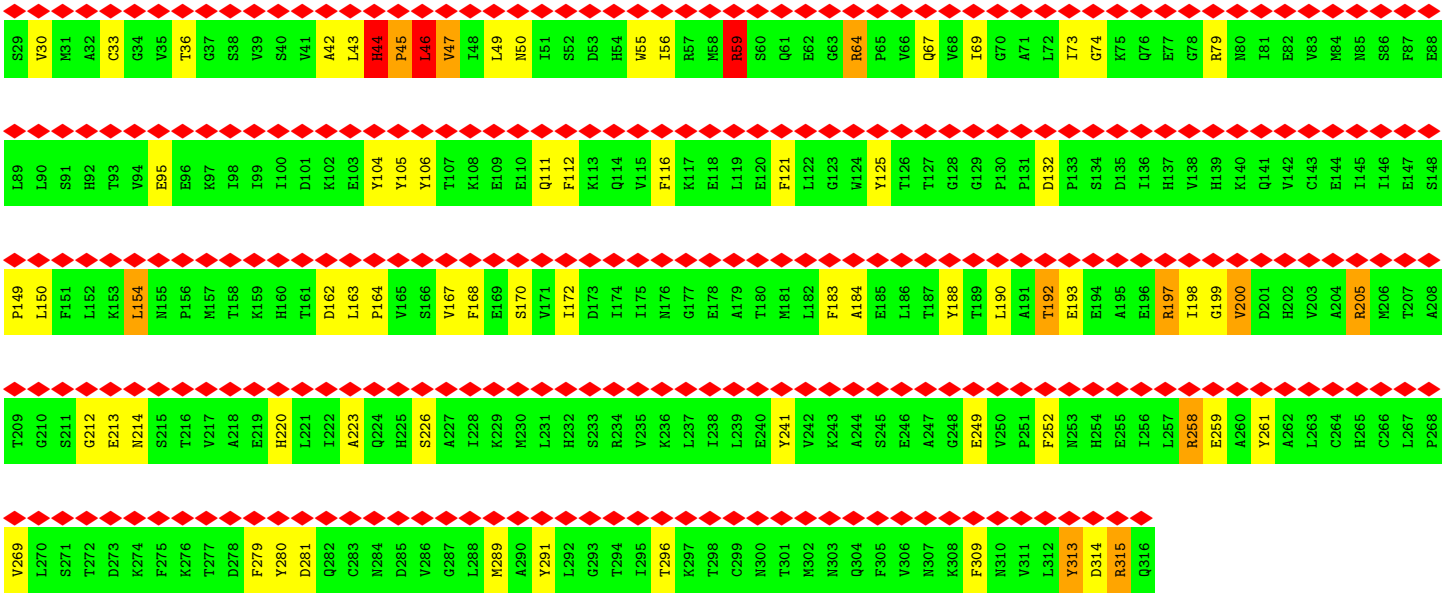
Chain E:



• Molecule 6: COP9 signalosome complex subunit 6

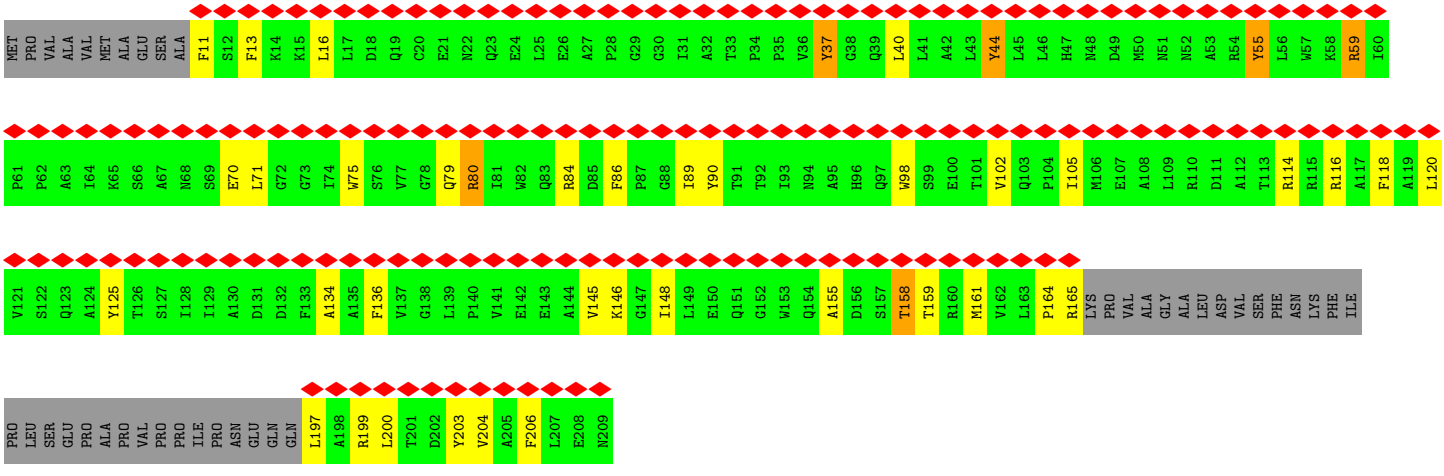
Chain F:





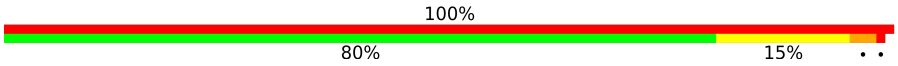
• Molecule 7: COP9 signalosome complex subunit 8

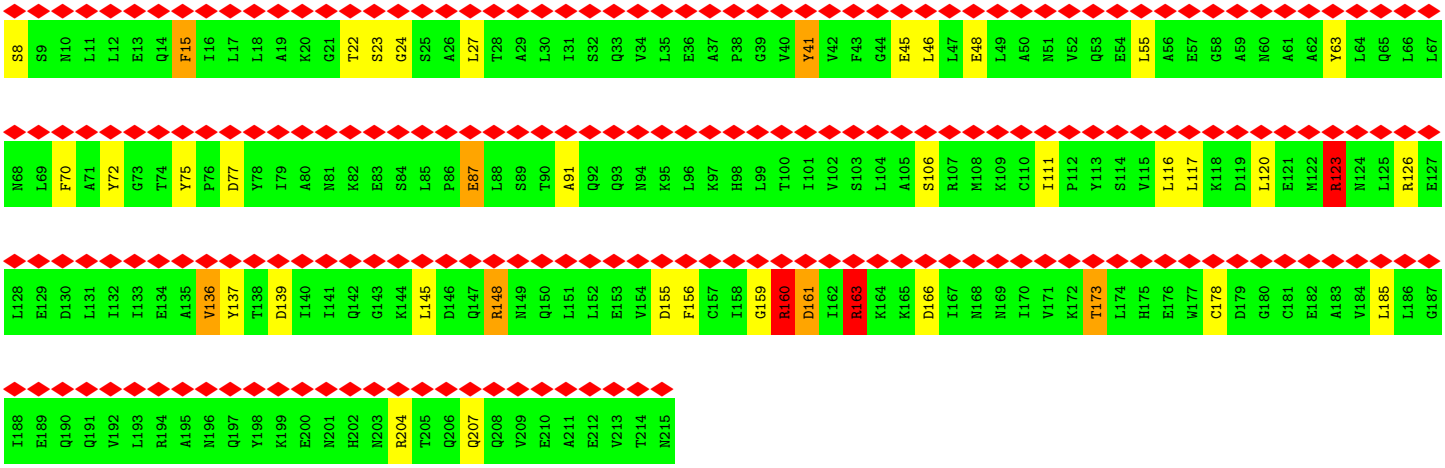
Chain H:



• Molecule 8: COP9 signalosome complex subunit 7b

Chain G:



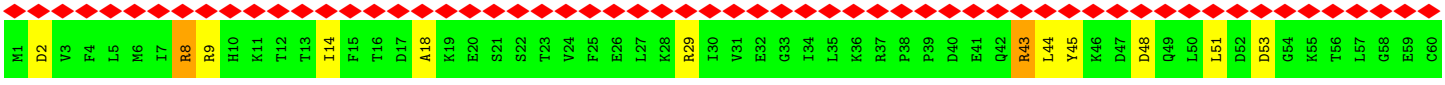


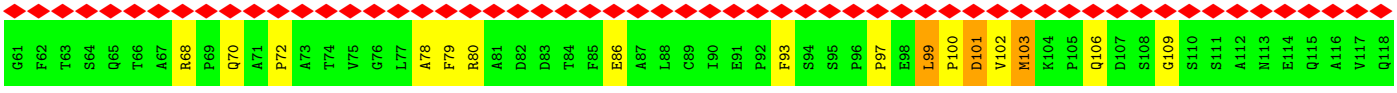
• Molecule 9: von Hippel-Lindau disease tumor suppressor

Chain V:

• Molecule 10: Elongin-B

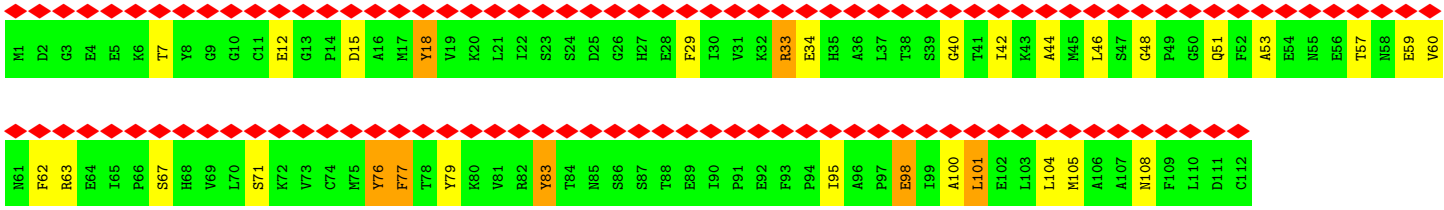
Chain P:





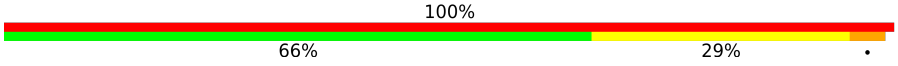
• Molecule 11: Elongin-C

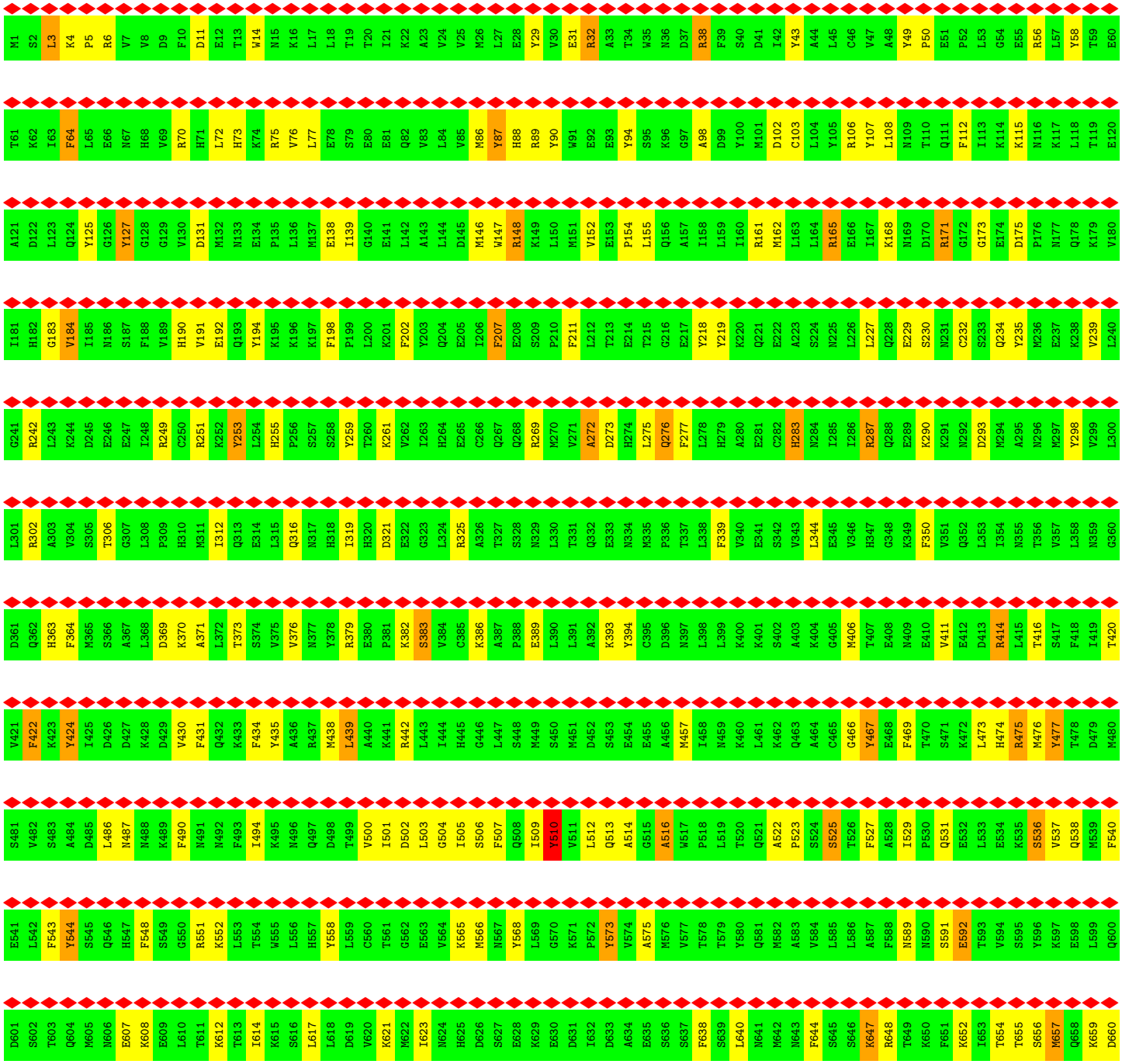
Chain Q:

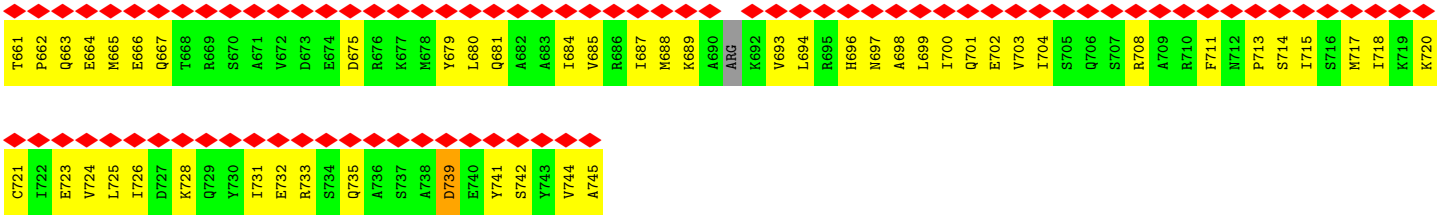


• Molecule 12: Cullin-2

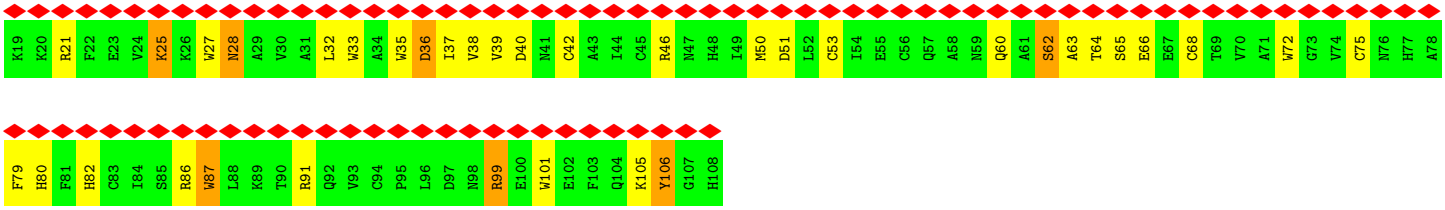
Chain O:



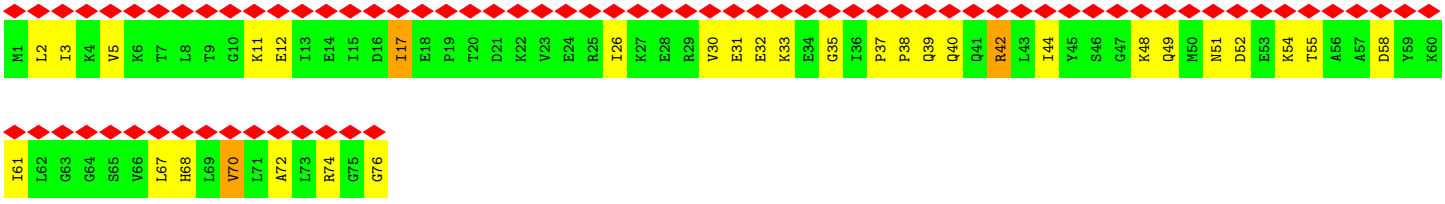




• Molecule 13: E3 ubiquitin-protein ligase RBX1



• Molecule 14: NEDD8



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	17.442	Depositor
Minimum map value	-4.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.70	38/3509 (1.1%)	1.85	69/4733 (1.5%)
2	B	2.07	30/3444 (0.9%)	1.94	86/4634 (1.9%)
3	C	1.63	20/3264 (0.6%)	1.85	65/4407 (1.5%)
4	D	1.69	31/3303 (0.9%)	1.87	71/4460 (1.6%)
5	E	2.67	31/2526 (1.2%)	1.94	64/3411 (1.9%)
6	F	1.68	15/2327 (0.6%)	1.99	56/3153 (1.8%)
7	H	1.71	14/1372 (1.0%)	1.91	29/1865 (1.6%)
8	G	1.60	7/1665 (0.4%)	1.90	30/2253 (1.3%)
9	V	1.05	0/1341	1.07	0/1824
10	P	1.75	8/938 (0.9%)	1.93	21/1267 (1.7%)
11	Q	1.72	8/892 (0.9%)	1.82	19/1204 (1.6%)
12	O	1.60	37/6207 (0.6%)	1.84	131/8358 (1.6%)
13	R	2.63	12/768 (1.6%)	1.93	20/1040 (1.9%)
14	N	0.36	0/596	0.56	0/800
All	All	1.80	251/32152 (0.8%)	1.84	661/43409 (1.5%)

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	12
2	B	0	15
3	C	0	6
4	D	0	10
5	E	0	10
6	F	0	7
7	H	0	7
8	G	0	9
10	P	0	2
11	Q	0	5
12	O	0	17

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	R	0	2
All	All	0	102

All (251) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	309	LYS	CA-CB	85.10	3.41	1.53
2	B	294	PHE	CA-C	70.42	3.36	1.52
5	E	203	TYR	CE1-CZ	26.85	1.73	1.38
5	E	203	TYR	CG-CD2	26.55	1.73	1.39
13	R	106	TYR	CG-CD2	26.45	1.73	1.39
5	E	203	TYR	CE2-CZ	26.29	1.72	1.38
13	R	106	TYR	CE2-CZ	26.03	1.72	1.38
13	R	106	TYR	CG-CD1	23.80	1.70	1.39
5	E	203	TYR	CG-CD1	23.06	1.69	1.39
13	R	106	TYR	CE1-CZ	21.68	1.66	1.38
13	R	106	TYR	CD1-CE1	21.12	1.71	1.39
5	E	203	TYR	CD1-CE1	20.54	1.70	1.39
5	E	203	TYR	CD2-CE2	19.39	1.68	1.39
13	R	106	TYR	CD2-CE2	19.39	1.68	1.39
11	Q	71	SER	CA-CB	9.10	1.66	1.52
10	P	86	GLU	CD-OE1	8.56	1.35	1.25
6	F	45	PRO	CA-C	8.55	1.70	1.52
3	C	223	SER	CA-CB	8.38	1.65	1.52
1	A	269	CYS	CB-SG	8.09	1.96	1.82
5	E	261	TYR	CE2-CZ	8.04	1.49	1.38
1	A	103	ARG	CD-NE	8.04	1.60	1.46
2	B	37	TYR	CG-CD1	8.03	1.49	1.39
11	Q	40	GLY	N-CA	-7.78	1.34	1.46
2	B	401	ARG	CZ-NH2	7.77	1.43	1.33
1	A	96	ARG	CD-NE	7.72	1.59	1.46
2	B	159	TYR	CE2-CZ	7.43	1.48	1.38
2	B	164	GLU	CG-CD	7.42	1.63	1.51
10	P	9	ARG	CZ-NH1	7.40	1.42	1.33
7	H	44	TYR	CE1-CZ	7.36	1.48	1.38
4	D	121	ARG	NE-CZ	7.29	1.42	1.33
1	A	319	PHE	CG-CD1	7.28	1.49	1.38
1	A	156	SER	CA-CB	7.27	1.63	1.52
5	E	233	LEU	C-N	7.27	1.50	1.34
8	G	41	TYR	CG-CD2	7.27	1.48	1.39
4	D	274	ARG	NE-CZ	7.17	1.42	1.33
12	O	192	GLU	CD-OE2	7.09	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	92	TYR	CG-CD2	7.06	1.48	1.39
3	C	338	VAL	CB-CG1	7.06	1.67	1.52
2	B	302	TYR	CG-CD2	7.06	1.48	1.39
2	B	114	SER	CA-CB	7.05	1.63	1.52
1	A	461	ARG	CZ-NH1	7.04	1.42	1.33
2	B	273	ARG	NE-CZ	7.03	1.42	1.33
6	F	74	GLY	CA-C	-7.00	1.40	1.51
1	A	449	ARG	NE-CZ	6.99	1.42	1.33
13	R	86	ARG	NE-CZ	6.98	1.42	1.33
6	F	106	TYR	CE1-CZ	6.98	1.47	1.38
7	H	13	PHE	CG-CD2	6.91	1.49	1.38
1	A	119	SER	CA-CB	6.89	1.63	1.52
2	B	252	GLU	CB-CG	6.84	1.65	1.52
5	E	187	ARG	CD-NE	6.80	1.58	1.46
4	D	302	ARG	NE-CZ	6.76	1.41	1.33
1	A	410	GLU	CD-OE2	6.75	1.33	1.25
4	D	170	ARG	NE-CZ	6.73	1.41	1.33
12	O	249	ARG	CZ-NH1	6.72	1.41	1.33
12	O	302	ARG	NE-CZ	6.70	1.41	1.33
4	D	364	ARG	CD-NE	6.67	1.57	1.46
2	B	294	PHE	CA-CB	6.67	1.68	1.53
1	A	433	SER	CA-CB	6.67	1.62	1.52
6	F	309	PHE	CG-CD2	6.66	1.48	1.38
12	O	302	ARG	CD-NE	6.62	1.57	1.46
12	O	161	ARG	CD-NE	6.57	1.57	1.46
5	E	228	TYR	CE1-CZ	6.55	1.47	1.38
3	C	205	TYR	CG-CD1	6.55	1.47	1.39
6	F	45	PRO	N-CD	6.55	1.57	1.47
3	C	95	TYR	CE1-CZ	6.52	1.47	1.38
5	E	115	GLU	CG-CD	6.50	1.61	1.51
3	C	331	PRO	N-CD	6.50	1.56	1.47
5	E	234	ASP	CA-C	6.49	1.69	1.52
6	F	79	ARG	CZ-NH2	6.47	1.41	1.33
12	O	506	SER	CA-CB	6.46	1.62	1.52
8	G	8	SER	CA-CB	6.44	1.62	1.52
12	O	422	PHE	CG-CD2	6.42	1.48	1.38
7	H	98	TRP	CB-CG	6.42	1.61	1.50
13	R	99	ARG	CZ-NH2	6.42	1.41	1.33
12	O	229	GLU	CG-CD	6.41	1.61	1.51
12	O	287	ARG	CZ-NH2	6.38	1.41	1.33
1	A	363	ARG	CD-NE	6.29	1.57	1.46
2	B	218	TYR	CE1-CZ	6.29	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	98	TRP	CD2-CE3	-6.28	1.30	1.40
12	O	525	SER	CA-CB	6.21	1.62	1.52
10	P	68	ARG	NE-CZ	6.19	1.41	1.33
2	B	92	TYR	CE2-CZ	6.19	1.46	1.38
12	O	31	GLU	CG-CD	6.16	1.61	1.51
10	P	80	ARG	NE-CZ	6.16	1.41	1.33
1	A	56	ARG	CZ-NH1	6.16	1.41	1.33
3	C	231	SER	CA-CB	6.14	1.62	1.52
7	H	165	ARG	CZ-NH1	6.14	1.41	1.33
3	C	114	ARG	CZ-NH2	6.13	1.41	1.33
5	E	221	TYR	CG-CD1	6.12	1.47	1.39
8	G	87	GLU	CG-CD	6.11	1.61	1.51
3	C	187	TYR	CG-CD1	6.11	1.47	1.39
1	A	333	PHE	CG-CD2	6.09	1.47	1.38
13	R	86	ARG	CZ-NH1	6.07	1.41	1.33
4	D	222	ARG	CZ-NH1	6.06	1.41	1.33
4	D	187	TYR	CG-CD2	6.04	1.47	1.39
1	A	135	ARG	CZ-NH1	6.03	1.40	1.33
2	B	318	TYR	CG-CD2	6.01	1.47	1.39
13	R	91	ARG	CA-CB	6.00	1.67	1.53
4	D	244	ARG	CZ-NH2	5.99	1.40	1.33
4	D	199	ARG	NE-CZ	5.98	1.40	1.33
11	Q	67	SER	CA-CB	5.97	1.61	1.52
1	A	416	ARG	NE-CZ	5.96	1.40	1.33
7	H	164	PRO	CA-C	-5.96	1.41	1.52
1	A	448	ARG	NE-CZ	5.95	1.40	1.33
7	H	44	TYR	CZ-OH	5.94	1.48	1.37
12	O	544	TYR	CG-CD1	5.92	1.46	1.39
4	D	170	ARG	CD-NE	5.92	1.56	1.46
4	D	95	ARG	CZ-NH1	5.91	1.40	1.33
11	Q	79	TYR	CE2-CZ	5.90	1.46	1.38
6	F	162	ASP	CB-CG	5.90	1.64	1.51
11	Q	18	TYR	CG-CD1	5.89	1.46	1.39
2	B	100	ARG	NE-CZ	5.88	1.40	1.33
1	A	414	SER	CA-CB	5.88	1.61	1.52
6	F	226	SER	CA-CB	5.87	1.61	1.52
6	F	64	ARG	CZ-NH2	5.85	1.40	1.33
12	O	165	ARG	CZ-NH2	5.83	1.40	1.33
12	O	325	ARG	CZ-NH1	5.83	1.40	1.33
4	D	347	ARG	NE-CZ	5.82	1.40	1.33
5	E	54	TYR	CE2-CZ	5.82	1.46	1.38
5	E	51	TYR	CD2-CE2	5.81	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	389	ARG	NE-CZ	5.80	1.40	1.33
5	E	230	LYS	C-N	5.80	1.47	1.34
1	A	315	SER	CA-CB	5.78	1.61	1.52
1	A	308	ARG	CZ-NH1	5.75	1.40	1.33
7	H	203	TYR	CE2-CZ	5.74	1.46	1.38
1	A	187	ARG	CZ-NH2	5.73	1.40	1.33
12	O	147	TRP	CB-CG	5.73	1.60	1.50
5	E	136	TRP	CD2-CE2	5.72	1.48	1.41
5	E	85	VAL	N-CA	-5.70	1.34	1.46
12	O	573	TYR	CB-CG	-5.69	1.43	1.51
5	E	55	CYS	CB-SG	5.68	1.92	1.82
10	P	109	GLY	CA-C	-5.67	1.42	1.51
2	B	289	SER	CA-CB	5.64	1.61	1.52
1	A	427	ARG	NE-CZ	5.63	1.40	1.33
5	E	174	ARG	NE-CZ	5.63	1.40	1.33
11	Q	34	GLU	CG-CD	5.63	1.60	1.51
4	D	55	GLU	CD-OE1	5.63	1.31	1.25
3	C	276	ARG	CZ-NH2	5.62	1.40	1.33
7	H	165	ARG	CD-NE	5.62	1.56	1.46
12	O	232	CYS	CB-SG	5.62	1.91	1.82
12	O	38	ARG	CZ-NH1	5.61	1.40	1.33
5	E	120	TYR	CA-CB	5.59	1.66	1.53
7	H	116	ARG	CZ-NH2	5.58	1.40	1.33
12	O	107	TYR	CG-CD2	5.58	1.46	1.39
4	D	69	PHE	CG-CD2	5.58	1.47	1.38
6	F	170	SER	CA-CB	5.58	1.61	1.52
4	D	197	TYR	CG-CD1	5.57	1.46	1.39
4	D	27	ARG	NE-CZ	5.56	1.40	1.33
2	B	219	GLU	N-CA	5.56	1.57	1.46
10	P	43	ARG	CZ-NH2	5.55	1.40	1.33
6	F	59	ARG	CD-NE	5.54	1.55	1.46
2	B	132	TYR	CE2-CZ	5.53	1.45	1.38
3	C	140	SER	CA-CB	5.52	1.61	1.52
4	D	336	GLU	CG-CD	5.51	1.60	1.51
4	D	133	GLU	CD-OE1	5.50	1.31	1.25
3	C	172	GLU	CD-OE2	5.49	1.31	1.25
12	O	6	ARG	CD-NE	5.49	1.55	1.46
4	D	316	TYR	CD2-CE2	5.48	1.47	1.39
3	C	84	PHE	CG-CD1	5.47	1.47	1.38
13	R	62	SER	CA-CB	5.47	1.61	1.52
1	A	366	TYR	CG-CD1	5.46	1.46	1.39
4	D	376	SER	CA-CB	5.46	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	56	ARG	CZ-NH1	5.46	1.40	1.33
5	E	193	TYR	CB-CG	5.45	1.59	1.51
1	A	52	SER	C-N	5.43	1.42	1.33
6	F	281	ASP	CA-CB	5.42	1.65	1.53
12	O	383	SER	CA-CB	5.42	1.61	1.52
12	O	523	PRO	N-CD	-5.41	1.40	1.47
3	C	31	SER	CA-CB	5.40	1.61	1.52
2	B	238	ARG	CZ-NH2	5.39	1.40	1.33
12	O	207	PHE	CE1-CZ	5.39	1.47	1.37
12	O	475	ARG	CZ-NH1	5.38	1.40	1.33
5	E	239	GLU	CG-CD	5.38	1.60	1.51
12	O	70	ARG	CD-NE	5.37	1.55	1.46
3	C	47	GLY	CA-C	-5.36	1.43	1.51
2	B	272	ARG	NE-CZ	5.35	1.40	1.33
2	B	272	ARG	CZ-NH2	5.34	1.40	1.33
1	A	335	GLU	CD-OE2	5.34	1.31	1.25
5	E	222	TYR	CB-CG	5.32	1.59	1.51
12	O	269	ARG	NE-CZ	5.31	1.40	1.33
5	E	294	ARG	NE-CZ	5.31	1.40	1.33
8	G	207	GLN	N-CA	-5.29	1.35	1.46
2	B	164	GLU	CA-CB	5.29	1.65	1.53
2	B	205	TYR	CE1-CZ	5.29	1.45	1.38
11	Q	79	TYR	CZ-OH	5.29	1.46	1.37
5	E	221	TYR	CE2-CZ	5.28	1.45	1.38
7	H	59	ARG	NE-CZ	5.27	1.39	1.33
10	P	68	ARG	CD-NE	5.26	1.55	1.46
12	O	510	TYR	CZ-OH	5.26	1.46	1.37
7	H	114	ARG	CZ-NH1	5.26	1.39	1.33
3	C	346	GLU	CB-CG	5.25	1.62	1.52
12	O	87	TYR	CE2-CZ	5.25	1.45	1.38
7	H	84	ARG	NE-CZ	5.24	1.39	1.33
7	H	70	GLU	CB-CG	5.24	1.62	1.52
1	A	162	ARG	CZ-NH2	5.22	1.39	1.33
3	C	288	ARG	CZ-NH2	5.22	1.39	1.33
12	O	251	ARG	CZ-NH1	5.22	1.39	1.33
5	E	221	TYR	CB-CG	5.22	1.59	1.51
1	A	338	TYR	CE2-CZ	5.21	1.45	1.38
12	O	516	ALA	CA-CB	5.21	1.63	1.52
4	D	203	GLU	CD-OE2	5.20	1.31	1.25
4	D	143	TYR	CG-CD2	5.20	1.46	1.39
6	F	197	ARG	NE-CZ	5.20	1.39	1.33
6	F	33	CYS	C-N	5.19	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	251	PHE	CB-CG	-5.19	1.42	1.51
4	D	85	TYR	CG-CD1	5.19	1.45	1.39
3	C	67	SER	CA-CB	5.19	1.60	1.52
4	D	316	TYR	CE2-CZ	5.19	1.45	1.38
12	O	32	ARG	CZ-NH2	5.19	1.39	1.33
4	D	401	GLU	CG-CD	5.18	1.59	1.51
1	A	71	ARG	CD-NE	5.18	1.55	1.46
1	A	293	GLY	CA-C	-5.18	1.43	1.51
4	D	170	ARG	CZ-NH2	5.18	1.39	1.33
8	G	163	ARG	CZ-NH1	5.17	1.39	1.33
3	C	309	ARG	CZ-NH1	5.17	1.39	1.33
13	R	46	ARG	CZ-NH2	5.17	1.39	1.33
1	A	240	SER	CA-CB	5.16	1.60	1.52
12	O	43	TYR	CE1-CZ	5.15	1.45	1.38
11	Q	18	TYR	CZ-OH	5.15	1.46	1.37
1	A	313	SER	CB-OG	-5.13	1.35	1.42
1	A	100	GLU	N-CA	-5.12	1.36	1.46
4	D	323	GLU	CG-CD	5.12	1.59	1.51
1	A	86	PHE	CE2-CZ	5.11	1.47	1.37
5	E	136	TRP	CD1-NE1	5.11	1.46	1.38
6	F	315	ARG	NE-CZ	5.10	1.39	1.33
2	B	36	TYR	CE1-CZ	5.09	1.45	1.38
3	C	78	PHE	CB-CG	-5.08	1.42	1.51
1	A	426	ALA	C-N	5.08	1.45	1.34
8	G	148	ARG	CD-NE	5.08	1.55	1.46
1	A	334	TYR	CE2-CZ	5.08	1.45	1.38
5	E	106	ARG	CZ-NH1	5.08	1.39	1.33
12	O	38	ARG	NE-CZ	5.08	1.39	1.33
1	A	45	GLU	CG-CD	5.07	1.59	1.51
2	B	345	GLU	N-CA	-5.06	1.36	1.46
1	A	469	PRO	N-CD	5.06	1.54	1.47
8	G	55	LEU	CA-CB	5.05	1.65	1.53
2	B	109	GLU	CB-CG	5.05	1.61	1.52
12	O	591	SER	CA-CB	5.04	1.60	1.52
4	D	321	PHE	CG-CD2	5.04	1.46	1.38
12	O	504	GLY	N-CA	5.03	1.53	1.46
4	D	311	SER	CA-CB	5.03	1.60	1.52
12	O	259	TYR	CE1-CZ	5.02	1.45	1.38
1	A	437	GLU	CG-CD	5.02	1.59	1.51
5	E	143	TYR	CD1-CE1	5.02	1.46	1.39
2	B	91	ARG	CD-NE	5.02	1.54	1.46
10	P	68	ARG	CZ-NH1	5.02	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	416	ARG	CZ-NH2	5.01	1.39	1.33
1	A	372	ARG	NE-CZ	5.01	1.39	1.33
2	B	273	ARG	CZ-NH1	5.01	1.39	1.33
4	D	95	ARG	CZ-NH2	5.01	1.39	1.33
4	D	363	THR	N-CA	-5.01	1.36	1.46

All (661) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	98	TYR	CB-CG-CD2	-18.83	109.70	121.00
6	F	205	ARG	NE-CZ-NH1	-16.75	111.93	120.30
4	D	6	ARG	NE-CZ-NH2	-16.17	112.22	120.30
6	F	45	PRO	N-CA-C	15.86	153.33	112.10
12	O	87	TYR	CB-CG-CD2	-15.76	111.55	121.00
8	G	123	ARG	NE-CZ-NH2	-15.56	112.52	120.30
12	O	6	ARG	NE-CZ-NH1	15.39	128.00	120.30
3	C	286	PHE	CB-CG-CD1	15.09	131.36	120.80
6	F	205	ARG	NE-CZ-NH2	13.88	127.24	120.30
12	O	253	TYR	CB-CG-CD2	-13.87	112.68	121.00
12	O	269	ARG	NE-CZ-NH2	13.34	126.97	120.30
12	O	6	ARG	NE-CZ-NH2	-13.26	113.67	120.30
12	O	424	TYR	CB-CG-CD2	-13.17	113.10	121.00
1	A	96	ARG	NE-CZ-NH1	12.49	126.55	120.30
6	F	44	HIS	N-CA-CB	-12.48	88.14	110.60
7	H	55	TYR	CB-CG-CD1	-12.44	113.54	121.00
3	C	325	ARG	NE-CZ-NH1	12.42	126.51	120.30
5	E	137	TYR	CB-CG-CD1	-12.11	113.74	121.00
5	E	52	PHE	CB-CG-CD1	-11.89	112.48	120.80
2	B	279	TYR	CB-CG-CD1	11.86	128.12	121.00
4	D	121	ARG	NE-CZ-NH1	11.81	126.20	120.30
2	B	279	TYR	CB-CG-CD2	-11.79	113.92	121.00
3	C	161	TYR	CB-CG-CD1	11.79	128.07	121.00
12	O	253	TYR	CB-CG-CD1	11.54	127.92	121.00
12	O	148	ARG	NE-CZ-NH2	-11.53	114.53	120.30
6	F	64	ARG	NE-CZ-NH2	-11.47	114.56	120.30
7	H	86	PHE	CB-CG-CD1	11.45	128.81	120.80
12	O	43	TYR	CB-CG-CD2	-11.42	114.14	121.00
12	O	435	TYR	CB-CG-CD2	-11.40	114.16	121.00
6	F	44	HIS	CA-CB-CG	11.39	132.96	113.60
12	O	431	PHE	CB-CG-CD2	11.31	128.71	120.80
4	D	26	TYR	CB-CG-CD2	-11.23	114.26	121.00
4	D	254	ARG	NE-CZ-NH1	11.13	125.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	303	ALA	N-CA-CB	11.05	125.58	110.10
1	A	301	PHE	CB-CG-CD1	10.98	128.49	120.80
4	D	26	TYR	CB-CG-CD1	10.86	127.52	121.00
2	B	159	TYR	CB-CG-CD2	-10.78	114.53	121.00
3	C	161	TYR	CB-CG-CD2	-10.74	114.55	121.00
4	D	271	ARG	NE-CZ-NH2	-10.72	114.94	120.30
12	O	287	ARG	NE-CZ-NH2	-10.68	114.96	120.30
2	B	420	ARG	NE-CZ-NH1	10.67	125.64	120.30
3	C	200	ARG	NE-CZ-NH1	-10.56	115.02	120.30
12	O	431	PHE	CB-CG-CD1	-10.48	113.46	120.80
12	O	467	TYR	CB-CG-CD2	-10.47	114.72	121.00
2	B	85	PHE	CB-CG-CD1	-10.39	113.53	120.80
6	F	64	ARG	NE-CZ-NH1	10.28	125.44	120.30
10	P	29	ARG	NE-CZ-NH1	10.23	125.42	120.30
6	F	241	TYR	CB-CG-CD2	10.20	127.12	121.00
2	B	262	PHE	CB-CG-CD2	10.18	127.92	120.80
8	G	15	PHE	CB-CG-CD2	-10.17	113.68	120.80
2	B	416	ARG	NE-CZ-NH2	-10.17	115.22	120.30
3	C	163	ASP	CB-CG-OD2	-10.17	109.15	118.30
3	C	286	PHE	CB-CG-CD2	-10.15	113.70	120.80
10	P	53	ASP	CB-CG-OD2	10.07	127.36	118.30
2	B	85	PHE	CB-CG-CD2	10.05	127.84	120.80
7	H	55	TYR	CB-CG-CD2	10.04	127.02	121.00
12	O	442	ARG	NE-CZ-NH1	9.97	125.28	120.30
3	C	8	PHE	CB-CG-CD2	-9.94	113.84	120.80
6	F	241	TYR	CB-CG-CD1	-9.92	115.05	121.00
5	E	282	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	A	301	PHE	CB-CG-CD2	-9.89	113.88	120.80
6	F	44	HIS	CA-C-N	9.89	144.78	117.10
2	B	146	ARG	NE-CZ-NH2	-9.85	115.37	120.30
12	O	259	TYR	CB-CG-CD2	-9.80	115.12	121.00
2	B	344	ARG	NE-CZ-NH1	9.74	125.17	120.30
12	O	269	ARG	NE-CZ-NH1	-9.73	115.44	120.30
2	B	294	PHE	O-C-N	-9.66	107.24	122.70
12	O	112	PHE	CB-CG-CD1	9.66	127.56	120.80
4	D	199	ARG	NE-CZ-NH2	9.65	125.12	120.30
1	A	338	TYR	CB-CG-CD1	-9.57	115.26	121.00
1	A	71	ARG	NE-CZ-NH1	9.56	125.08	120.30
12	O	543	PHE	CB-CG-CD1	9.53	127.47	120.80
2	B	262	PHE	CB-CG-CD1	-9.47	114.17	120.80
1	A	115	ALA	N-CA-CB	9.47	123.36	110.10
11	Q	83	TYR	CB-CG-CD1	-9.41	115.35	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	285	MET	CG-SD-CE	-9.38	85.19	100.20
12	O	29	TYR	CB-CG-CD1	-9.35	115.39	121.00
8	G	123	ARG	NE-CZ-NH1	9.34	124.97	120.30
2	B	92	TYR	CB-CG-CD2	-9.31	115.42	121.00
10	P	2	ASP	CB-CG-OD2	-9.29	109.94	118.30
8	G	41	TYR	CB-CG-CD2	-9.24	115.45	121.00
8	G	15	PHE	CB-CG-CD1	9.20	127.24	120.80
4	D	243	SER	N-CA-CB	9.19	124.29	110.50
1	A	162	ARG	NE-CZ-NH1	9.15	124.87	120.30
10	P	43	ARG	NE-CZ-NH1	9.10	124.85	120.30
10	P	93	PHE	CB-CG-CD2	-9.07	114.45	120.80
8	G	156	PHE	CB-CG-CD1	9.04	127.13	120.80
5	E	309	LYS	CA-CB-CG	8.98	133.17	113.40
4	D	196	ASP	CB-CG-OD1	8.91	126.32	118.30
2	B	294	PHE	N-CA-CB	-8.89	94.61	110.60
1	A	96	ARG	NE-CZ-NH2	-8.87	115.87	120.30
13	R	51	ASP	CB-CG-OD1	8.84	126.25	118.30
3	C	348	PHE	CB-CG-CD1	8.79	126.96	120.80
12	O	302	ARG	NE-CZ-NH2	-8.79	115.91	120.30
4	D	8	ASP	CB-CG-OD1	-8.77	110.41	118.30
10	P	93	PHE	CB-CG-CD1	8.75	126.93	120.80
6	F	44	HIS	O-C-N	-8.75	104.47	121.10
4	D	351	PHE	CB-CG-CD2	8.63	126.84	120.80
12	O	171	ARG	NE-CZ-NH2	8.61	124.61	120.30
3	C	337	TYR	CB-CG-CD2	-8.52	115.89	121.00
2	B	401	ARG	NE-CZ-NH1	8.50	124.55	120.30
4	D	85	TYR	CB-CG-CD1	8.49	126.10	121.00
1	A	170	ASP	CB-CG-OD1	8.45	125.90	118.30
1	A	333	PHE	CB-CG-CD2	8.44	126.71	120.80
6	F	45	PRO	CA-C-N	8.42	135.72	117.20
1	A	62	PHE	CB-CG-CD1	8.40	126.68	120.80
13	R	91	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	B	98	TYR	CB-CG-CD1	8.35	126.01	121.00
2	B	162	ARG	NE-CZ-NH1	8.35	124.47	120.30
6	F	55	TRP	CB-CG-CD2	-8.31	115.79	126.60
1	A	59	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	C	184	TYR	CB-CG-CD2	-8.27	116.04	121.00
8	G	166	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	319	PHE	CB-CG-CD1	-8.20	115.06	120.80
4	D	8	ASP	CB-CG-OD2	8.19	125.67	118.30
7	H	84	ARG	NE-CZ-NH2	-8.19	116.21	120.30
11	Q	29	PHE	CB-CG-CD1	8.18	126.53	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	78	ALA	N-CA-CB	8.17	121.54	110.10
2	B	126	ASP	CB-CG-OD1	-8.16	110.95	118.30
12	O	568	TYR	CB-CG-CD2	8.16	125.90	121.00
3	C	260	TYR	CB-CG-CD2	8.16	125.89	121.00
6	F	55	TRP	CB-CG-CD1	8.15	137.59	127.00
12	O	394	TYR	CB-CG-CD2	-8.14	116.11	121.00
13	R	87	TRP	CB-CG-CD2	-8.14	116.02	126.60
5	E	232	SER	CA-C-N	8.11	135.04	117.20
5	E	235	ARG	NE-CZ-NH2	-8.10	116.25	120.30
12	O	644	PHE	CB-CG-CD2	8.08	126.46	120.80
3	C	8	PHE	CB-CG-CD1	8.08	126.46	120.80
5	E	116	TYR	CB-CG-CD2	-8.08	116.15	121.00
12	O	89	ARG	NE-CZ-NH1	8.06	124.33	120.30
3	C	260	TYR	CB-CG-CD1	-8.05	116.17	121.00
2	B	294	PHE	CB-CA-C	8.02	126.44	110.40
12	O	87	TYR	CB-CG-CD1	8.02	125.81	121.00
12	O	442	ARG	NE-CZ-NH2	-8.02	116.29	120.30
6	F	252	PHE	CB-CG-CD1	-8.01	115.19	120.80
6	F	252	PHE	CB-CG-CD2	8.01	126.41	120.80
7	H	136	PHE	CB-CG-CD2	8.00	126.40	120.80
12	O	558	TYR	CB-CG-CD1	7.97	125.78	121.00
4	D	78	ASP	CB-CG-OD2	7.96	125.46	118.30
5	E	309	LYS	CB-CA-C	7.94	126.28	110.40
1	A	388	ARG	NE-CZ-NH2	7.94	124.27	120.30
3	C	314	PHE	CB-CG-CD2	7.91	126.33	120.80
12	O	94	TYR	CB-CG-CD1	-7.87	116.28	121.00
12	O	544	TYR	CB-CG-CD2	-7.86	116.28	121.00
12	O	272	ALA	N-CA-CB	7.85	121.09	110.10
6	F	45	PRO	O-C-N	-7.84	110.15	122.70
1	A	261	ARG	NE-CZ-NH2	7.83	124.22	120.30
4	D	302	ARG	CA-C-N	7.82	134.41	117.20
5	E	309	LYS	N-CA-CB	7.82	124.67	110.60
1	A	363	ARG	NE-CZ-NH2	-7.80	116.40	120.30
6	F	45	PRO	N-CA-CB	-7.78	93.96	103.30
4	D	366	ALA	N-CA-CB	7.74	120.93	110.10
7	H	203	TYR	CB-CG-CD1	7.74	125.64	121.00
2	B	373	PHE	CB-CG-CD1	7.71	126.20	120.80
2	B	256	THR	CA-CB-CG2	-7.70	101.63	112.40
2	B	54	PHE	CB-CG-CD2	7.69	126.18	120.80
6	F	258	ARG	NE-CZ-NH2	-7.67	116.47	120.30
8	G	120	LEU	CB-CG-CD1	7.65	124.01	111.00
2	B	36	TYR	CB-CG-CD1	-7.65	116.41	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	PHE	CB-CG-CD2	7.59	126.11	120.80
3	C	94	ARG	NE-CZ-NH1	-7.59	116.50	120.30
12	O	90	TYR	CB-CG-CD1	-7.56	116.46	121.00
1	A	333	PHE	CB-CG-CD1	-7.53	115.53	120.80
8	G	75	TYR	CB-CG-CD2	-7.51	116.49	121.00
6	F	289	MET	CG-SD-CE	-7.49	88.22	100.20
4	D	274	ARG	NE-CZ-NH2	-7.48	116.56	120.30
3	C	337	TYR	CG-CD1-CE1	-7.47	115.33	121.30
10	P	45	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	A	327	ARG	NE-CZ-NH2	7.44	124.02	120.30
6	F	168	PHE	CB-CG-CD1	-7.42	115.60	120.80
5	E	96	PHE	CB-CG-CD1	-7.40	115.62	120.80
2	B	384	ASP	CB-CG-OD2	7.38	124.94	118.30
8	G	70	PHE	CB-CG-CD2	7.38	125.96	120.80
7	H	161	MET	CG-SD-CE	-7.37	88.40	100.20
12	O	527	PHE	CB-CG-CD1	7.36	125.95	120.80
10	P	18	ALA	N-CA-CB	7.35	120.40	110.10
12	O	165	ARG	NE-CZ-NH1	7.34	123.97	120.30
12	O	249	ARG	NE-CZ-NH1	-7.31	116.65	120.30
1	A	172	TYR	CB-CG-CD1	-7.30	116.62	121.00
12	O	89	ARG	NE-CZ-NH2	-7.30	116.65	120.30
5	E	100	VAL	CA-CB-CG1	7.27	121.81	110.90
8	G	126	ARG	NE-CZ-NH2	-7.27	116.67	120.30
6	F	121	PHE	CB-CG-CD2	-7.25	115.72	120.80
1	A	292	TYR	CG-CD2-CE2	-7.24	115.51	121.30
1	A	90	MET	CG-SD-CE	7.22	111.75	100.20
2	B	258	PHE	CB-CG-CD1	-7.20	115.76	120.80
5	E	305	ARG	NE-CZ-NH2	-7.17	116.72	120.30
12	O	32	ARG	NE-CZ-NH1	7.13	123.87	120.30
3	C	114	ARG	NE-CZ-NH2	-7.13	116.74	120.30
10	P	43	ARG	NE-CZ-NH2	-7.11	116.75	120.30
11	Q	77	PHE	CB-CG-CD2	-7.10	115.83	120.80
5	E	232	SER	N-CA-C	7.08	130.11	111.00
7	H	11	PHE	CB-CG-CD1	-7.08	115.85	120.80
2	B	53	SER	N-CA-CB	7.05	121.08	110.50
12	O	184	VAL	CA-CB-CG1	7.03	121.45	110.90
12	O	467	TYR	CG-CD1-CE1	-7.03	115.67	121.30
4	D	365	GLU	N-CA-C	7.00	129.91	111.00
12	O	298	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	B	198	TYR	CB-CG-CD1	6.99	125.20	121.00
4	D	170	ARG	NE-CZ-NH2	-6.98	116.81	120.30
6	F	291	TYR	CB-CG-CD2	-6.98	116.81	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	280	LEU	CB-CG-CD1	6.96	122.84	111.00
10	P	51	LEU	CB-CG-CD1	-6.96	99.16	111.00
3	C	185	TYR	CB-CG-CD1	-6.96	116.82	121.00
12	O	573	TYR	CB-CG-CD1	6.95	125.17	121.00
2	B	182	ASP	CB-CG-OD1	6.94	124.55	118.30
5	E	32	ASP	CB-CG-OD2	-6.94	112.05	118.30
13	R	21	ARG	NE-CZ-NH1	6.94	123.77	120.30
12	O	435	TYR	CB-CG-CD1	6.92	125.15	121.00
2	B	146	ARG	NE-CZ-NH1	6.92	123.76	120.30
5	E	174	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	B	159	TYR	CB-CG-CD1	6.90	125.14	121.00
5	E	237	LEU	CB-CA-C	-6.88	97.12	110.20
4	D	196	ASP	CB-CG-OD2	-6.88	112.11	118.30
3	C	288	ARG	NE-CZ-NH1	6.84	123.72	120.30
6	F	315	ARG	NE-CZ-NH2	-6.84	116.88	120.30
13	R	36	ASP	CB-CA-C	6.83	124.06	110.40
3	C	206	GLU	N-CA-CB	6.82	122.88	110.60
4	D	85	TYR	CB-CG-CD2	-6.81	116.91	121.00
12	O	507	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	A	162	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
4	D	167	TYR	CG-CD2-CE2	-6.80	115.86	121.30
2	B	105	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	B	90	ASN	N-CA-CB	6.79	122.83	110.60
2	B	92	TYR	CB-CG-CD1	6.77	125.06	121.00
4	D	317	ASN	N-CA-C	6.77	129.28	111.00
8	G	160	ARG	NE-CZ-NH2	-6.77	116.92	120.30
3	C	389	ARG	NE-CZ-NH2	6.76	123.68	120.30
6	F	188	TYR	CB-CG-CD1	6.76	125.06	121.00
12	O	184	VAL	CA-CB-CG2	-6.76	100.76	110.90
5	E	261	TYR	CB-CG-CD2	-6.75	116.95	121.00
6	F	46	LEU	CA-CB-CG	6.75	130.81	115.30
13	R	36	ASP	N-CA-CB	6.75	122.74	110.60
2	B	105	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	C	251	ARG	NE-CZ-NH1	6.74	123.67	120.30
4	D	268	TYR	CB-CG-CD1	6.73	125.04	121.00
5	E	234	ASP	N-CA-C	6.72	129.14	111.00
1	A	221	TYR	CB-CG-CD1	6.72	125.03	121.00
3	C	190	MET	N-CA-CB	6.71	122.67	110.60
7	H	206	PHE	CB-CG-CD2	-6.71	116.11	120.80
4	D	213	TYR	CG-CD1-CE1	-6.70	115.94	121.30
3	C	360	PHE	CB-CG-CD1	-6.69	116.12	120.80
5	E	233	LEU	N-CA-C	6.69	129.05	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	527	PHE	CB-CG-CD2	-6.67	116.13	120.80
12	O	544	TYR	CG-CD1-CE1	-6.67	115.96	121.30
6	F	280	TYR	CZ-CE2-CD2	-6.66	113.81	119.80
8	G	136	VAL	CA-CB-CG1	6.66	120.89	110.90
2	B	149	PHE	CB-CG-CD2	-6.65	116.14	120.80
8	G	160	ARG	NE-CZ-NH1	6.65	123.62	120.30
12	O	190	HIS	N-CA-CB	6.62	122.52	110.60
7	H	136	PHE	CB-CG-CD1	-6.62	116.17	120.80
5	E	242	TRP	CB-CG-CD1	6.60	135.58	127.00
2	B	131	PHE	CG-CD1-CE1	6.60	128.06	120.80
5	E	237	LEU	CB-CG-CD2	6.60	122.22	111.00
12	O	434	PHE	CB-CG-CD1	-6.60	116.18	120.80
12	O	424	TYR	CB-CG-CD1	6.59	124.96	121.00
12	O	43	TYR	CB-CG-CD1	6.58	124.95	121.00
2	B	191	GLY	N-CA-C	-6.57	96.67	113.10
3	C	367	TYR	CB-CG-CD2	6.57	124.94	121.00
1	A	292	TYR	CD1-CE1-CZ	-6.55	113.90	119.80
12	O	277	PHE	CB-CG-CD1	6.55	125.39	120.80
1	A	81	PHE	CB-CG-CD1	6.54	125.38	120.80
5	E	237	LEU	N-CA-CB	6.53	123.45	110.40
3	C	100	PHE	CB-CG-CD1	-6.53	116.23	120.80
5	E	334	SER	N-CA-CB	6.51	120.27	110.50
4	D	6	ARG	NE-CZ-NH1	6.50	123.55	120.30
12	O	369	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	C	44	THR	CA-CB-CG2	-6.49	103.31	112.40
4	D	300	LEU	N-CA-C	6.49	128.52	111.00
3	C	176	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	A	276	ASP	CB-CG-OD1	-6.47	112.48	118.30
6	F	261	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	B	62	GLY	N-CA-C	-6.46	96.94	113.10
8	G	22	THR	CA-CB-CG2	-6.46	103.36	112.40
13	R	21	ARG	CD-NE-CZ	-6.45	114.57	123.60
6	F	105	TYR	CG-CD1-CE1	6.43	126.44	121.30
4	D	364	ARG	N-CA-C	6.43	128.35	111.00
8	G	46	LEU	CB-CG-CD2	6.42	121.92	111.00
2	B	162	ARG	NE-CZ-NH2	-6.41	117.09	120.30
6	F	42	ALA	C-N-CA	6.41	137.74	121.70
4	D	134	THR	CA-CB-CG2	-6.41	103.43	112.40
12	O	457	MET	CG-SD-CE	-6.40	89.96	100.20
12	O	551	ARG	NE-CZ-NH1	-6.40	117.10	120.30
5	E	52	PHE	CB-CG-CD2	6.39	125.28	120.80
2	B	391	GLN	CA-CB-CG	6.39	127.45	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Q	33	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	205	TYR	CG-CD1-CE1	-6.38	116.19	121.30
13	R	87	TRP	CB-CG-CD1	6.38	135.29	127.00
11	Q	15	ASP	CB-CG-OD1	-6.36	112.58	118.30
3	C	172	GLU	N-CA-CB	6.35	122.04	110.60
3	C	136	ASN	N-CA-CB	6.34	122.01	110.60
12	O	566	MET	CG-SD-CE	-6.33	90.07	100.20
1	A	59	ARG	NE-CZ-NH1	6.33	123.46	120.30
3	C	97	THR	N-CA-CB	6.30	122.27	110.30
1	A	177	ASP	CB-CG-OD1	-6.30	112.63	118.30
12	O	194	TYR	CB-CG-CD1	6.29	124.78	121.00
11	Q	7	THR	CA-CB-CG2	-6.29	103.60	112.40
10	P	8	ARG	NE-CZ-NH2	6.29	123.44	120.30
5	E	197	ASP	CB-CG-OD2	-6.28	112.65	118.30
7	H	199	ARG	NE-CZ-NH1	6.28	123.44	120.30
10	P	103	MET	CG-SD-CE	-6.27	90.17	100.20
3	C	372	MET	CG-SD-CE	-6.27	90.17	100.20
5	E	137	TYR	CB-CG-CD2	6.26	124.76	121.00
2	B	424	LEU	CB-CA-C	-6.26	98.31	110.20
1	A	453	MET	CG-SD-CE	-6.24	90.21	100.20
11	Q	77	PHE	CB-CG-CD1	6.24	125.17	120.80
2	B	320	ASN	N-CA-CB	6.23	121.81	110.60
5	E	31	TYR	CG-CD2-CE2	-6.22	116.33	121.30
5	E	29	TYR	CB-CG-CD2	6.21	124.73	121.00
13	R	86	ARG	NE-CZ-NH1	6.19	123.39	120.30
6	F	46	LEU	N-CA-C	6.18	127.69	111.00
13	R	33	TRP	N-CA-CB	6.18	121.72	110.60
10	P	68	ARG	NE-CZ-NH2	-6.17	117.21	120.30
12	O	490	PHE	CB-CG-CD2	-6.17	116.48	120.80
3	C	167	MET	CG-SD-CE	-6.16	90.34	100.20
5	E	250	LEU	CB-CA-C	-6.16	98.50	110.20
2	B	277	LEU	CB-CG-CD1	6.15	121.46	111.00
12	O	544	TYR	CB-CG-CD1	6.15	124.69	121.00
10	P	48	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	426	ALA	N-CA-CB	6.14	118.70	110.10
2	B	268	SER	N-CA-CB	-6.14	101.30	110.50
2	B	259	PHE	CB-CG-CD1	6.13	125.09	120.80
3	C	13	ARG	NE-CZ-NH2	6.13	123.36	120.30
4	D	199	ARG	NE-CZ-NH1	-6.11	117.25	120.30
4	D	348	MET	CG-SD-CE	-6.10	90.44	100.20
3	C	163	ASP	CB-CG-OD1	6.09	123.78	118.30
8	G	63	TYR	CB-CG-CD1	6.09	124.65	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	414	ARG	NE-CZ-NH2	-6.08	117.26	120.30
6	F	296	THR	CA-CB-CG2	-6.07	103.90	112.40
1	A	81	PHE	CB-CG-CD2	-6.06	116.56	120.80
7	H	86	PHE	CB-CG-CD2	-6.05	116.57	120.80
12	O	273	ASP	CB-CG-OD1	-6.05	112.86	118.30
5	E	90	MET	CG-SD-CE	-6.04	90.53	100.20
12	O	648	ARG	NE-CZ-NH1	6.03	123.31	120.30
5	E	51	TYR	CB-CG-CD1	-6.02	117.39	121.00
4	D	302	ARG	O-C-N	-6.02	113.07	122.70
12	O	198	PHE	CB-CG-CD2	-6.02	116.59	120.80
12	O	540	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	A	37	VAL	CG1-CB-CG2	6.01	120.52	110.90
3	C	183	CYS	N-CA-CB	6.01	121.41	110.60
5	E	67	MET	CG-SD-CE	-6.01	90.59	100.20
12	O	202	PHE	CD1-CE1-CZ	-6.00	112.90	120.10
2	B	84	ASN	N-CA-CB	6.00	121.39	110.60
3	C	390	LEU	CB-CA-C	-5.99	98.82	110.20
12	O	87	TYR	CG-CD2-CE2	-5.99	116.51	121.30
3	C	218	HIS	CA-CB-CG	-5.98	103.44	113.60
12	O	90	TYR	CG-CD1-CE1	-5.97	116.53	121.30
5	E	56	LYS	N-CA-CB	5.96	121.33	110.60
1	A	336	SER	N-CA-CB	5.96	119.44	110.50
12	O	273	ASP	CB-CG-OD2	5.95	123.66	118.30
5	E	242	TRP	CB-CG-CD2	-5.94	118.88	126.60
12	O	638	PHE	CB-CG-CD1	-5.94	116.64	120.80
12	O	106	ARG	NE-CZ-NH2	5.93	123.27	120.30
4	D	230	LEU	CB-CG-CD1	5.93	121.08	111.00
8	G	77	ASP	CB-CG-OD1	-5.93	112.97	118.30
2	B	64	LYS	C-N-CA	5.92	134.74	122.30
7	H	199	ARG	NE-CZ-NH2	-5.92	117.34	120.30
4	D	191	TYR	CG-CD1-CE1	-5.92	116.56	121.30
4	D	287	PRO	N-CA-CB	5.92	110.41	103.30
4	D	142	ASP	CB-CG-OD1	5.92	123.63	118.30
12	O	14	TRP	CE3-CZ3-CH2	-5.92	114.69	121.20
12	O	339	PHE	CZ-CE2-CD2	-5.91	113.01	120.10
7	H	59	ARG	NE-CZ-NH1	5.90	123.25	120.30
12	O	536	SER	N-CA-CB	5.89	119.33	110.50
2	B	37	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	426	ALA	CB-CA-C	-5.88	101.28	110.10
4	D	68	ASP	CB-CG-OD2	-5.87	113.02	118.30
4	D	315	LEU	CB-CA-C	-5.87	99.06	110.20
5	E	233	LEU	C-N-CA	5.87	136.36	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	279	PHE	CG-CD1-CE1	-5.87	114.35	120.80
6	F	313	TYR	CD1-CE1-CZ	-5.87	114.52	119.80
6	F	183	PHE	CZ-CE2-CD2	5.86	127.14	120.10
2	B	126	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	298	GLU	C-N-CA	5.86	136.35	121.70
4	D	114	TYR	CB-CG-CD2	5.86	124.52	121.00
5	E	136	TRP	CE2-CD2-CG	5.86	111.99	107.30
12	O	239	VAL	CA-CB-CG1	5.85	119.68	110.90
3	C	74	PHE	CB-CG-CD1	5.85	124.90	120.80
4	D	107	ARG	NE-CZ-NH2	-5.85	117.38	120.30
4	D	224	GLU	OE1-CD-OE2	5.85	130.32	123.30
12	O	476	MET	CG-SD-CE	-5.84	90.85	100.20
7	H	114	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	388	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
4	D	217	VAL	CA-CB-CG2	-5.83	102.15	110.90
3	C	267	TYR	CB-CG-CD1	5.83	124.50	121.00
5	E	185	ALA	N-CA-C	-5.83	95.27	111.00
6	F	46	LEU	CB-CG-CD2	5.83	120.90	111.00
13	R	105	LYS	N-CA-CB	5.83	121.09	110.60
4	D	302	ARG	NE-CZ-NH2	-5.82	117.39	120.30
6	F	149	PRO	N-CA-CB	5.82	110.29	103.30
13	R	28	ASN	N-CA-CB	5.82	121.07	110.60
8	G	139	ASP	CB-CG-OD1	5.81	123.53	118.30
12	O	640	LEU	CB-CG-CD1	5.81	120.87	111.00
5	E	156	MET	CA-CB-CG	-5.79	103.45	113.30
1	A	69	THR	CA-CB-CG2	-5.79	104.30	112.40
13	R	40	ASP	N-CA-CB	5.77	120.99	110.60
12	O	371	ALA	CB-CA-C	-5.77	101.45	110.10
7	H	120	LEU	CB-CG-CD1	5.76	120.80	111.00
11	Q	98	GLU	O-C-N	5.76	131.92	122.70
1	A	135	ARG	NE-CZ-NH1	5.76	123.18	120.30
12	O	543	PHE	CD1-CE1-CZ	-5.75	113.20	120.10
4	D	170	ARG	NE-CZ-NH1	5.75	123.17	120.30
12	O	487	ASN	CA-CB-CG	5.73	126.02	113.40
2	B	421	TYR	CB-CG-CD2	-5.73	117.56	121.00
11	Q	101	LEU	N-CA-CB	5.73	121.86	110.40
12	O	477	TYR	CB-CG-CD2	5.72	124.43	121.00
7	H	203	TYR	CG-CD2-CE2	5.71	125.87	121.30
12	O	477	TYR	CB-CG-CD1	-5.71	117.58	121.00
3	C	227	TYR	CB-CG-CD2	5.71	124.42	121.00
5	E	73	GLY	N-CA-C	-5.70	98.84	113.10
4	D	213	TYR	CB-CG-CD2	-5.70	117.58	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ARG	NE-CZ-NH1	5.70	123.15	120.30
12	O	321	ASP	CB-CG-OD1	5.69	123.42	118.30
12	O	573	TYR	CG-CD1-CE1	5.69	125.85	121.30
7	H	158	THR	N-CA-CB	5.68	121.10	110.30
1	A	162	ARG	NE-CZ-NH2	5.68	123.14	120.30
4	D	360	HIS	CB-CA-C	-5.67	99.05	110.40
4	D	364	ARG	C-N-CA	5.67	135.89	121.70
7	H	37	TYR	CG-CD2-CE2	5.67	125.84	121.30
2	B	98	TYR	CG-CD2-CE2	-5.67	116.76	121.30
11	Q	62	PHE	CB-CG-CD1	5.67	124.77	120.80
12	O	146	MET	CG-SD-CE	-5.64	91.18	100.20
6	F	184	ALA	N-CA-CB	5.64	117.99	110.10
1	A	211	TYR	N-CA-CB	5.63	120.74	110.60
6	F	33	CYS	N-CA-CB	5.63	120.74	110.60
12	O	339	PHE	CG-CD2-CE2	5.63	127.00	120.80
12	O	70	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	454	MET	CG-SD-CE	-5.63	91.20	100.20
5	E	174	ARG	NH1-CZ-NH2	-5.62	113.21	119.40
2	B	384	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	A	113	PRO	N-CA-CB	5.61	110.04	103.30
5	E	189	TYR	CB-CG-CD2	-5.61	117.64	121.00
12	O	486	LEU	CB-CG-CD2	-5.60	101.47	111.00
12	O	98	ALA	CB-CA-C	-5.60	101.70	110.10
5	E	285	PHE	CB-CG-CD1	5.60	124.72	120.80
12	O	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
10	P	79	PHE	CB-CG-CD1	-5.60	116.88	120.80
10	P	51	LEU	CB-CG-CD2	5.59	120.51	111.00
8	G	173	THR	CA-CB-CG2	-5.59	104.57	112.40
10	P	72	PRO	N-CD-CG	5.59	111.58	103.20
4	D	323	GLU	OE1-CD-OE2	-5.58	116.60	123.30
8	G	91	ALA	CB-CA-C	-5.58	101.73	110.10
1	A	366	TYR	CB-CG-CD1	5.58	124.34	121.00
2	B	198	TYR	CB-CG-CD2	-5.57	117.66	121.00
12	O	414	ARG	NE-CZ-NH1	5.57	123.08	120.30
7	H	148	ILE	CA-CB-CG2	-5.56	99.78	110.90
6	F	46	LEU	CB-CG-CD1	-5.56	101.55	111.00
2	B	44	GLU	N-CA-CB	5.55	120.60	110.60
11	Q	12	GLU	N-CA-C	-5.55	96.00	111.00
3	C	330	GLY	N-CA-C	-5.55	99.22	113.10
3	C	247	GLN	C-N-CA	5.54	135.56	121.70
3	C	184	TYR	CG-CD2-CE2	-5.54	116.86	121.30
7	H	79	GLN	CB-CA-C	-5.54	99.33	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	LYS	C-N-CA	5.53	135.53	121.70
2	B	269	GLY	C-N-CA	5.53	135.53	121.70
4	D	213	TYR	CD1-CE1-CZ	5.53	124.78	119.80
12	O	276	GLN	CA-CB-CG	5.53	125.56	113.40
1	A	75	LEU	CB-CG-CD1	5.53	120.39	111.00
4	D	313	SER	N-CA-CB	5.52	118.78	110.50
6	F	150	LEU	CB-CA-C	-5.51	99.73	110.20
3	C	185	TYR	CB-CG-CD2	5.51	124.31	121.00
2	B	185	GLU	C-N-CA	5.50	135.45	121.70
1	A	338	TYR	CG-CD2-CE2	-5.50	116.90	121.30
6	F	313	TYR	CG-CD2-CE2	-5.50	116.90	121.30
8	G	106	SER	N-CA-CB	5.50	118.74	110.50
2	B	174	GLN	CB-CA-C	-5.49	99.42	110.40
4	D	283	ALA	N-CA-CB	5.48	117.78	110.10
5	E	267	PHE	CG-CD2-CE2	-5.48	114.77	120.80
7	H	134	ALA	CB-CA-C	-5.48	101.88	110.10
4	D	160	ASP	CB-CG-OD1	-5.48	113.37	118.30
2	B	352	ARG	NE-CZ-NH1	-5.47	117.56	120.30
12	O	544	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
12	O	566	MET	CA-CB-CG	5.47	122.60	113.30
3	C	348	PHE	CB-CG-CD2	-5.46	116.97	120.80
12	O	406	MET	CG-SD-CE	-5.46	91.47	100.20
11	Q	57	THR	CA-CB-CG2	-5.45	104.77	112.40
12	O	3	LEU	C-N-CA	5.45	135.32	121.70
12	O	416	THR	CA-CB-CG2	-5.45	104.77	112.40
6	F	313	TYR	CB-CG-CD2	-5.44	117.73	121.00
11	Q	46	LEU	CB-CG-CD2	5.44	120.25	111.00
12	O	127	TYR	CD1-CE1-CZ	-5.44	114.91	119.80
1	A	62	PHE	CB-CG-CD2	-5.44	117.00	120.80
5	E	307	SER	N-CA-CB	5.44	118.65	110.50
1	A	152	TYR	O-C-N	5.43	131.39	122.70
2	B	205	TYR	CD1-CE1-CZ	-5.43	114.91	119.80
2	B	172	LEU	CB-CG-CD2	5.43	120.22	111.00
12	O	548	PHE	CG-CD1-CE1	-5.42	114.84	120.80
7	H	102	VAL	CA-CB-CG2	-5.41	102.78	110.90
10	P	68	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	188	ALA	CB-CA-C	-5.41	101.98	110.10
2	B	368	ARG	NE-CZ-NH1	5.41	123.00	120.30
12	O	192	GLU	N-CA-CB	5.41	120.33	110.60
13	R	27	TRP	CG-CD2-CE3	-5.41	129.03	133.90
12	O	102	ASP	CB-CG-OD2	-5.40	113.44	118.30
12	O	369	ASP	CB-CG-OD1	5.40	123.16	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	227	LEU	CB-CG-CD1	5.40	120.17	111.00
4	D	362	GLU	N-CA-C	-5.39	96.44	111.00
2	B	281	VAL	CB-CA-C	-5.39	101.16	111.40
12	O	86	MET	CG-SD-CE	-5.39	91.58	100.20
5	E	174	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	338	TYR	CD1-CG-CD2	5.37	123.81	117.90
2	B	265	TYR	N-CA-CB	5.37	120.27	110.60
12	O	430	VAL	CA-CB-CG1	-5.36	102.86	110.90
6	F	125	TYR	CB-CG-CD1	5.36	124.21	121.00
3	C	349	ALA	N-CA-CB	5.35	117.59	110.10
12	O	242	ARG	NE-CZ-NH1	5.35	122.98	120.30
12	O	568	TYR	CZ-CE2-CD2	5.34	124.61	119.80
3	C	309	ARG	NE-CZ-NH2	-5.34	117.63	120.30
6	F	121	PHE	CB-CG-CD1	5.34	124.54	120.80
11	Q	53	ALA	CB-CA-C	-5.34	102.10	110.10
1	A	379	SER	N-CA-CB	5.33	118.50	110.50
1	A	395	THR	CA-CB-CG2	-5.33	104.94	112.40
4	D	1	MET	CG-SD-CE	-5.33	91.67	100.20
4	D	254	ARG	NE-CZ-NH2	-5.33	117.64	120.30
6	F	36	THR	CA-CB-CG2	-5.33	104.94	112.40
4	D	363	THR	C-N-CA	5.33	135.02	121.70
1	A	418	ASP	CB-CG-OD2	5.32	123.09	118.30
6	F	167	VAL	CB-CA-C	-5.32	101.30	111.40
5	E	267	PHE	CB-CG-CD2	-5.32	117.08	120.80
2	B	366	TYR	CB-CG-CD1	-5.32	117.81	121.00
4	D	360	HIS	C-N-CA	5.32	134.99	121.70
3	C	281	LYS	C-N-CA	5.31	134.97	121.70
12	O	127	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
4	D	139	TYR	CG-CD2-CE2	5.30	125.54	121.30
3	C	203	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
2	B	182	ASP	CB-CG-OD2	-5.30	113.53	118.30
4	D	193	ARG	O-C-N	-5.29	114.23	122.70
4	D	198	ARG	NE-CZ-NH2	-5.29	117.65	120.30
6	F	223	ALA	N-CA-CB	5.29	117.51	110.10
12	O	259	TYR	CG-CD1-CE1	-5.28	117.07	121.30
11	Q	63	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	75	MET	O-C-N	5.28	131.14	122.70
2	B	248	GLU	CB-CG-CD	-5.27	99.97	114.20
12	O	438	MET	N-CA-CB	5.27	120.09	110.60
12	O	527	PHE	O-C-N	-5.27	114.27	122.70
1	A	78	ALA	CB-CA-C	5.26	118.00	110.10
4	D	329	GLU	N-CA-CB	5.26	120.06	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	54	TYR	CB-CG-CD1	-5.26	117.85	121.00
12	O	589	ASN	N-CA-CB	5.26	120.06	110.60
11	Q	62	PHE	CB-CG-CD2	-5.25	117.12	120.80
13	R	38	VAL	CA-CB-CG2	-5.25	103.02	110.90
1	A	239	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	395	THR	N-CA-C	-5.25	96.84	111.00
5	E	183	LEU	N-CA-C	-5.25	96.84	111.00
5	E	228	TYR	CB-CG-CD1	-5.25	117.85	121.00
13	R	63	ALA	N-CA-CB	5.25	117.44	110.10
12	O	218	TYR	CB-CG-CD2	-5.25	117.85	121.00
13	R	79	PHE	CB-CG-CD1	5.24	124.47	120.80
5	E	249	THR	CA-CB-OG1	5.24	120.01	109.00
8	G	145	LEU	CB-CG-CD1	5.24	119.91	111.00
3	C	267	TYR	CB-CG-CD2	-5.23	117.86	121.00
3	C	204	PHE	CB-CG-CD2	5.23	124.46	120.80
2	B	221	SER	CB-CA-C	-5.23	100.17	110.10
12	O	494	ILE	CA-CB-CG2	5.23	121.36	110.90
1	A	284	LEU	O-C-N	-5.23	114.34	122.70
4	D	394	GLU	N-CA-CB	5.22	120.00	110.60
2	B	176	HIS	C-N-CA	5.22	134.75	121.70
2	B	232	LEU	CB-CA-C	-5.21	100.31	110.20
2	B	168	LEU	CB-CG-CD2	5.21	119.85	111.00
2	B	159	TYR	CG-CD2-CE2	-5.20	117.14	121.30
5	E	165	PHE	CB-CG-CD1	-5.20	117.16	120.80
7	H	75	TRP	CD1-CG-CD2	5.20	110.46	106.30
13	R	65	SER	O-C-N	-5.20	114.39	122.70
1	A	390	ALA	CB-CA-C	-5.20	102.31	110.10
5	E	117	MET	CG-SD-CE	-5.20	91.89	100.20
12	O	64	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
4	D	370	TRP	CG-CD2-CE3	-5.19	129.23	133.90
1	A	283	LEU	CA-C-N	5.19	128.62	117.20
12	O	344	LEU	N-CA-CB	5.19	120.79	110.40
2	B	281	VAL	CA-CB-CG2	5.19	118.69	110.90
6	F	154	LEU	CB-CG-CD2	5.19	119.83	111.00
1	A	359	ALA	N-CA-C	5.19	125.00	111.00
6	F	106	TYR	N-CA-CB	5.19	119.94	110.60
5	E	163	GLU	OE1-CD-OE2	5.18	129.51	123.30
4	D	270	ASP	CB-CG-OD1	5.18	122.96	118.30
12	O	283	HIS	CA-CB-CG	5.18	122.40	113.60
1	A	310	VAL	CA-CB-CG1	-5.17	103.14	110.90
6	F	44	HIS	N-CA-C	5.17	124.96	111.00
2	B	439	VAL	CA-CB-CG2	-5.17	103.15	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	31	TYR	CZ-CE2-CD2	5.17	124.45	119.80
3	C	50	ASP	C-N-CA	5.16	134.60	121.70
6	F	116	PHE	CB-CG-CD1	-5.16	117.19	120.80
5	E	232	SER	CA-C-O	-5.15	109.28	120.10
12	O	373	THR	N-CA-CB	5.15	120.09	110.30
4	D	52	MET	N-CA-CB	5.15	119.86	110.60
1	A	81	PHE	CA-CB-CG	-5.15	101.55	113.90
3	C	266	VAL	CA-CB-CG2	-5.15	103.18	110.90
12	O	608	LYS	C-N-CA	5.15	134.56	121.70
5	E	174	ARG	CA-C-O	5.14	130.88	120.10
8	G	48	GLU	CA-CB-CG	5.14	124.70	113.40
11	Q	101	LEU	CB-CG-CD1	5.13	119.72	111.00
5	E	233	LEU	CB-CA-C	-5.13	100.45	110.20
2	B	118	TYR	CB-CG-CD1	5.13	124.08	121.00
5	E	38	GLU	O-C-N	-5.13	114.50	122.70
12	O	500	VAL	CA-CB-CG2	5.13	118.59	110.90
12	O	592	GLU	CA-CB-CG	5.13	124.68	113.40
8	G	185	LEU	CB-CA-C	-5.12	100.47	110.20
8	G	207	GLN	CB-CG-CD	-5.12	98.29	111.60
3	C	403	PHE	CZ-CE2-CD2	5.12	126.24	120.10
1	A	289	VAL	N-CA-CB	5.12	122.76	111.50
12	O	558	TYR	CB-CG-CD2	-5.12	117.93	121.00
3	C	4	ALA	CB-CA-C	-5.12	102.42	110.10
4	D	356	ASP	N-CA-CB	5.12	119.81	110.60
8	G	161	ASP	CB-CG-OD2	-5.12	113.70	118.30
6	F	45	PRO	CA-N-CD	-5.11	104.34	111.50
5	E	106	ARG	NE-CZ-NH1	-5.11	117.75	120.30
10	P	101	ASP	CB-CG-OD2	-5.11	113.70	118.30
7	H	159	THR	C-N-CA	5.11	134.47	121.70
5	E	228	TYR	CB-CG-CD2	5.10	124.06	121.00
11	Q	48	GLY	N-CA-C	-5.10	100.35	113.10
2	B	148	TRP	CZ3-CH2-CZ2	-5.10	115.48	121.60
3	C	161	TYR	CA-CB-CG	-5.09	103.72	113.40
12	O	235	TYR	CB-CG-CD2	5.09	124.06	121.00
11	Q	18	TYR	CD1-CG-CD2	-5.09	112.30	117.90
12	O	371	ALA	N-CA-CB	5.09	117.23	110.10
13	R	101	TRP	CB-CG-CD1	5.09	133.62	127.00
5	E	282	ARG	NH1-CZ-NH2	5.08	124.99	119.40
7	H	118	PHE	CG-CD2-CE2	5.08	126.39	120.80
7	H	116	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	B	307	GLU	O-C-N	5.07	130.81	122.70
4	D	212	SER	N-CA-CB	5.07	118.10	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	543	PHE	CB-CG-CD2	-5.07	117.25	120.80
6	F	200	VAL	CA-CB-CG2	-5.06	103.31	110.90
6	F	69	ILE	N-CA-C	-5.06	97.34	111.00
1	A	214	ASN	C-N-CA	5.06	134.34	121.70
2	B	205	TYR	CB-CG-CD2	-5.06	117.97	121.00
5	E	98	LEU	CB-CA-C	-5.06	100.59	110.20
3	C	68	MET	CG-SD-CE	-5.05	92.12	100.20
1	A	187	ARG	NE-CZ-NH1	5.05	122.83	120.30
5	E	236	LYS	N-CA-CB	5.05	119.69	110.60
8	G	63	TYR	CG-CD1-CE1	5.05	125.34	121.30
6	F	279	PHE	CD1-CE1-CZ	5.04	126.15	120.10
1	A	130	TRP	CG-CD2-CE3	-5.04	129.36	133.90
12	O	230	SER	N-CA-CB	5.04	118.06	110.50
1	A	157	ILE	N-CA-C	-5.04	97.39	111.00
8	G	139	ASP	CB-CG-OD2	-5.04	113.76	118.30
4	D	109	HIS	CB-CA-C	-5.04	100.33	110.40
7	H	145	VAL	CA-CB-CG1	-5.04	103.35	110.90
4	D	250	PHE	CG-CD1-CE1	5.03	126.34	120.80
12	O	575	ALA	N-CA-CB	5.03	117.15	110.10
13	R	86	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	B	304	ASN	CA-CB-CG	-5.03	102.33	113.40
8	G	116	LEU	CB-CG-CD1	5.03	119.55	111.00
4	D	121	ARG	CG-CD-NE	-5.03	101.24	111.80
5	E	180	LYS	N-CA-CB	5.03	119.65	110.60
2	B	227	ALA	CB-CA-C	-5.03	102.56	110.10
12	O	139	ILE	CA-CB-CG2	5.03	120.96	110.90
12	O	466	GLY	N-CA-C	-5.03	100.53	113.10
3	C	367	TYR	CG-CD1-CE1	5.02	125.32	121.30
1	A	331	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	410	GLU	CG-CD-OE2	-5.02	108.26	118.30
3	C	160	PRO	N-CD-CG	5.02	110.73	103.20
10	P	80	ARG	NE-CZ-NH1	-5.02	117.79	120.30
12	O	439	LEU	CB-CG-CD1	5.02	119.53	111.00
2	B	163	GLU	N-CA-CB	5.01	119.63	110.60
3	C	84	PHE	CB-CG-CD2	5.01	124.31	120.80
3	C	13	ARG	NE-CZ-NH1	-5.01	117.79	120.30
3	C	156	LYS	CA-C-N	5.01	131.13	117.10
7	H	155	ALA	N-CA-CB	5.00	117.10	110.10
12	O	235	TYR	CG-CD1-CE1	5.00	125.30	121.30
12	O	435	TYR	CA-CB-CG	-5.00	103.89	113.40

There are no chirality outliers.

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ARG	Sidechain
1	A	152	TYR	Sidechain
1	A	187	ARG	Sidechain
1	A	221	TYR	Sidechain
1	A	238	ARG	Sidechain
1	A	263	TYR	Sidechain
1	A	363	ARG	Sidechain
1	A	370	ARG	Sidechain
1	A	425	TYR	Peptide
1	A	432	ARG	Sidechain
1	A	449	ARG	Sidechain
1	A	66	HIS	Sidechain
2	B	118	TYR	Sidechain
2	B	146	ARG	Sidechain
2	B	162	ARG	Sidechain
2	B	165	TYR	Sidechain
2	B	180	GLN	Peptide
2	B	218	TYR	Sidechain
2	B	259	PHE	Sidechain
2	B	279	TYR	Sidechain
2	B	342	PHE	Sidechain
2	B	352	ARG	Sidechain
2	B	36	TYR	Sidechain
2	B	410	GLU	Peptide,Mainchain
2	B	416	ARG	Sidechain
2	B	83	THR	Mainchain
3	C	114	ARG	Sidechain
3	C	119	ARG	Sidechain
3	C	185	TYR	Sidechain
3	C	224	TYR	Sidechain
3	C	276	ARG	Sidechain
3	C	337	TYR	Sidechain
4	D	114	TYR	Sidechain
4	D	155	TYR	Sidechain
4	D	187	TYR	Sidechain
4	D	198	ARG	Sidechain
4	D	242	ARG	Sidechain
4	D	250	PHE	Sidechain
4	D	299	ILE	Peptide
4	D	300	LEU	Mainchain
4	D	85	TYR	Sidechain
4	D	95	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	E	114	TYR	Sidechain
5	E	116	TYR	Sidechain
5	E	143	TYR	Sidechain
5	E	189	TYR	Sidechain
5	E	193	TYR	Sidechain
5	E	222	TYR	Sidechain
5	E	229	PHE	Sidechain
5	E	261	TYR	Sidechain
5	E	282	ARG	Sidechain
5	E	54	TYR	Sidechain
6	F	104	TYR	Sidechain
6	F	205	ARG	Sidechain
6	F	212	GLY	Peptide
6	F	313	TYR	Sidechain
6	F	43	LEU	Mainchain
6	F	44	HIS	Peptide
6	F	59	ARG	Sidechain
8	G	123	ARG	Sidechain
8	G	137	TYR	Sidechain
8	G	15	PHE	Sidechain
8	G	160	ARG	Peptide,Sidechain
8	G	163	ARG	Sidechain
8	G	204	ARG	Sidechain
8	G	41	TYR	Sidechain
8	G	72	TYR	Sidechain
7	H	125	TYR	Sidechain
7	H	37	TYR	Sidechain
7	H	44	TYR	Sidechain
7	H	55	TYR	Sidechain
7	H	59	ARG	Sidechain
7	H	80	ARG	Sidechain
7	H	90	TYR	Sidechain
12	O	125	TYR	Sidechain
12	O	127	TYR	Sidechain
12	O	152	VAL	Peptide
12	O	165	ARG	Sidechain
12	O	207	PHE	Sidechain
12	O	219	TYR	Sidechain
12	O	253	TYR	Sidechain
12	O	364	PHE	Sidechain
12	O	38	ARG	Sidechain
12	O	382	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	O	414	ARG	Sidechain
12	O	422	PHE	Sidechain
12	O	467	TYR	Sidechain
12	O	469	PHE	Sidechain
12	O	544	TYR	Sidechain
12	O	573	TYR	Sidechain
12	O	64	PHE	Sidechain
10	P	43	ARG	Sidechain
10	P	8	ARG	Sidechain
11	Q	18	TYR	Sidechain
11	Q	33	ARG	Sidechain
11	Q	76	TYR	Sidechain
11	Q	77	PHE	Sidechain
11	Q	83	TYR	Sidechain
13	R	25	LYS	Peptide
13	R	35	TRP	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	3450	0	3482	2	0
2	B	3386	0	3424	37	0
3	C	3205	0	3225	15	0
4	D	3251	0	3253	13	0
5	E	2472	0	2444	74	0
6	F	2280	0	2263	35	0
7	H	1340	0	1324	2	0
8	G	1645	0	1667	3	0
9	V	1308	0	1299	327	0
10	P	921	0	908	92	0
11	Q	873	0	845	90	0
12	O	6090	0	6071	181	0
13	R	746	0	705	29	0
14	N	591	0	616	45	0
All	All	31558	0	31526	644	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 (644) 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)
9:V:178:LEU:CD2	10:P:103:MET:HG3	1.06	1.53
9:V:171:LYS:NZ	10:P:106:GLN:CB	1.70	1.52
9:V:178:LEU:CD2	10:P:103:MET:CG	1.75	1.50
9:V:178:LEU:HD21	10:P:103:MET:CG	1.27	1.50
9:V:178:LEU:HD13	10:P:103:MET:CE	1.32	1.50
9:V:171:LYS:NZ	10:P:106:GLN:HB3	1.19	1.47
9:V:178:LEU:HD21	10:P:103:MET:CB	1.43	1.46
9:V:174:ASN:HB3	10:P:102:VAL:CA	1.48	1.42
9:V:178:LEU:CG	10:P:103:MET:HG3	1.49	1.40
9:V:180:ILE:CG1	11:Q:101:LEU:HD23	1.13	1.40
9:V:180:ILE:N	11:Q:101:LEU:HD22	1.38	1.36
12:O:612:LYS:HB3	12:O:657:MET:CE	1.57	1.34
9:V:180:ILE:HG12	11:Q:101:LEU:CD2	1.22	1.32
9:V:178:LEU:CD1	10:P:103:MET:CE	2.09	1.31
5:E:203:TYR:CG	5:E:309:LYS:HA	1.63	1.30
12:O:654:THR:HG1	12:O:655:THR:N	1.28	1.28
9:V:182:ARG:H	12:O:5:PRO:CD	1.44	1.28
9:V:178:LEU:HA	10:P:100:PRO:CG	1.62	1.28
12:O:370:LYS:HG3	14:N:32:GLU:O	1.18	1.27
9:V:163:LEU:CD2	11:Q:104:LEU:CD1	2.14	1.24
9:V:163:LEU:CD2	11:Q:104:LEU:HD11	1.64	1.24
9:V:163:LEU:CD2	11:Q:104:LEU:CD2	2.16	1.24
2:B:294:PHE:HA	13:R:106:TYR:CG	1.73	1.24
9:V:163:LEU:CD2	11:Q:104:LEU:HD21	1.67	1.23
9:V:174:ASN:CB	10:P:102:VAL:O	1.87	1.22
9:V:159:LYS:HD3	11:Q:104:LEU:CD1	1.68	1.22
9:V:171:LYS:CE	10:P:106:GLN:HB3	1.73	1.19
12:O:389:GLU:OE2	12:O:665:MET:HB3	1.04	1.19
9:V:174:ASN:HB2	10:P:102:VAL:O	1.35	1.18
12:O:654:THR:OG1	12:O:655:THR:N	1.77	1.18
9:V:159:LYS:HD3	11:Q:104:LEU:HD12	1.21	1.16
9:V:181:VAL:HG21	12:O:3:LEU:HB3	1.23	1.15
5:E:115:GLU:HG3	12:O:693:VAL:HB	1.16	1.15
12:O:680:LEU:HD21	12:O:718:ILE:HA	1.18	1.15
12:O:389:GLU:OE2	12:O:665:MET:CB	1.97	1.13
9:V:163:LEU:HD21	11:Q:104:LEU:HD11	1.20	1.12
9:V:142:VAL:HG23	9:V:144:GLY:H	1.10	1.12
9:V:174:ASN:HB3	10:P:102:VAL:HA	1.16	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:685:VAL:HG12	12:O:689:LYS:HE3	1.29	1.12
12:O:370:LYS:CG	14:N:32:GLU:O	1.96	1.11
9:V:182:ARG:N	12:O:5:PRO:HD3	1.40	1.11
9:V:178:LEU:HA	10:P:100:PRO:HG2	1.29	1.11
9:V:163:LEU:HD21	11:Q:104:LEU:HD21	1.33	1.10
9:V:178:LEU:CD1	10:P:103:MET:HG3	1.80	1.10
2:B:294:PHE:CA	13:R:106:TYR:CZ	2.34	1.10
9:V:171:LYS:CD	10:P:106:GLN:HB3	1.82	1.09
9:V:170:VAL:HG21	10:P:103:MET:HG2	1.26	1.09
9:V:178:LEU:CD1	10:P:103:MET:CG	2.31	1.08
5:E:203:TYR:CZ	5:E:309:LYS:CA	2.37	1.08
12:O:702:GLU:OE2	14:N:74:ARG:HD3	1.53	1.08
5:E:203:TYR:CD1	5:E:309:LYS:CA	2.37	1.08
2:B:294:PHE:CA	13:R:106:TYR:CD1	2.37	1.07
5:E:203:TYR:CD2	5:E:309:LYS:CA	2.38	1.07
12:O:654:THR:C	12:O:655:THR:HB	1.72	1.07
9:V:174:ASN:HB3	10:P:102:VAL:C	1.75	1.07
2:B:294:PHE:HA	13:R:106:TYR:CD2	1.90	1.06
12:O:370:LYS:HG2	14:N:33:LYS:HA	1.10	1.06
5:E:203:TYR:CE2	5:E:309:LYS:CA	2.39	1.06
12:O:654:THR:CA	12:O:655:THR:HB	1.86	1.06
9:V:178:LEU:CD1	10:P:103:MET:HE2	1.82	1.06
12:O:681:GLN:HG3	12:O:725:LEU:HD21	1.10	1.06
2:B:294:PHE:CA	13:R:106:TYR:CE2	2.39	1.05
9:V:163:LEU:HD21	11:Q:104:LEU:CD1	1.81	1.05
9:V:178:LEU:HD22	10:P:103:MET:CG	1.78	1.05
5:E:203:TYR:CG	5:E:309:LYS:CA	2.40	1.05
12:O:654:THR:C	12:O:655:THR:CB	2.24	1.04
5:E:203:TYR:CE1	5:E:309:LYS:CA	2.40	1.04
2:B:294:PHE:CA	13:R:106:TYR:CE1	2.41	1.04
2:B:294:PHE:CA	13:R:106:TYR:CG	2.41	1.04
2:B:294:PHE:CA	13:R:106:TYR:CD2	2.41	1.03
12:O:688:MET:HG3	12:O:731:ILE:HD13	1.38	1.03
5:E:203:TYR:CE1	5:E:309:LYS:CB	2.42	1.02
5:E:203:TYR:CE2	5:E:309:LYS:CB	2.43	1.02
5:E:115:GLU:HG3	12:O:693:VAL:CB	1.89	1.02
9:V:171:LYS:NZ	10:P:106:GLN:HB2	1.71	1.02
9:V:178:LEU:CB	11:Q:101:LEU:HD21	1.90	1.01
12:O:612:LYS:HB3	12:O:657:MET:HE2	1.02	1.01
9:V:178:LEU:HB3	11:Q:101:LEU:HD21	1.42	1.01
2:B:294:PHE:C	13:R:106:TYR:CE1	2.34	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:203:TYR:CZ	5:E:309:LYS:CB	2.44	1.01
9:V:159:LYS:NZ	11:Q:108:ASN:HB2	1.75	1.00
5:E:203:TYR:CG	5:E:309:LYS:CB	2.45	1.00
9:V:163:LEU:CG	11:Q:104:LEU:HD11	1.92	0.99
9:V:178:LEU:HD21	10:P:103:MET:CA	1.92	0.99
12:O:316:GLN:CD	14:N:32:GLU:OE1	2.00	0.99
5:E:203:TYR:CD1	5:E:309:LYS:CB	2.45	0.99
5:E:203:TYR:CD2	5:E:309:LYS:CB	2.46	0.98
9:V:181:VAL:HG21	12:O:3:LEU:CB	1.93	0.98
9:V:178:LEU:CD2	10:P:103:MET:CB	2.18	0.97
9:V:162:CYS:SG	11:Q:95:ILE:HD13	2.03	0.97
9:V:181:VAL:HA	12:O:4:LYS:HA	1.47	0.97
9:V:178:LEU:CD1	10:P:103:MET:HE3	1.81	0.97
9:V:184:LEU:HD21	11:Q:105:MET:N	1.79	0.97
9:V:163:LEU:HD21	11:Q:104:LEU:CD2	1.89	0.97
9:V:163:LEU:HD23	11:Q:104:LEU:CD2	1.90	0.97
2:B:294:PHE:C	13:R:106:TYR:CG	2.39	0.96
9:V:178:LEU:HD23	10:P:100:PRO:HG2	1.46	0.96
2:B:294:PHE:C	13:R:106:TYR:CZ	2.39	0.96
9:V:179:ASP:H	10:P:100:PRO:HG3	1.25	0.96
12:O:612:LYS:CB	12:O:657:MET:CE	2.43	0.96
2:B:294:PHE:C	13:R:106:TYR:CD2	2.40	0.95
2:B:294:PHE:C	13:R:106:TYR:CE2	2.40	0.95
5:E:203:TYR:CD2	5:E:309:LYS:HA	2.00	0.95
9:V:174:ASN:CB	10:P:102:VAL:HA	1.95	0.95
9:V:159:LYS:CD	11:Q:104:LEU:HD12	1.97	0.94
2:B:294:PHE:C	13:R:106:TYR:CD1	2.41	0.94
9:V:174:ASN:CB	10:P:102:VAL:CA	2.45	0.94
9:V:177:ARG:O	10:P:100:PRO:HB2	1.67	0.94
9:V:178:LEU:HD11	10:P:103:MET:CG	1.96	0.93
9:V:179:ASP:N	10:P:100:PRO:HG3	1.82	0.93
12:O:370:LYS:CG	14:N:33:LYS:HA	1.97	0.93
9:V:177:ARG:HB3	10:P:102:VAL:H	1.33	0.93
5:E:115:GLU:CG	12:O:693:VAL:HB	1.99	0.92
9:V:74:VAL:HG22	9:V:147:ILE:CG2	1.99	0.92
9:V:181:VAL:HG22	12:O:4:LYS:N	1.84	0.92
9:V:171:LYS:NZ	10:P:106:GLN:CG	2.33	0.92
9:V:177:ARG:HB2	10:P:102:VAL:CA	1.65	0.92
9:V:181:VAL:CG1	12:O:3:LEU:O	2.17	0.92
9:V:178:LEU:HA	10:P:100:PRO:HG3	1.49	0.91
12:O:660:ASP:HA	12:O:663:GLN:HG2	1.49	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:680:LEU:CD2	12:O:718:ILE:HA	2.00	0.91
12:O:370:LYS:HG2	14:N:33:LYS:CA	1.99	0.91
9:V:163:LEU:HD23	11:Q:104:LEU:CD1	2.01	0.90
9:V:178:LEU:HD13	10:P:103:MET:HE3	0.91	0.90
9:V:159:LYS:HZ1	11:Q:108:ASN:CB	1.85	0.89
9:V:178:LEU:CD2	10:P:103:MET:HB2	2.03	0.89
9:V:178:LEU:HD11	10:P:103:MET:HE2	1.53	0.89
9:V:163:LEU:HD21	11:Q:104:LEU:CG	2.03	0.88
12:O:694:LEU:HD13	14:N:74:ARG:NH1	1.86	0.88
9:V:178:LEU:HD11	10:P:103:MET:HG2	1.56	0.87
9:V:180:ILE:N	11:Q:101:LEU:CD2	2.33	0.87
9:V:175:TYR:C	10:P:102:VAL:HG11	1.90	0.87
9:V:159:LYS:CD	11:Q:104:LEU:CD1	2.50	0.87
9:V:159:LYS:HZ1	11:Q:108:ASN:HB2	1.34	0.86
9:V:159:LYS:HD3	11:Q:104:LEU:HD11	1.53	0.86
9:V:184:LEU:HD23	11:Q:104:LEU:HD23	1.55	0.86
9:V:163:LEU:CD2	11:Q:104:LEU:CG	2.52	0.86
12:O:612:LYS:HB3	12:O:657:MET:HE1	1.57	0.86
12:O:680:LEU:HD23	12:O:721:CYS:SG	2.14	0.86
12:O:681:GLN:CG	12:O:725:LEU:HD21	2.03	0.86
9:V:142:VAL:HG23	9:V:144:GLY:N	1.91	0.86
9:V:171:LYS:NZ	10:P:106:GLN:CD	2.29	0.86
9:V:112:TYR:HB2	9:V:115:HIS:CE1	2.11	0.85
9:V:181:VAL:CG2	12:O:3:LEU:CB	2.53	0.85
9:V:181:VAL:HG11	12:O:3:LEU:O	1.75	0.85
9:V:180:ILE:CA	11:Q:101:LEU:HD22	1.96	0.85
9:V:180:ILE:CD1	11:Q:101:LEU:HD23	2.07	0.84
9:V:177:ARG:CB	10:P:102:VAL:N	2.40	0.84
9:V:159:LYS:NZ	11:Q:108:ASN:CB	2.39	0.84
12:O:316:GLN:NE2	14:N:32:GLU:OE1	2.11	0.84
9:V:76:PHE:CE2	9:V:109:ILE:HG12	2.13	0.83
9:V:203:GLN:O	9:V:206:ILE:HG13	1.79	0.83
9:V:178:LEU:HD22	10:P:103:MET:SD	2.19	0.83
5:E:203:TYR:CD1	5:E:309:LYS:HA	2.08	0.82
9:V:163:LEU:HG	11:Q:104:LEU:CD1	2.09	0.82
9:V:178:LEU:CA	10:P:100:PRO:CG	2.52	0.81
12:O:654:THR:HA	12:O:655:THR:HB	1.60	0.81
9:V:180:ILE:HD13	11:Q:101:LEU:HG	1.63	0.80
12:O:681:GLN:HG3	12:O:725:LEU:CD2	2.04	0.80
9:V:102:PRO:O	9:V:105:THR:HG22	1.81	0.80
12:O:688:MET:HG3	12:O:731:ILE:CD1	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:87:VAL:HB	9:V:118:LEU:CD1	2.12	0.80
9:V:90:ASN:HD21	9:V:92:ASP:HB2	1.44	0.79
9:V:163:LEU:CG	11:Q:104:LEU:CD1	2.57	0.79
9:V:178:LEU:HD13	10:P:103:MET:SD	2.21	0.79
12:O:680:LEU:HD11	12:O:703:VAL:HG11	1.65	0.79
9:V:115:HIS:O	9:V:137:VAL:HG23	1.83	0.79
12:O:612:LYS:CB	12:O:657:MET:HE1	2.09	0.79
5:E:203:TYR:CD1	5:E:309:LYS:HB2	2.16	0.78
9:V:162:CYS:SG	11:Q:95:ILE:CD1	2.70	0.78
9:V:181:VAL:CG2	12:O:3:LEU:HB3	2.06	0.78
12:O:316:GLN:CG	14:N:32:GLU:OE1	2.32	0.78
9:V:108:ARG:C	9:V:109:ILE:HD12	2.04	0.77
9:V:178:LEU:CD2	10:P:100:PRO:HG2	2.15	0.77
9:V:177:ARG:H	10:P:102:VAL:CG1	1.98	0.77
9:V:178:LEU:CA	10:P:100:PRO:HG3	2.11	0.77
12:O:680:LEU:HD11	12:O:718:ILE:HD12	1.66	0.77
12:O:657:MET:SD	12:O:660:ASP:HB3	2.25	0.77
5:E:203:TYR:CZ	5:E:309:LYS:HB3	2.19	0.77
5:E:115:GLU:HG3	12:O:693:VAL:CG1	2.15	0.76
5:E:106:ARG:NH1	14:N:76:GLY:C	2.38	0.76
9:V:171:LYS:CD	10:P:106:GLN:CB	2.63	0.76
9:V:159:LYS:NZ	11:Q:108:ASN:CG	2.38	0.76
9:V:163:LEU:HD23	11:Q:104:LEU:HD22	1.65	0.76
12:O:700:ILE:HD11	12:O:715:ILE:HD12	1.67	0.76
9:V:134:GLU:OE1	9:V:201:LEU:HD21	1.85	0.76
9:V:179:ASP:C	11:Q:101:LEU:HD22	2.05	0.76
12:O:661:THR:HG23	12:O:662:PRO:HD3	1.68	0.75
12:O:702:GLU:CD	14:N:74:ARG:HD3	2.05	0.75
12:O:660:ASP:HA	12:O:663:GLN:CG	2.15	0.75
4:D:240:GLN:O	4:D:303:ALA:HB2	1.87	0.75
9:V:206:ILE:HD12	9:V:207:ALA:N	2.02	0.75
9:V:163:LEU:HG	11:Q:104:LEU:HD11	1.65	0.74
9:V:181:VAL:HG13	12:O:3:LEU:O	1.87	0.74
12:O:654:THR:C	12:O:655:THR:OG1	2.26	0.74
12:O:370:LYS:NZ	14:N:32:GLU:C	2.40	0.74
12:O:370:LYS:NZ	14:N:35:GLY:H	1.85	0.73
9:V:77:CYS:HB3	9:V:79:ARG:NH1	2.04	0.73
5:E:235:ARG:H	6:F:46:LEU:H	1.35	0.73
9:V:184:LEU:HD23	11:Q:104:LEU:CD2	2.18	0.73
12:O:660:ASP:CA	12:O:663:GLN:HG2	2.19	0.73
9:V:177:ARG:HB2	10:P:102:VAL:N	2.03	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:697:ASN:O	12:O:700:ILE:HG22	1.89	0.72
9:V:62:VAL:CG1	9:V:205:ARG:HD2	2.18	0.72
9:V:163:LEU:HD22	11:Q:104:LEU:HD21	1.68	0.72
9:V:159:LYS:HE3	11:Q:104:LEU:HG	1.71	0.72
9:V:70:GLU:OE1	9:V:140:LEU:HD21	1.90	0.72
12:O:316:GLN:HG2	14:N:32:GLU:OE1	1.90	0.72
12:O:685:VAL:O	12:O:689:LYS:HG3	1.90	0.72
9:V:130:VAL:O	9:V:133:THR:HG22	1.91	0.71
9:V:171:LYS:HE3	10:P:106:GLN:OE1	1.91	0.71
9:V:163:LEU:CD2	11:Q:104:LEU:HD13	2.20	0.70
9:V:172:PRO:HA	9:V:175:TYR:CE2	2.26	0.70
9:V:75:ILE:HG21	9:V:148:PHE:CE2	2.26	0.70
9:V:61:PRO:O	9:V:64:ARG:HD3	1.91	0.70
9:V:184:LEU:HD23	11:Q:104:LEU:CG	2.22	0.70
5:E:98:LEU:HD22	5:E:113:ALA:HB1	1.74	0.70
9:V:163:LEU:HD23	11:Q:104:LEU:CG	2.20	0.69
12:O:700:ILE:CD1	12:O:715:ILE:HD12	2.22	0.69
12:O:731:ILE:HG23	12:O:742:SER:O	1.92	0.69
2:B:295:ASP:N	13:R:106:TYR:CE2	2.61	0.69
9:V:87:VAL:HB	9:V:118:LEU:HD11	1.74	0.69
9:V:177:ARG:HB3	10:P:102:VAL:N	2.00	0.69
9:V:180:ILE:HD13	11:Q:101:LEU:CG	2.22	0.69
5:E:203:TYR:CE1	5:E:309:LYS:HB3	2.24	0.69
9:V:158:LEU:HD23	11:Q:76:TYR:CD1	2.27	0.69
9:V:180:ILE:H	11:Q:101:LEU:HD22	1.53	0.69
12:O:680:LEU:CD1	12:O:703:VAL:HG11	2.22	0.69
9:V:184:LEU:HD22	11:Q:101:LEU:O	1.92	0.69
9:V:63:LEU:HD13	9:V:205:ARG:CZ	2.22	0.69
2:B:294:PHE:N	13:R:106:TYR:CE2	2.60	0.69
9:V:200:ARG:O	9:V:203:GLN:HG2	1.93	0.69
9:V:162:CYS:O	9:V:165:VAL:HG12	1.92	0.68
9:V:181:VAL:CG2	12:O:3:LEU:C	2.62	0.68
5:E:203:TYR:CE1	5:E:309:LYS:N	2.61	0.68
12:O:654:THR:OG1	12:O:655:THR:CB	2.41	0.68
12:O:684:ILE:HB	12:O:725:LEU:HD11	1.76	0.68
9:V:177:ARG:H	10:P:102:VAL:HG11	1.60	0.67
9:V:181:VAL:HG13	12:O:4:LYS:CA	2.25	0.67
12:O:685:VAL:CG1	12:O:689:LYS:HE3	2.15	0.67
9:V:62:VAL:HG12	9:V:205:ARG:HH11	1.58	0.67
9:V:163:LEU:HD22	9:V:188:LEU:HD23	1.76	0.67
12:O:657:MET:HG2	12:O:660:ASP:H	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:ARG:HD3	14:N:72:ALA:HA	1.76	0.67
9:V:63:LEU:HD21	9:V:202:THR:HA	1.76	0.67
5:E:112:ALA:CB	14:N:76:GLY:HA2	2.24	0.67
9:V:176:ARG:N	10:P:102:VAL:HG11	2.09	0.67
5:E:203:TYR:CE2	5:E:309:LYS:C	2.68	0.66
9:V:142:VAL:CG2	9:V:144:GLY:H	2.00	0.66
5:E:112:ALA:HB2	14:N:76:GLY:HA2	1.76	0.66
12:O:708:ARG:NH1	14:N:40:GLN:OE1	2.26	0.66
9:V:178:LEU:HB3	11:Q:101:LEU:HD11	1.77	0.66
9:V:182:ARG:H	12:O:5:PRO:HD3	0.57	0.66
9:V:181:VAL:HG22	12:O:3:LEU:C	2.15	0.66
9:V:163:LEU:HD23	11:Q:104:LEU:HD13	1.77	0.65
9:V:184:LEU:HD23	11:Q:104:LEU:HB3	1.77	0.65
12:O:662:PRO:O	12:O:666:GLU:HG3	1.97	0.65
9:V:74:VAL:HG22	9:V:147:ILE:HG22	1.76	0.65
12:O:680:LEU:HD11	12:O:718:ILE:CD1	2.24	0.65
9:V:170:VAL:CG1	10:P:103:MET:HA	2.26	0.65
9:V:159:LYS:HG2	11:Q:104:LEU:O	1.96	0.64
9:V:78:ASN:ND2	9:V:84:VAL:HG23	2.13	0.64
5:E:237:LEU:N	6:F:44:HIS:HB2	2.13	0.63
9:V:145:GLN:HB3	9:V:146:PRO:HD2	1.80	0.63
9:V:177:ARG:O	10:P:100:PRO:CB	2.43	0.63
9:V:182:ARG:N	12:O:5:PRO:CD	2.22	0.63
12:O:717:MET:HA	12:O:717:MET:CE	2.28	0.63
12:O:694:LEU:HD23	12:O:699:LEU:HA	1.80	0.63
9:V:171:LYS:HD2	10:P:106:GLN:CB	2.29	0.62
5:E:203:TYR:CG	5:E:309:LYS:HB2	2.32	0.62
9:V:63:LEU:HD13	9:V:205:ARG:NH2	2.14	0.62
9:V:80:SER:HB2	9:V:81:PRO:HD2	1.82	0.62
2:B:294:PHE:CB	13:R:106:TYR:CD1	2.83	0.62
9:V:159:LYS:CD	11:Q:104:LEU:HD11	2.25	0.62
9:V:178:LEU:HB2	11:Q:101:LEU:HD21	1.81	0.62
2:B:294:PHE:CB	13:R:106:TYR:CE1	2.82	0.61
9:V:170:VAL:CG2	10:P:103:MET:HG2	2.16	0.61
12:O:684:ILE:HB	12:O:725:LEU:CD1	2.31	0.61
12:O:744:VAL:HG12	12:O:745:ALA:O	2.00	0.61
9:V:57:GLY:O	9:V:59:PRO:HD3	1.99	0.61
9:V:167:ARG:HD3	9:V:191:HIS:CD2	2.35	0.61
12:O:393:LYS:NZ	12:O:661:THR:OG1	2.33	0.61
12:O:654:THR:OG1	12:O:655:THR:CA	2.47	0.61
12:O:694:LEU:CD1	14:N:74:ARG:NH1	2.62	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:PHE:HB3	13:R:106:TYR:CD1	2.35	0.61
9:V:178:LEU:HD21	10:P:103:MET:N	2.15	0.61
12:O:370:LYS:NZ	14:N:31:GLU:O	2.33	0.61
9:V:77:CYS:HB3	9:V:79:ARG:HH12	1.65	0.60
9:V:170:VAL:CG2	10:P:103:MET:HA	2.30	0.60
9:V:181:VAL:CG2	12:O:3:LEU:HB2	2.29	0.60
9:V:184:LEU:HD23	11:Q:104:LEU:CB	2.31	0.60
12:O:720:LYS:O	12:O:724:VAL:HG23	2.02	0.60
9:V:166:VAL:CG2	11:Q:100:ALA:HB1	2.31	0.60
9:V:69:ARG:O	9:V:71:PRO:HD3	2.00	0.60
9:V:145:GLN:HB3	9:V:146:PRO:CD	2.31	0.60
9:V:178:LEU:CD1	10:P:103:MET:SD	2.86	0.60
5:E:138:HIS:CE1	5:E:169:VAL:HG22	2.36	0.60
9:V:135:LEU:HD11	9:V:201:LEU:HD13	1.83	0.60
9:V:158:LEU:HD13	9:V:158:LEU:O	2.02	0.59
12:O:700:ILE:HD11	12:O:715:ILE:CD1	2.32	0.59
12:O:612:LYS:CB	12:O:657:MET:HE2	1.99	0.59
9:V:163:LEU:O	9:V:167:ARG:HG3	2.02	0.59
12:O:370:LYS:NZ	14:N:35:GLY:N	2.50	0.59
3:C:138:LEU:HD11	3:C:184:TYR:CE2	2.38	0.59
9:V:109:ILE:HD12	9:V:109:ILE:N	2.16	0.59
9:V:78:ASN:HD21	9:V:84:VAL:HG23	1.67	0.59
9:V:121:ASP:HB2	9:V:126:ASP:OD1	2.02	0.59
9:V:171:LYS:HD3	10:P:106:GLN:HB3	1.82	0.59
9:V:178:LEU:HD21	10:P:103:MET:HG3	0.95	0.59
12:O:680:LEU:HD21	12:O:718:ILE:CA	2.13	0.59
9:V:153:LEU:HD11	9:V:156:TYR:HE2	1.68	0.59
9:V:130:VAL:HG11	9:V:136:PHE:HB2	1.83	0.58
14:N:3:ILE:HG12	14:N:17:ILE:HD13	1.84	0.58
4:D:243:SER:HB2	4:D:303:ALA:HB3	1.85	0.58
9:V:90:ASN:ND2	9:V:92:ASP:H	2.01	0.58
9:V:181:VAL:CA	12:O:4:LYS:HA	2.28	0.58
9:V:102:PRO:HD2	9:V:105:THR:HG21	1.85	0.58
9:V:184:LEU:CD2	11:Q:101:LEU:O	2.51	0.58
9:V:170:VAL:CG1	10:P:102:VAL:O	2.51	0.58
12:O:656:SER:HB2	12:O:660:ASP:OD2	2.03	0.58
5:E:63:LEU:HD22	6:F:46:LEU:HD13	1.85	0.58
9:V:184:LEU:CD2	11:Q:104:LEU:HB3	2.33	0.58
9:V:171:LYS:CE	10:P:106:GLN:CD	2.72	0.58
5:E:106:ARG:HH12	14:N:76:GLY:C	2.06	0.58
5:E:235:ARG:H	6:F:46:LEU:N	2.00	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:696:HIS:HB2	12:O:739:ASP:HB3	1.86	0.58
9:V:178:LEU:HB3	11:Q:101:LEU:CD2	2.27	0.57
12:O:647:LYS:H	12:O:647:LYS:HD2	1.70	0.57
2:B:30:VAL:HG23	2:B:31:ASP:H	1.70	0.57
9:V:80:SER:O	9:V:103:PRO:HB3	2.04	0.57
5:E:232:SER:HA	6:F:45:PRO:HB3	1.86	0.57
9:V:90:ASN:HD21	9:V:92:ASP:CB	2.16	0.56
9:V:159:LYS:CE	11:Q:104:LEU:CD1	2.82	0.56
9:V:159:LYS:HZ2	11:Q:108:ASN:CB	2.18	0.56
4:D:243:SER:CA	4:D:303:ALA:HB3	2.35	0.56
9:V:158:LEU:HD23	11:Q:76:TYR:CG	2.39	0.56
12:O:661:THR:CG2	12:O:662:PRO:HD3	2.35	0.56
5:E:203:TYR:CD2	5:E:309:LYS:CG	2.88	0.56
9:V:121:ASP:HB3	9:V:124:THR:OG1	2.05	0.56
9:V:174:ASN:CB	10:P:102:VAL:C	2.46	0.56
9:V:178:LEU:CD2	10:P:103:MET:N	2.68	0.56
12:O:660:ASP:O	12:O:663:GLN:HG2	2.04	0.56
9:V:130:VAL:O	9:V:130:VAL:HG13	2.06	0.56
12:O:694:LEU:HD23	12:O:699:LEU:CA	2.35	0.56
4:D:316:TYR:HB2	4:D:365:GLU:HA	1.87	0.56
14:N:55:THR:OG1	14:N:58:ASP:OD1	2.23	0.56
9:V:144:GLY:O	9:V:145:GLN:HB2	2.06	0.56
9:V:155:VAL:HG23	9:V:155:VAL:O	2.06	0.56
9:V:170:VAL:HG13	10:P:102:VAL:O	2.06	0.56
5:E:233:LEU:O	6:F:44:HIS:CD2	2.59	0.56
9:V:184:LEU:HD21	11:Q:105:MET:H	1.65	0.56
12:O:723:GLU:O	12:O:726:ILE:HG12	2.06	0.55
12:O:685:VAL:HG12	12:O:689:LYS:CE	2.20	0.55
2:B:294:PHE:N	13:R:106:TYR:CZ	2.73	0.55
4:D:243:SER:H	4:D:303:ALA:H	1.53	0.55
5:E:106:ARG:NH1	14:N:76:GLY:H	2.04	0.55
9:V:177:ARG:NE	10:P:102:VAL:N	2.54	0.55
12:O:694:LEU:HG	12:O:698:ALA:HB3	1.88	0.55
5:E:234:ASP:HA	6:F:44:HIS:CE1	2.42	0.55
9:V:166:VAL:HG22	11:Q:100:ALA:HB1	1.86	0.55
14:N:11:LYS:HG3	14:N:12:GLU:H	1.71	0.55
12:O:717:MET:HE2	12:O:720:LYS:HD2	1.88	0.55
9:V:85:LEU:C	9:V:85:LEU:HD13	2.28	0.55
9:V:159:LYS:HZ2	11:Q:108:ASN:CG	2.09	0.54
9:V:75:ILE:O	9:V:75:ILE:HG23	2.06	0.54
9:V:178:LEU:C	11:Q:101:LEU:HD21	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:181:VAL:HG13	12:O:4:LYS:HA	1.89	0.54
4:D:316:TYR:HB2	4:D:365:GLU:H	1.72	0.54
5:E:237:LEU:HD22	6:F:190:LEU:HA	1.90	0.54
9:V:159:LYS:HG3	11:Q:108:ASN:HB2	1.88	0.54
14:N:5:VAL:HG22	14:N:67:LEU:HB2	1.88	0.54
9:V:63:LEU:HD23	9:V:202:THR:OG1	2.08	0.54
9:V:159:LYS:CE	11:Q:104:LEU:HG	2.36	0.54
5:E:233:LEU:CB	6:F:47:VAL:HG22	2.38	0.54
9:V:87:VAL:HB	9:V:118:LEU:HD12	1.85	0.54
12:O:700:ILE:HG23	12:O:701:GLN:N	2.23	0.54
3:C:64:VAL:HG12	3:C:64:VAL:O	2.08	0.53
5:E:237:LEU:HG	6:F:44:HIS:CG	2.44	0.53
5:E:233:LEU:O	6:F:44:HIS:O	2.27	0.53
9:V:88:TRP:HB3	9:V:98:TYR:HE2	1.73	0.53
9:V:163:LEU:HG	11:Q:104:LEU:HD13	1.88	0.53
9:V:178:LEU:C	10:P:100:PRO:HG3	2.27	0.53
12:O:693:VAL:HG13	12:O:741:TYR:O	2.08	0.53
2:B:295:ASP:N	13:R:106:TYR:CZ	2.77	0.53
5:E:106:ARG:HH11	14:N:76:GLY:H	1.56	0.53
2:B:270:SER:HB2	2:B:271:PRO:HA	1.90	0.53
9:V:180:ILE:CD1	11:Q:101:LEU:CD2	2.77	0.53
12:O:72:LEU:O	12:O:76:VAL:HG23	2.08	0.53
9:V:67:ASN:HA	9:V:91:PHE:HE1	1.73	0.53
9:V:79:ARG:HB2	9:V:151:ILE:O	2.08	0.53
9:V:112:TYR:HB2	9:V:115:HIS:ND1	2.24	0.53
9:V:181:VAL:CG1	12:O:3:LEU:C	2.77	0.53
9:V:74:VAL:HG22	9:V:147:ILE:HG23	1.87	0.53
12:O:657:MET:HG2	12:O:660:ASP:N	2.23	0.53
12:O:726:ILE:HG22	12:O:731:ILE:O	2.09	0.53
9:V:142:VAL:HG23	9:V:143:ASP:N	2.24	0.53
7:H:80:ARG:HB2	7:H:89:ILE:HD13	1.90	0.53
12:O:675:ASP:O	12:O:679:TYR:HD1	1.92	0.53
5:E:112:ALA:HB2	14:N:76:GLY:CA	2.37	0.52
9:V:76:PHE:HE2	9:V:109:ILE:HG12	1.68	0.52
11:Q:59:GLU:HG2	12:O:32:ARG:HE	1.75	0.52
12:O:700:ILE:CD1	12:O:715:ILE:HG23	2.39	0.52
9:V:118:LEU:HD12	9:V:118:LEU:C	2.29	0.52
5:E:237:LEU:H	6:F:44:HIS:HB2	1.74	0.52
5:E:316:HIS:CE1	6:F:220:HIS:HB2	2.45	0.52
9:V:90:ASN:ND2	9:V:92:ASP:HB2	2.19	0.52
12:O:88:HIS:CG	12:O:183:GLY:HA3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:237:LEU:HG	6:F:44:HIS:CB	2.40	0.52
12:O:699:LEU:O	12:O:703:VAL:HG23	2.10	0.52
2:B:180:GLN:HB2	2:B:181:THR:HG23	1.92	0.52
9:V:159:LYS:NZ	11:Q:108:ASN:ND2	2.58	0.52
9:V:70:GLU:CD	9:V:113:ARG:HE	2.13	0.52
9:V:159:LYS:HZ2	11:Q:108:ASN:HB2	1.68	0.51
9:V:165:VAL:HG13	9:V:166:VAL:N	2.25	0.51
14:N:44:ILE:HD11	14:N:70:VAL:HG12	1.92	0.51
9:V:62:VAL:HG11	9:V:205:ARG:HD2	1.91	0.51
12:O:667:GLN:HA	12:O:667:GLN:OE1	2.11	0.51
5:E:239:GLU:HG3	6:F:200:VAL:HG11	1.91	0.51
9:V:59:PRO:O	9:V:60:ARG:HB2	2.10	0.51
9:V:206:ILE:HD12	9:V:206:ILE:C	2.30	0.51
2:B:294:PHE:O	13:R:106:TYR:CD1	2.62	0.51
5:E:235:ARG:N	6:F:46:LEU:H	2.07	0.51
12:O:654:THR:OG1	12:O:655:THR:OG1	2.26	0.51
9:V:76:PHE:HD1	9:V:149:ALA:HB3	1.74	0.51
9:V:118:LEU:HD12	9:V:118:LEU:O	2.11	0.51
12:O:684:ILE:HG21	12:O:725:LEU:HD12	1.92	0.51
14:N:3:ILE:HD12	14:N:67:LEU:HD13	1.93	0.51
12:O:717:MET:HA	12:O:717:MET:HE2	1.93	0.50
9:V:159:LYS:HZ1	11:Q:108:ASN:CG	2.09	0.50
12:O:77:LEU:HD22	12:O:155:LEU:HD13	1.93	0.50
9:V:74:VAL:HG12	9:V:75:ILE:N	2.26	0.50
11:Q:42:ILE:HG23	11:Q:60:VAL:HG21	1.93	0.50
12:O:660:ASP:C	12:O:663:GLN:HG2	2.31	0.50
9:V:76:PHE:CD2	9:V:109:ILE:CD1	2.95	0.50
9:V:159:LYS:HG3	11:Q:108:ASN:CA	2.41	0.50
4:D:168:ILE:HG21	4:D:194:VAL:HG21	1.93	0.50
9:V:176:ARG:HH21	9:V:185:TYR:HE2	1.56	0.50
12:O:660:ASP:HA	12:O:663:GLN:CD	2.31	0.50
9:V:75:ILE:CG2	9:V:148:PHE:CD2	2.95	0.50
9:V:147:ILE:HG23	9:V:147:ILE:O	2.12	0.50
9:V:177:ARG:N	10:P:102:VAL:HG11	2.26	0.50
12:O:370:LYS:CG	14:N:33:LYS:CA	2.72	0.50
9:V:159:LYS:CE	11:Q:108:ASN:HB2	2.43	0.49
12:O:509:ILE:HG22	13:R:28:ASN:HB2	1.94	0.49
14:N:26:ILE:O	14:N:30:VAL:HG23	2.11	0.49
9:V:101:LEU:HB3	9:V:105:THR:CG2	2.41	0.49
9:V:181:VAL:HG13	12:O:3:LEU:C	2.32	0.49
12:O:687:ILE:HG21	12:O:702:GLU:OE1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:312:ILE:HD13	12:O:363:HIS:CD2	2.47	0.49
12:O:708:ARG:NH1	14:N:40:GLN:CD	2.66	0.49
4:D:243:SER:CB	4:D:303:ALA:HB3	2.43	0.49
9:V:120:ARG:HD2	9:V:127:GLY:HA2	1.94	0.49
9:V:178:LEU:CD2	10:P:103:MET:SD	2.84	0.49
5:E:233:LEU:HB2	6:F:47:VAL:HG22	1.93	0.49
5:E:203:TYR:CE2	5:E:309:LYS:CG	2.95	0.49
12:O:661:THR:HG23	12:O:662:PRO:CD	2.42	0.49
12:O:661:THR:N	12:O:662:PRO:HD2	2.28	0.49
12:O:723:GLU:HA	12:O:726:ILE:HG12	1.95	0.48
12:O:700:ILE:HD11	12:O:715:ILE:HG23	1.95	0.48
2:B:72:LEU:HB3	2:B:95:LEU:HD21	1.94	0.48
3:C:305:LYS:HA	3:C:308:GLN:HG2	1.96	0.48
12:O:376:VAL:HG21	12:O:424:TYR:CD2	2.48	0.48
12:O:514:ALA:HA	13:R:32:LEU:HD22	1.95	0.48
5:E:236:LYS:HB3	6:F:44:HIS:HA	1.96	0.48
5:E:234:ASP:H	6:F:47:VAL:H	1.60	0.48
9:V:66:VAL:O	9:V:66:VAL:HG23	2.14	0.47
9:V:65:SER:HA	9:V:116:LEU:HD13	1.96	0.47
9:V:67:ASN:HA	9:V:91:PHE:CE1	2.49	0.47
9:V:154:PRO:HG2	9:V:156:TYR:CE1	2.49	0.47
9:V:158:LEU:HD13	9:V:162:CYS:SG	2.53	0.47
12:O:701:GLN:HE22	14:N:39:GLN:NE2	2.13	0.47
3:C:39:LEU:HB3	3:C:58:VAL:HG13	1.95	0.47
3:C:71:VAL:HB	3:C:72:PRO:HD2	1.95	0.47
9:V:76:PHE:O	9:V:106:GLY:HA2	2.15	0.47
9:V:170:VAL:HG13	10:P:103:MET:HA	1.95	0.47
9:V:172:PRO:HA	9:V:175:TYR:CD2	2.49	0.47
1:A:247:THR:HG23	1:A:274:SER:H	1.80	0.47
2:B:214:LEU:HD22	2:B:240:CYS:SG	2.55	0.47
2:B:294:PHE:O	13:R:106:TYR:CG	2.67	0.47
2:B:300:LYS:H	2:B:301:PRO:HD2	1.79	0.47
5:E:238:LEU:H	5:E:238:LEU:HG	1.43	0.47
12:O:694:LEU:CD2	12:O:699:LEU:HA	2.44	0.47
9:V:130:VAL:HA	9:V:150:ASN:O	2.15	0.47
3:C:205:TYR:CZ	3:C:226:LYS:HB3	2.50	0.47
14:N:54:LYS:NZ	14:N:58:ASP:OD2	2.31	0.47
9:V:208:HIS:O	9:V:210:ARG:HD2	2.15	0.47
9:V:159:LYS:O	9:V:163:LEU:HG	2.15	0.46
9:V:163:LEU:HD22	9:V:188:LEU:CD2	2.43	0.46
12:O:700:ILE:O	12:O:704:ILE:HD13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:137:VAL:O	9:V:137:VAL:HG13	2.15	0.46
5:E:236:LYS:HB2	6:F:45:PRO:HD2	1.96	0.46
5:E:237:LEU:CA	6:F:44:HIS:HB2	2.44	0.46
12:O:503:LEU:H	13:R:25:LYS:HG3	1.79	0.46
5:E:92:ILE:HD13	5:E:134:ILE:HD13	1.98	0.46
12:O:612:LYS:HB2	12:O:657:MET:HE1	1.94	0.46
12:O:711:PHE:O	12:O:713:PRO:HD3	2.16	0.46
3:C:180:HIS:HA	3:C:183:CYS:SG	2.56	0.46
9:V:163:LEU:CD2	11:Q:104:LEU:HD22	2.23	0.46
9:V:177:ARG:CB	10:P:102:VAL:CA	2.50	0.46
12:O:660:ASP:O	12:O:664:GLU:HG3	2.16	0.46
12:O:732:GLU:HG2	12:O:733:ARG:N	2.30	0.46
9:V:67:ASN:CA	9:V:91:PHE:HE1	2.29	0.46
9:V:67:ASN:CA	9:V:91:PHE:CE1	2.99	0.46
9:V:178:LEU:HD23	10:P:103:MET:H	1.80	0.46
9:V:63:LEU:N	9:V:63:LEU:HD22	2.30	0.46
9:V:171:LYS:HE3	10:P:106:GLN:CD	2.36	0.46
9:V:184:LEU:HB3	11:Q:104:LEU:HD23	1.98	0.46
9:V:171:LYS:CE	10:P:106:GLN:OE1	2.63	0.46
12:O:654:THR:C	12:O:655:THR:CG2	2.84	0.46
9:V:158:LEU:HD13	9:V:158:LEU:C	2.35	0.45
2:B:282:LEU:HD11	2:B:346:HIS:CD2	2.52	0.45
9:V:62:VAL:HG12	9:V:205:ARG:HD2	1.95	0.45
12:O:680:LEU:CD1	12:O:703:VAL:CG1	2.94	0.45
12:O:681:GLN:HE22	12:O:728:LYS:NZ	2.14	0.45
9:V:109:ILE:HG22	9:V:110:HIS:N	2.30	0.45
9:V:162:CYS:O	9:V:166:VAL:HG23	2.15	0.45
12:O:509:ILE:O	12:O:510:TYR:CG	2.68	0.45
5:E:241:LEU:HG	6:F:192:THR:HA	1.99	0.45
11:Q:44:ALA:HB1	12:O:103:CYS:HB3	1.98	0.45
12:O:684:ILE:HG22	12:O:731:ILE:CD1	2.46	0.45
5:E:203:TYR:CD1	5:E:309:LYS:N	2.85	0.45
6:F:258:ARG:HB2	8:G:159:GLY:HA3	1.99	0.45
9:V:64:ARG:HG2	9:V:64:ARG:HH11	1.82	0.45
12:O:283:HIS:CE1	12:O:287:ARG:HH21	2.35	0.45
12:O:714:SER:HB2	12:O:717:MET:HG2	1.99	0.45
6:F:56:ILE:HG23	6:F:59:ARG:HH21	1.80	0.45
9:V:76:PHE:CD2	9:V:109:ILE:HD11	2.52	0.45
12:O:735:GLN:OE1	12:O:735:GLN:HA	2.15	0.45
9:V:70:GLU:HG3	9:V:113:ARG:HB3	1.99	0.45
9:V:159:LYS:HG3	11:Q:108:ASN:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:GLU:CB	12:O:538:GLN:HE22	2.30	0.45
4:D:175:GLN:HG3	4:D:187:TYR:CD2	2.51	0.45
5:E:236:LYS:HB2	6:F:45:PRO:CD	2.46	0.45
9:V:181:VAL:HG22	12:O:3:LEU:HB2	1.98	0.45
14:N:51:ASN:OD1	14:N:52:ASP:N	2.44	0.45
9:V:84:VAL:HG22	9:V:128:LEU:CD1	2.47	0.44
3:C:221:LEU:HD11	3:C:256:LEU:HD13	1.98	0.44
10:P:99:LEU:HD23	11:Q:98:GLU:HA	1.99	0.44
14:N:61:ILE:HD13	14:N:67:LEU:HD11	1.99	0.44
7:H:200:LEU:O	7:H:204:VAL:HG23	2.18	0.44
9:V:180:ILE:CG1	11:Q:101:LEU:CD2	1.87	0.44
12:O:717:MET:HA	12:O:717:MET:HE3	1.99	0.44
2:B:314:LEU:HD11	2:B:326:PHE:CZ	2.52	0.44
3:C:112:VAL:HG22	3:C:151:LEU:HD22	2.00	0.44
9:V:62:VAL:HG12	9:V:205:ARG:NH1	2.28	0.44
3:C:138:LEU:HD11	3:C:184:TYR:CD2	2.52	0.44
9:V:88:TRP:HE1	9:V:115:HIS:CD2	2.35	0.44
9:V:163:LEU:CG	11:Q:104:LEU:HD13	2.41	0.44
9:V:174:ASN:CG	10:P:102:VAL:HA	2.37	0.44
9:V:177:ARG:CB	10:P:102:VAL:H	1.96	0.44
3:C:12:VAL:HG21	3:C:54:HIS:HB2	2.00	0.44
9:V:60:ARG:HB3	9:V:61:PRO:HD2	1.99	0.43
3:C:263:LEU:HD12	3:C:275:LEU:HD11	2.00	0.43
9:V:178:LEU:CD2	10:P:103:MET:H	2.30	0.43
12:O:656:SER:HB3	12:O:657:MET:SD	2.58	0.43
3:C:153:LYS:H	3:C:153:LYS:HD2	1.83	0.43
9:V:73:GLN:HG2	9:V:146:PRO:HG3	2.00	0.43
5:E:175:THR:OG1	6:F:198:ILE:HD13	2.19	0.43
12:O:659:LYS:C	12:O:662:PRO:HD2	2.39	0.43
5:E:233:LEU:HB3	6:F:47:VAL:HG22	2.00	0.43
12:O:319:ILE:HD12	12:O:350:PHE:CG	2.52	0.43
14:N:37:PRO:HA	14:N:38:PRO:HD3	1.83	0.43
8:G:123:ARG:HG3	8:G:123:ARG:HH11	1.84	0.43
9:V:188:LEU:HD21	11:Q:104:LEU:HD22	2.00	0.43
12:O:654:THR:CB	12:O:655:THR:HB	2.44	0.43
12:O:684:ILE:CG2	12:O:725:LEU:CD1	2.97	0.43
9:V:124:THR:O	9:V:125:HIS:HB2	2.19	0.43
6:F:314:ASP:CG	6:F:315:ARG:H	2.21	0.43
9:V:74:VAL:HG13	9:V:147:ILE:O	2.19	0.43
9:V:177:ARG:CZ	10:P:101:ASP:C	2.67	0.43
4:D:317:ASN:HB2	4:D:368:PRO:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:TYR:CE2	6:F:111:GLN:HB2	2.53	0.42
9:V:171:LYS:HD2	10:P:106:GLN:H	1.84	0.42
12:O:370:LYS:NZ	14:N:32:GLU:O	2.52	0.42
12:O:617:LEU:HG	12:O:623:ILE:HD13	2.01	0.42
12:O:659:LYS:O	12:O:662:PRO:HD2	2.19	0.42
6:F:46:LEU:HD23	6:F:47:VAL:HA	2.01	0.42
9:V:166:VAL:HG13	10:P:103:MET:HE2	2.00	0.42
2:B:101:SER:HB3	2:B:102:ALA:H	1.62	0.42
9:V:159:LYS:CE	11:Q:104:LEU:HD11	2.49	0.42
12:O:654:THR:CA	12:O:655:THR:CB	2.73	0.42
12:O:680:LEU:CD1	12:O:718:ILE:CD1	2.94	0.42
9:V:142:VAL:CG2	9:V:143:ASP:N	2.82	0.42
1:A:141:LYS:HB3	1:A:141:LYS:HZ2	1.85	0.42
9:V:170:VAL:HG12	9:V:171:LYS:O	2.19	0.42
9:V:185:TYR:HD2	9:V:186:GLU:OE2	2.03	0.42
5:E:234:ASP:HA	6:F:44:HIS:CG	2.55	0.42
5:E:334:SER:H	8:G:173:THR:HG22	1.85	0.42
2:B:93:LYS:HA	2:B:96:LEU:HD12	2.02	0.42
5:E:181:VAL:HG21	6:F:199:GLY:HA2	2.01	0.42
12:O:700:ILE:CG2	12:O:701:GLN:N	2.82	0.42
2:B:229:PRO:CB	12:O:474:HIS:CE1	3.03	0.42
9:V:119:PHE:CD1	9:V:119:PHE:N	2.87	0.42
9:V:158:LEU:CD1	9:V:162:CYS:SG	3.07	0.42
2:B:363:ILE:HG13	2:B:411:LEU:HD21	2.02	0.41
9:V:170:VAL:HG22	10:P:103:MET:O	2.20	0.41
9:V:177:ARG:HD3	10:P:102:VAL:HA	2.01	0.41
12:O:73:HIS:CE1	12:O:77:LEU:HD11	2.54	0.41
5:E:150:ILE:H	5:E:150:ILE:HD12	1.85	0.41
9:V:109:ILE:N	9:V:109:ILE:CD1	2.83	0.41
9:V:165:VAL:CG1	9:V:166:VAL:N	2.82	0.41
9:V:181:VAL:HG22	12:O:3:LEU:CB	2.43	0.41
12:O:475:ARG:HE	13:R:66:GLU:HA	1.85	0.41
3:C:59:LEU:HD23	3:C:77:LEU:HD11	2.02	0.41
5:E:112:ALA:HB1	14:N:76:GLY:HA2	1.99	0.41
5:E:205:THR:HG21	5:E:261:TYR:CG	2.55	0.41
5:E:233:LEU:O	6:F:44:HIS:CG	2.73	0.41
5:E:300:LEU:HD23	5:E:300:LEU:HA	1.89	0.41
12:O:694:LEU:CG	12:O:698:ALA:HB3	2.50	0.41
9:V:111:SER:HB3	9:V:112:TYR:H	1.71	0.41
9:V:178:LEU:HA	10:P:100:PRO:CB	2.43	0.41
9:V:178:LEU:N	10:P:102:VAL:HB	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:44:LEU:HD23	10:P:44:LEU:HA	1.93	0.41
14:N:42:ARG:HG2	14:N:49:GLN:OE1	2.20	0.41
12:O:680:LEU:HD12	12:O:703:VAL:CG1	2.51	0.41
12:O:731:ILE:HG22	12:O:732:GLU:N	2.36	0.41
14:N:48:LYS:HE3	14:N:48:LYS:HB2	1.87	0.41
13:R:53:CYS:SG	13:R:80:HIS:CD2	3.13	0.41
9:V:109:ILE:CG2	9:V:110:HIS:N	2.84	0.41
5:E:237:LEU:HG	6:F:44:HIS:HB2	2.02	0.41
9:V:130:VAL:CG2	9:V:149:ALA:HB1	2.50	0.41
3:C:269:THR:O	3:C:270:ASN:HB2	2.20	0.41
4:D:316:TYR:CB	4:D:365:GLU:H	2.34	0.41
9:V:74:VAL:CG1	9:V:75:ILE:N	2.84	0.41
9:V:82:ARG:HD2	9:V:121:ASP:OD2	2.20	0.41
9:V:206:ILE:HD12	9:V:207:ALA:CA	2.51	0.41
12:O:473:LEU:N	12:O:473:LEU:HD22	2.36	0.41
9:V:170:VAL:HG12	9:V:171:LYS:N	2.35	0.41
12:O:512:LEU:HB2	13:R:32:LEU:HD23	2.01	0.41
12:O:725:LEU:HD23	12:O:725:LEU:HA	1.92	0.41
12:O:306:THR:CG2	14:N:2:LEU:HD21	2.51	0.40
2:B:418:GLY:O	2:B:422:THR:HG22	2.22	0.40
9:V:159:LYS:HZ1	11:Q:108:ASN:ND2	2.17	0.40
9:V:181:VAL:CG2	12:O:4:LYS:N	2.67	0.40
12:O:694:LEU:HD11	12:O:698:ALA:CB	2.51	0.40
2:B:171:ILE:HG13	2:B:172:LEU:N	2.37	0.40
4:D:131:PRO:HG3	12:O:552:LYS:NZ	2.36	0.40
6:F:200:VAL:O	6:F:200:VAL:HG12	2.22	0.40
9:V:107:ARG:HG2	9:V:108:ARG:N	2.37	0.40
12:O:513:GLN:HB2	12:O:516:ALA:HB3	2.03	0.40
9:V:129:LEU:O	9:V:151:ILE:HA	2.21	0.40
9:V:142:VAL:C	9:V:144:GLY:N	2.75	0.40
12:O:654:THR:CB	12:O:655:THR:CB	2.99	0.40
12:O:657:MET:CG	12:O:660:ASP:HB3	2.51	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	431/433 (100%)	399 (93%)	26 (6%)	6 (1%)	11 46
2	B	412/443 (93%)	364 (88%)	33 (8%)	15 (4%)	3 25
3	C	401/403 (100%)	361 (90%)	26 (6%)	14 (4%)	3 25
4	D	404/406 (100%)	387 (96%)	8 (2%)	9 (2%)	6 35
5	E	309/311 (99%)	290 (94%)	15 (5%)	4 (1%)	12 48
6	F	286/288 (99%)	272 (95%)	8 (3%)	6 (2%)	7 36
7	H	164/209 (78%)	158 (96%)	5 (3%)	1 (1%)	25 66
8	G	206/208 (99%)	189 (92%)	13 (6%)	4 (2%)	8 38
9	V	158/160 (99%)	154 (98%)	1 (1%)	3 (2%)	8 38
10	P	116/118 (98%)	109 (94%)	7 (6%)	0	100 100
11	Q	110/112 (98%)	102 (93%)	8 (7%)	0	100 100
12	O	738/745 (99%)	691 (94%)	29 (4%)	18 (2%)	6 33
13	R	88/90 (98%)	70 (80%)	13 (15%)	5 (6%)	1 18
14	N	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
All	All	3897/4002 (97%)	3617 (93%)	195 (5%)	85 (2%)	10 35

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ALA
1	A	426	ALA
2	B	61	GLU
2	B	141	ASP
2	B	186	ASP
2	B	411	LEU
3	C	51	VAL
3	C	70	SER
3	C	71	VAL
3	C	134	ASN
4	D	294	ALA
4	D	300	LEU
4	D	363	THR
4	D	364	ARG
6	F	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	193	GLU
7	H	158	THR
9	V	145	GLN
12	O	234	GLN
12	O	272	ALA
12	O	505	ILE
12	O	739	ASP
13	R	36	ASP
13	R	60	GLN
13	R	68	CYS
1	A	278	CYS
2	B	229	PRO
2	B	299	ALA
2	B	379	ASN
3	C	136	ASN
3	C	154	CYS
3	C	168	ASP
3	C	362	ASP
4	D	236	ALA
4	D	295	ASP
6	F	249	GLU
8	G	161	ASP
12	O	138	GLU
12	O	290	LYS
12	O	383	SER
12	O	522	ALA
12	O	525	SER
1	A	238	ARG
2	B	182	ASP
2	B	231	PRO
3	C	173	ASN
4	D	238	ALA
4	D	365	GLU
5	E	99	PRO
6	F	213	GLU
8	G	160	ARG
8	G	163	ARG
12	O	49	TYR
12	O	502	ASP
12	O	510	TYR
13	R	62	SER
1	A	86	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	163	GLU
2	B	185	GLU
2	B	270	SER
3	C	89	ASN
3	C	172	GLU
4	D	299	ILE
6	F	95	GLU
8	G	24	GLY
12	O	171	ARG
12	O	529	ILE
12	O	536	SER
13	R	42	CYS
2	B	300	LYS
2	B	301	PRO
3	C	67	SER
3	C	270	ASN
5	E	102	GLY
5	E	196	PRO
2	B	84	ASN
3	C	48	ALA
12	O	173	GLY
12	O	191	VAL
6	F	164	PRO
9	V	142	VAL
12	O	154	PRO
1	A	117	PRO
9	V	60	ARG
5	E	172	PRO

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	377/377 (100%)	363 (96%)	14 (4%)	34	58
2	B	376/405 (93%)	356 (95%)	20 (5%)	22	47
3	C	359/359 (100%)	348 (97%)	11 (3%)	40	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	347/347 (100%)	342 (99%)	5 (1%)	67 80
5	E	267/267 (100%)	250 (94%)	17 (6%)	17 42
6	F	255/255 (100%)	237 (93%)	18 (7%)	14 39
7	H	139/173 (80%)	133 (96%)	6 (4%)	29 53
8	G	181/181 (100%)	171 (94%)	10 (6%)	21 47
9	V	147/147 (100%)	145 (99%)	2 (1%)	67 80
10	P	103/103 (100%)	99 (96%)	4 (4%)	32 56
11	Q	96/96 (100%)	95 (99%)	1 (1%)	76 86
12	O	680/681 (100%)	644 (95%)	36 (5%)	22 47
13	R	79/79 (100%)	70 (89%)	9 (11%)	5 21
14	N	64/66 (97%)	60 (94%)	4 (6%)	18 43
All	All	3470/3536 (98%)	3313 (96%)	157 (4%)	31 52

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	87	ASN
1	A	89	ASP
1	A	140	LEU
1	A	174	ASP
1	A	178	LEU
1	A	238	ARG
1	A	258	LEU
1	A	275	PHE
1	A	280	PHE
1	A	283	LEU
1	A	348	MET
1	A	462	ASN
1	A	468	SER
2	B	42	LEU
2	B	66	GLU
2	B	69	PHE
2	B	70	LYS
2	B	83	THR
2	B	87	GLU
2	B	100	ARG
2	B	115	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	124	GLN
2	B	146	ARG
2	B	190	LYS
2	B	253	LYS
2	B	303	LYS
2	B	320	ASN
2	B	330	LEU
2	B	337	ILE
2	B	363	ILE
2	B	384	ASP
2	B	391	GLN
2	B	409	LEU
3	C	5	LEU
3	C	29	ASN
3	C	51	VAL
3	C	125	LYS
3	C	153	LYS
3	C	217	SER
3	C	302	LEU
3	C	337	TYR
3	C	363	ASN
3	C	385	GLU
3	C	402	GLN
4	D	202	ILE
4	D	300	LEU
4	D	316	TYR
4	D	368	PRO
4	D	385	LEU
5	E	80	LEU
5	E	85	VAL
5	E	130	LEU
5	E	131	GLU
5	E	165	PHE
5	E	191	LYS
5	E	206	ILE
5	E	213	ASP
5	E	219	LYS
5	E	227	SER
5	E	229	PHE
5	E	240	LEU
5	E	241	LEU
5	E	261	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	282	ARG
5	E	305	ARG
5	E	315	ILE
6	F	30	VAL
6	F	44	HIS
6	F	46	LEU
6	F	47	VAL
6	F	49	LEU
6	F	50	ASN
6	F	64	ARG
6	F	67	GLN
6	F	73	ILE
6	F	112	PHE
6	F	132	ASP
6	F	154	LEU
6	F	163	LEU
6	F	172	ILE
6	F	197	ARG
6	F	214	ASN
6	F	259	GLU
6	F	269	VAL
7	H	16	LEU
7	H	40	LEU
7	H	71	LEU
7	H	105	ILE
7	H	146	LYS
7	H	197	LEU
8	G	23	SER
8	G	27	LEU
8	G	45	GLU
8	G	87	GLU
8	G	111	ILE
8	G	117	LEU
8	G	136	VAL
8	G	148	ARG
8	G	155	ASP
8	G	178	CYS
9	V	54	MET
9	V	210	ARG
10	P	14	ILE
10	P	70	GLN
10	P	97	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	P	99	LEU
11	Q	51	GLN
12	O	11	ASP
12	O	50	PRO
12	O	58	TYR
12	O	75	ARG
12	O	87	TYR
12	O	108	LEU
12	O	115	LYS
12	O	131	ASP
12	O	148	ARG
12	O	162	MET
12	O	168	LYS
12	O	175	ASP
12	O	184	VAL
12	O	211	PHE
12	O	255	HIS
12	O	261	LYS
12	O	275	LEU
12	O	276	GLN
12	O	293	ASP
12	O	379	ARG
12	O	386	LYS
12	O	411	VAL
12	O	420	THR
12	O	439	LEU
12	O	477	TYR
12	O	501	ILE
12	O	531	GLN
12	O	537	VAL
12	O	565	LYS
12	O	592	GLU
12	O	607	GLU
12	O	614	ILE
12	O	621	LYS
12	O	647	LYS
12	O	652	LYS
12	O	657	MET
13	R	37	ILE
13	R	39	VAL
13	R	50	MET
13	R	64	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	R	72	TRP
13	R	75	CYS
13	R	82	HIS
13	R	87	TRP
13	R	99	ARG
14	N	17	ILE
14	N	42	ARG
14	N	68	HIS
14	N	70	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	171	HIS
1	A	197	HIS
1	A	307	GLN
2	B	35	GLN
2	B	297	GLN
2	B	320	ASN
2	B	333	ASN
2	B	346	HIS
3	C	14	GLN
3	C	132	GLN
4	D	231	HIS
4	D	380	GLN
5	E	36	GLN
5	E	50	HIS
5	E	138	HIS
5	E	316	HIS
6	F	114	GLN
6	F	202	HIS
6	F	214	ASN
6	F	225	HIS
6	F	316	GLN
8	G	33	GLN
8	G	190	GLN
8	G	203	ASN
9	V	90	ASN
9	V	115	HIS
9	V	145	GLN
11	Q	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	O	73	HIS
12	O	88	HIS
12	O	111	GLN
12	O	190	HIS
12	O	267	GLN
12	O	283	HIS
12	O	310	HIS
12	O	318	HIS
12	O	363	HIS
12	O	377	ASN
12	O	491	ASN
12	O	513	GLN
12	O	538	GLN
12	O	658	GLN
12	O	663	GLN
12	O	681	GLN
12	O	697	ASN
13	R	57	GLN
13	R	80	HIS
14	N	39	GLN
14	N	41	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	654:THR	C	655:THR	N	4.12

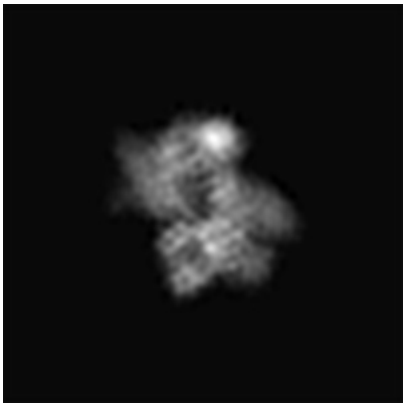
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4739. These allow visual inspection of the internal detail of the map and identification of artifacts.

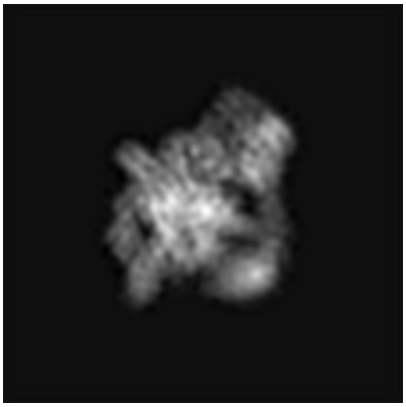
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

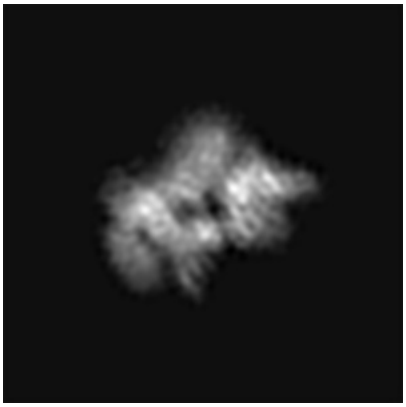
6.1.1 Primary map



X



Y

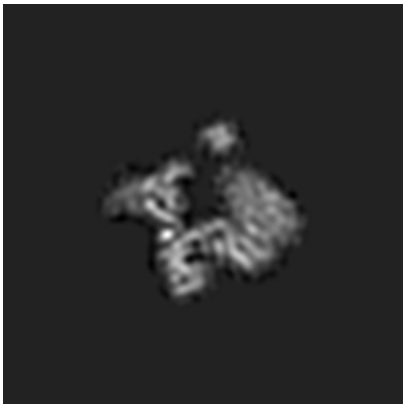


Z

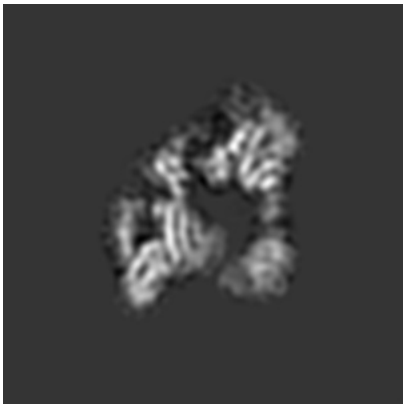
The images above show the map projected in three orthogonal directions.

6.2 Central slices

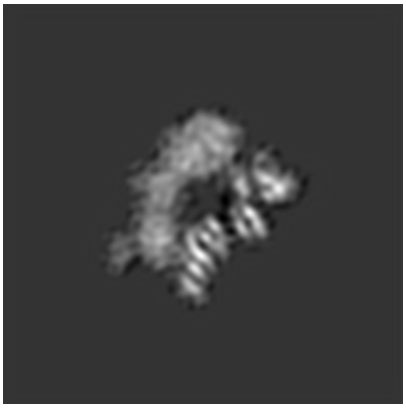
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 145

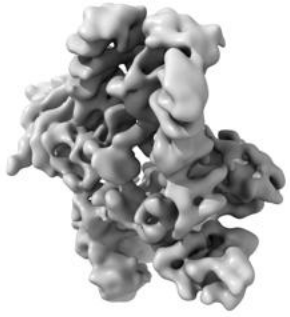
Y Index: 160

Z Index: 126

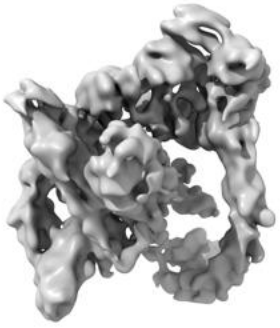
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

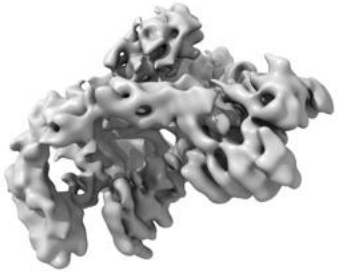
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

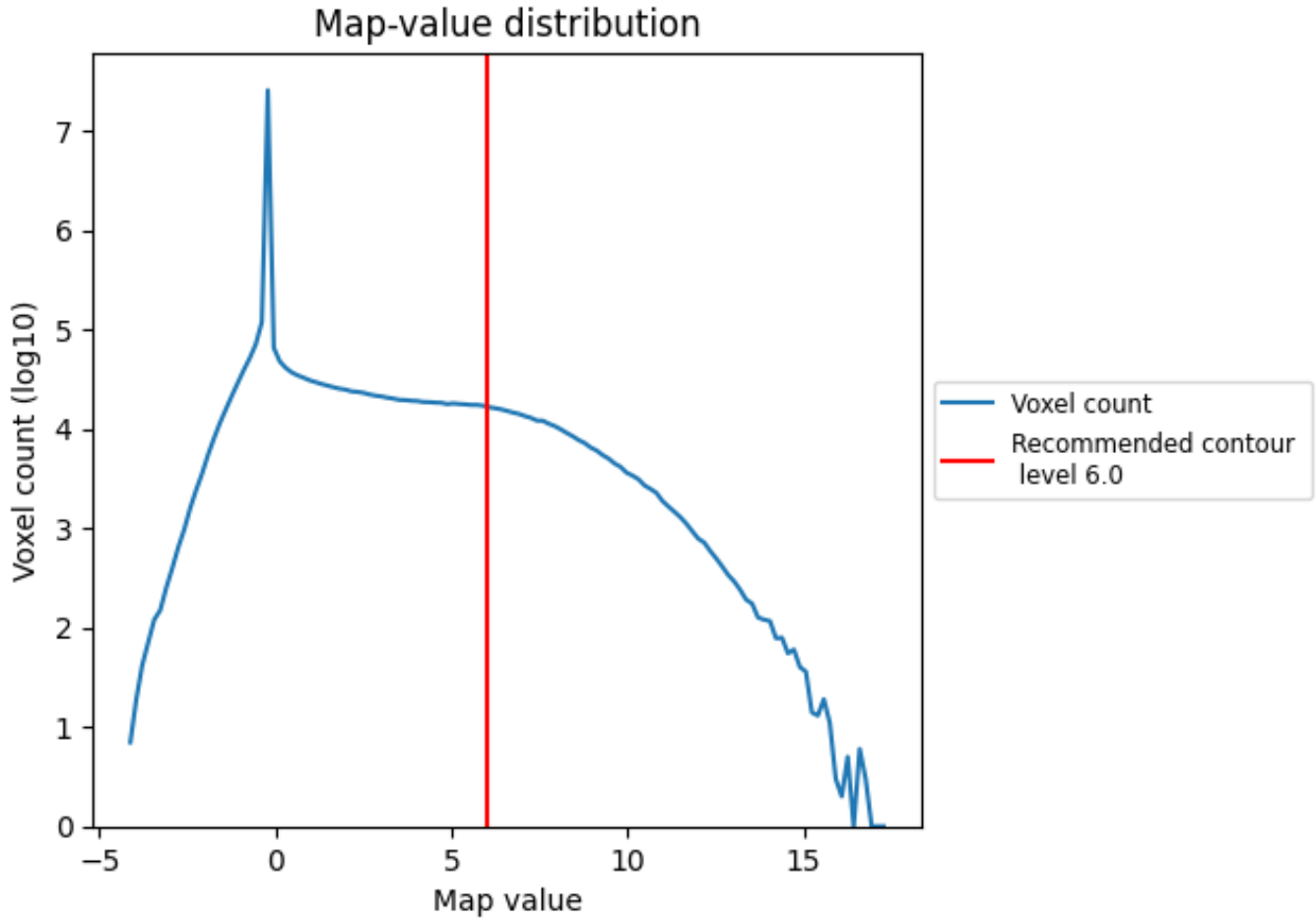
6.5 Mask visualisation (i)

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

7 Map analysis

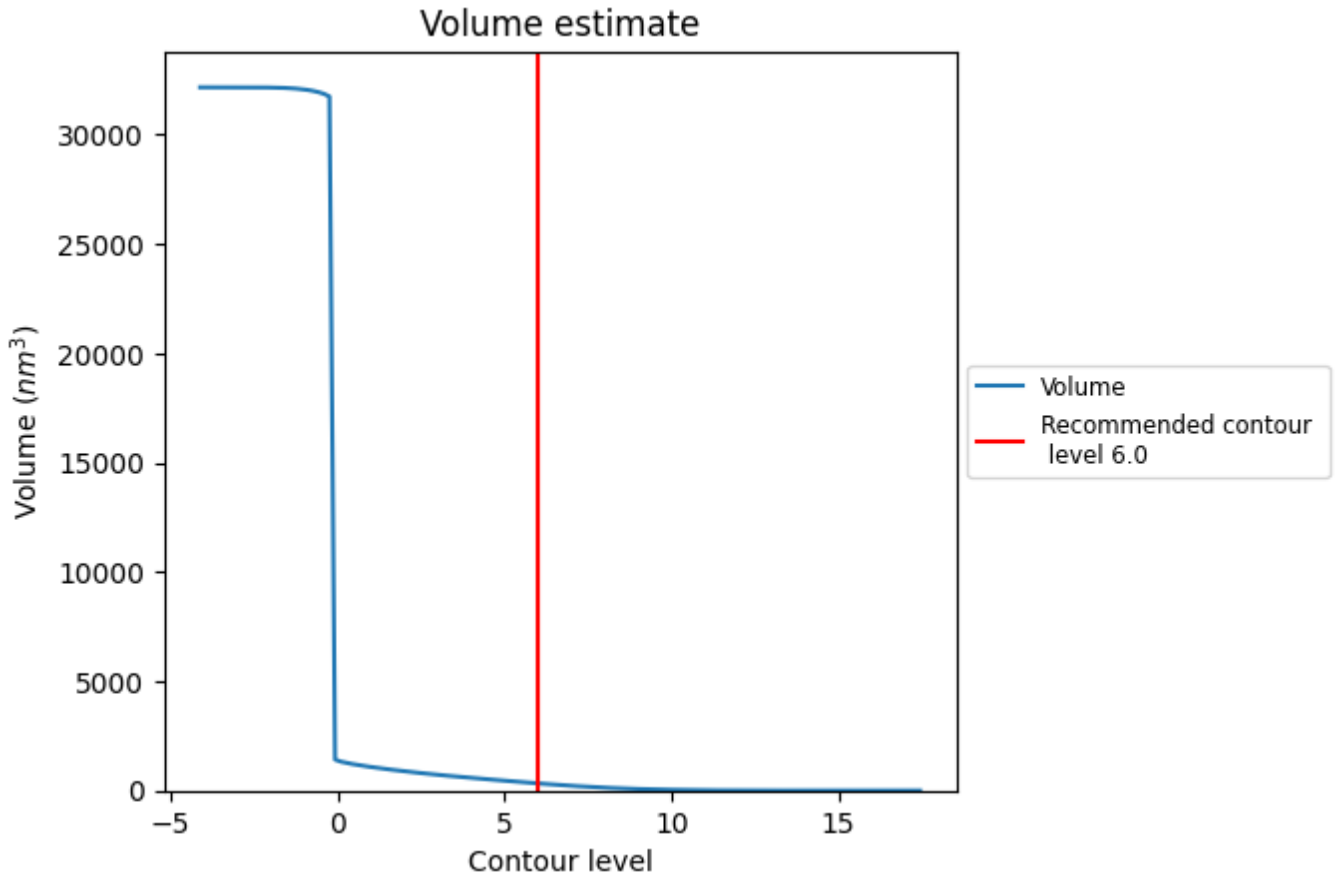
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

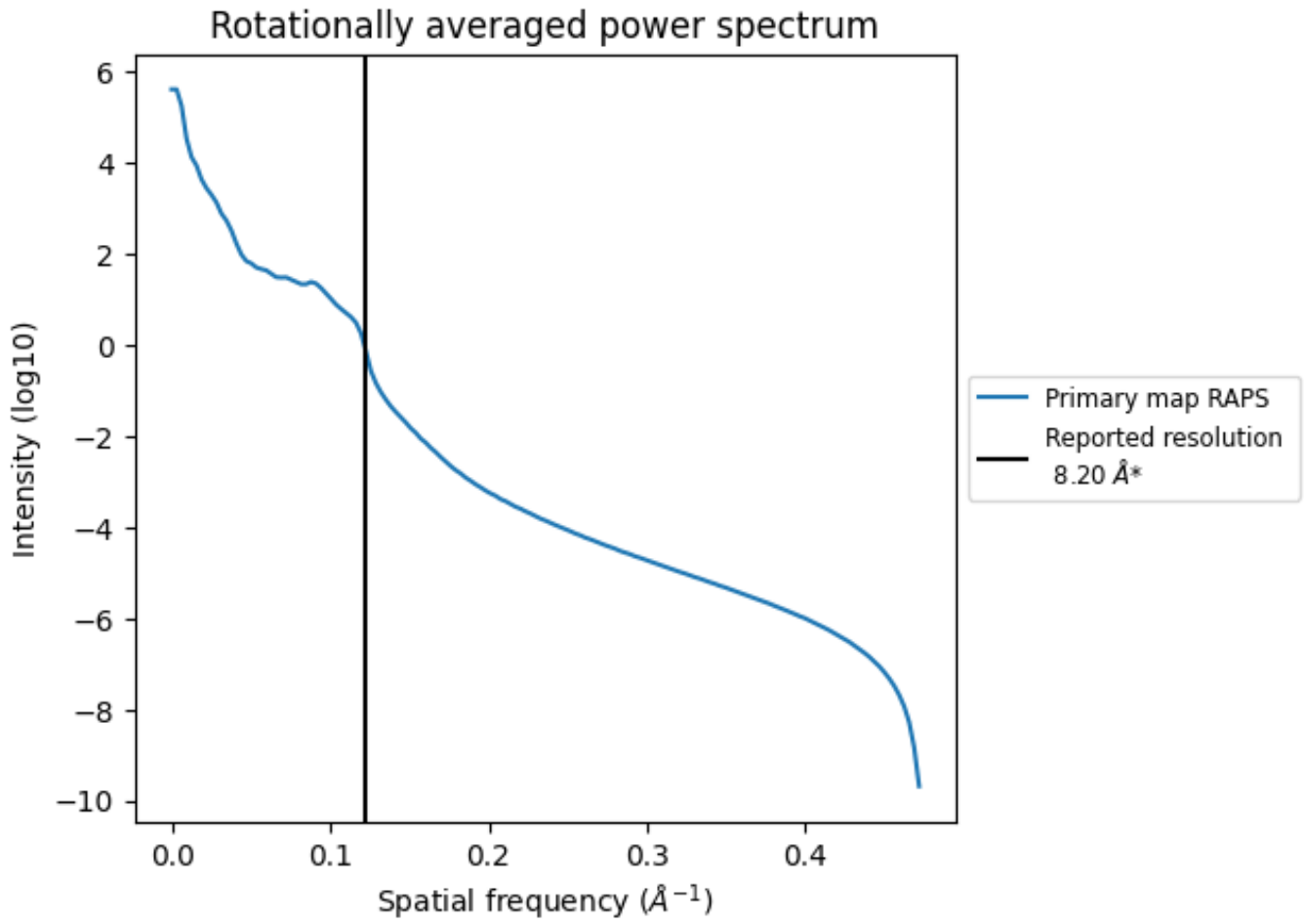
7.2 Volume estimate



The volume at the recommended contour level is 327 nm^3; this corresponds to an approximate mass of 296 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.122 Å^{-1}

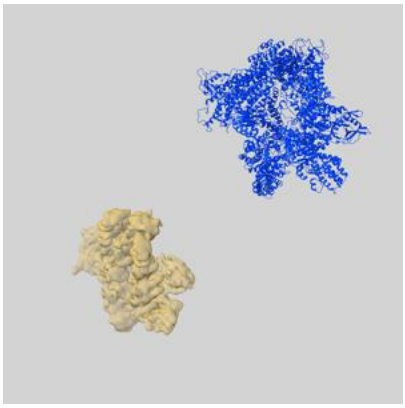
8 Fourier-Shell correlation

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

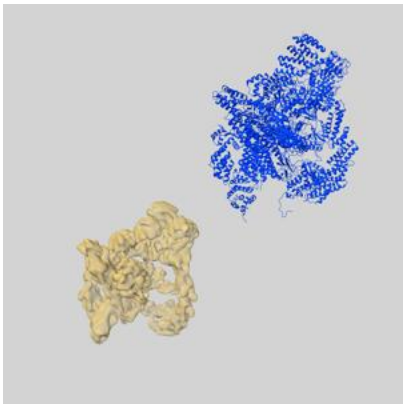
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4739 and PDB model 6R7F. Per-residue inclusion information can be found in section 3 on page 7.

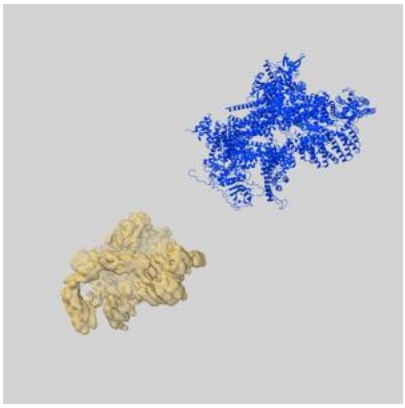
9.1 Map-model overlay



X



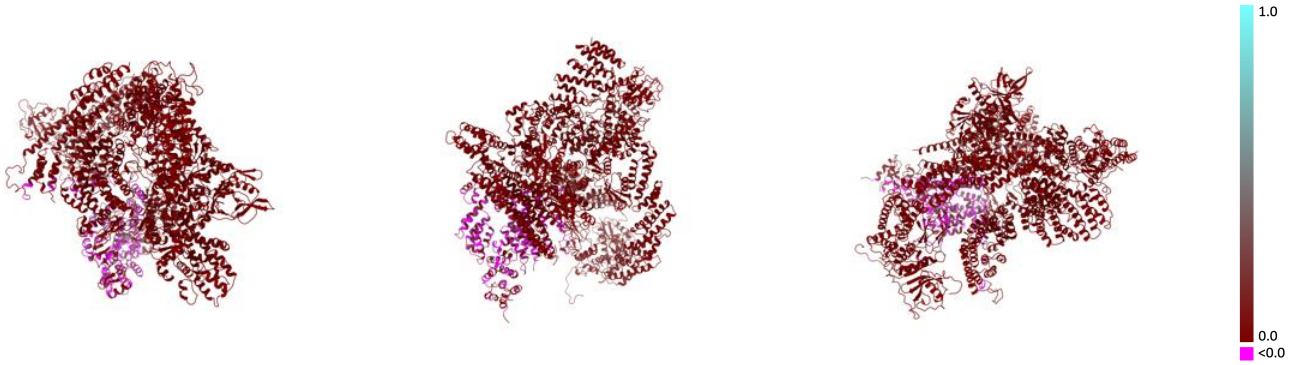
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

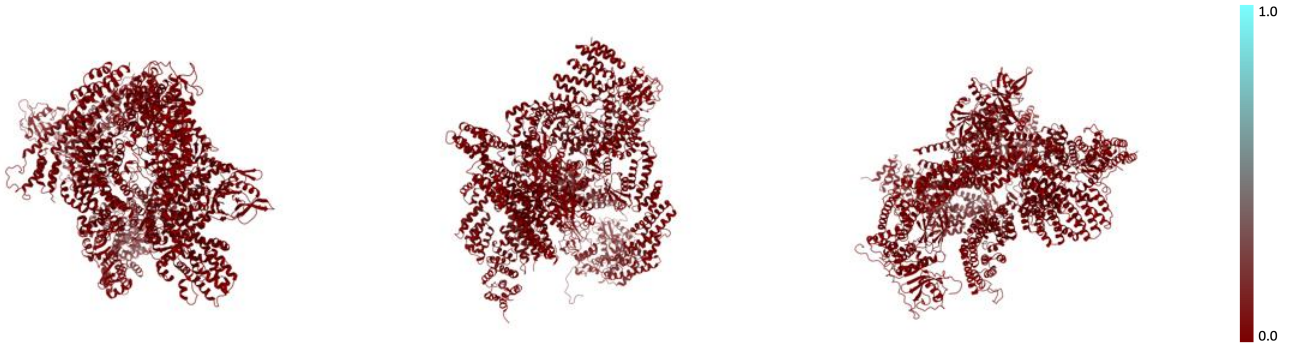
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

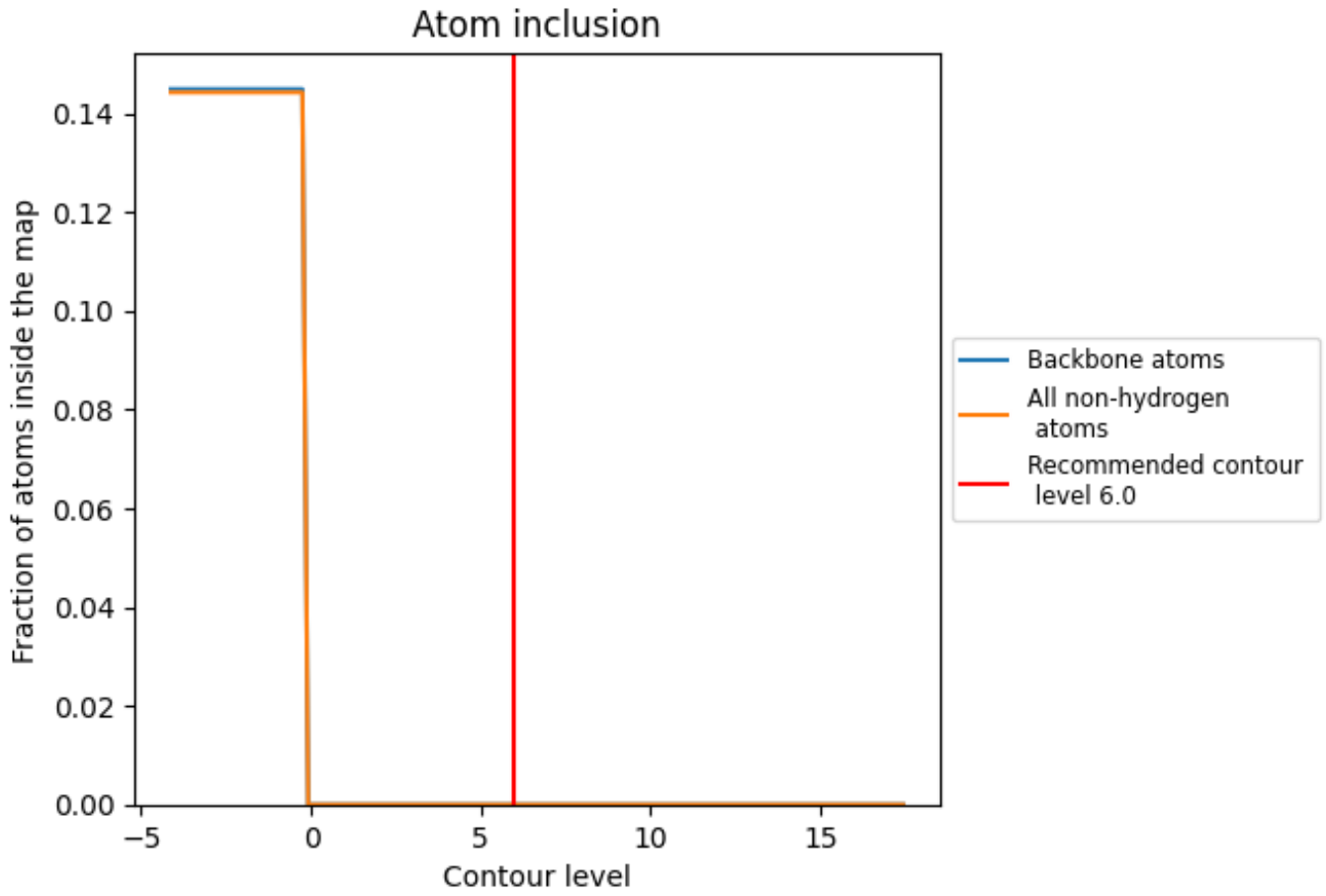
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0010
A	0.0000	0.0040
B	0.0000	0.0010
C	0.0000	0.0040
D	0.0000	0.0000
E	0.0000	-0.0010
F	0.0000	0.0030
G	0.0000	0.0000
H	0.0000	-0.0030
N	0.0000	0.0000
O	0.0000	0.0000
P	0.0000	0.0060
Q	0.0000	0.0000
R	0.0000	0.0000
V	0.0000	0.0070