wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:44 PM BST

PDB ID	:	3J4J
EMDB ID:	:	EMD-2448
Title	:	Model of full-length T. thermophilus Translation Initiation Factor 2 refined against its cryo-EM density from a 30S Initiation Complex map
Authors	:	Simonetti, A.; Marzi, S.; Billas, I.M.L.; Tsai, A.; Fabbretti, A.; Myasnikov, A.; Roblin, P.; Vaiana, A.C.; Hazemann, I.; Eiler, D.; Steitz, T.A.; Puglisi, J.D.; Gualerzi, C.O.; Klaholz, B.P.
Deposited on	:	2013-08-26
Resolution	:	11.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

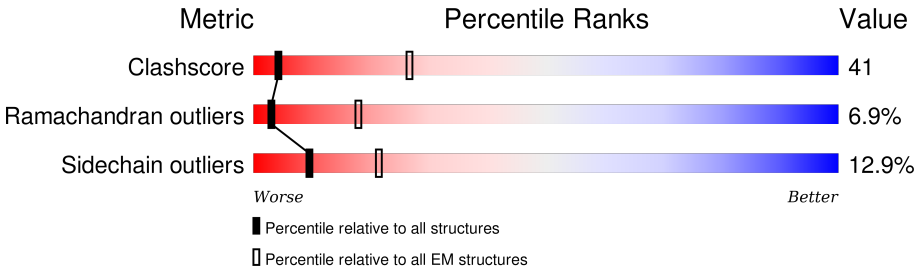
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 11.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	569	27% 35% 24% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4383 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 Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	569	4383	2747	778	841	17	0	0

There are 10 discrepancies between the modelled and reference sequences:

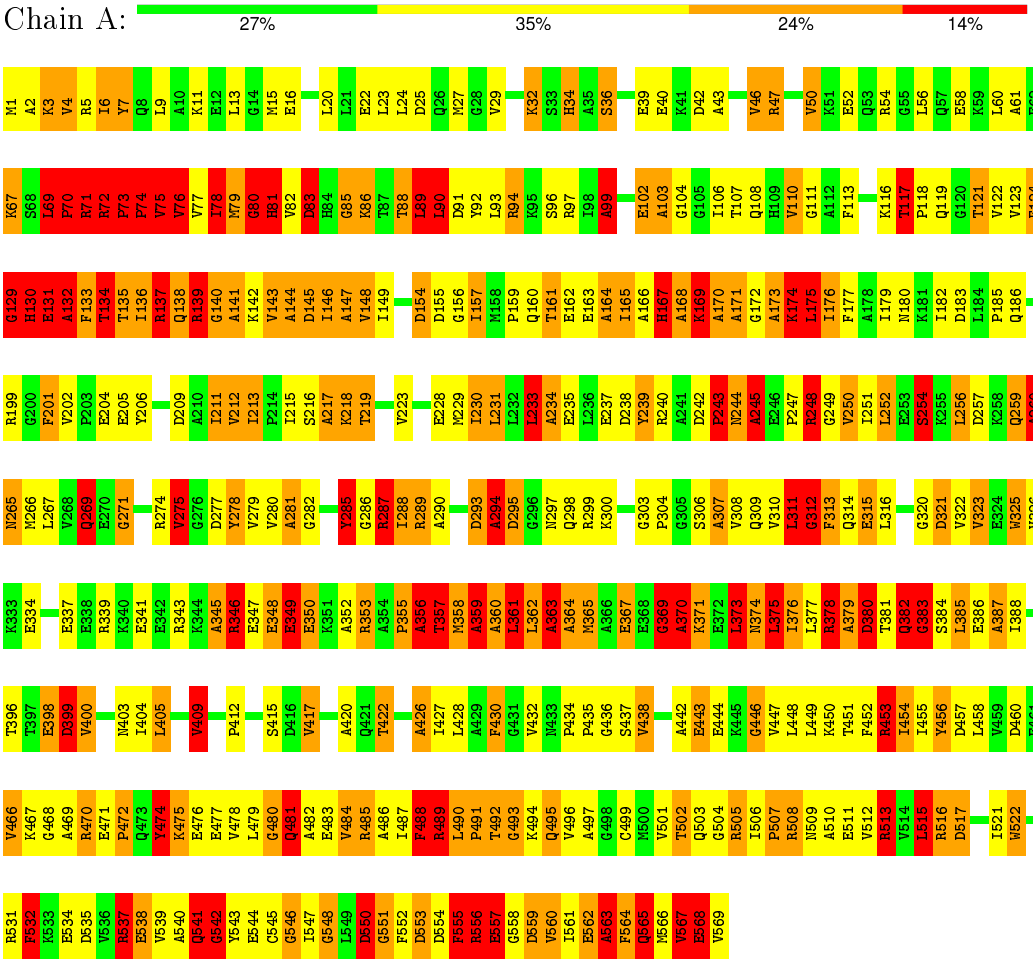
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	CONFLICT	UNP P48515
A	356	ALA	ARG	CONFLICT	UNP P48515
A	360	ALA	GLU	CONFLICT	UNP P48515
A	363	ALA	ARG	CONFLICT	UNP P48515
A	366	ALA	GLN	CONFLICT	UNP P48515
A	370	ALA	ARG	CONFLICT	UNP P48515
A	395	ALA	GLU	CONFLICT	UNP P48515
A	396	THR	SER	CONFLICT	UNP P48515
A	406	ALA	LEU	CONFLICT	UNP P48515
A	469	ALA	GLN	CONFLICT	UNP P48515

3 Residue-property plots (i)

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

- Molecule 1: Translation initiation factor IF-2

Chain A:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	150	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	59000	Depositor
Image detector	FEI CCD 4K*4K "EAGLE"	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	1.70	25/4440 (0.6%)	3.00	444/5985 (7.4%)

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	177

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ARG	CZ-NH2	-7.20	1.23	1.33
1	A	7	TYR	CE1-CZ	6.51	1.47	1.38
1	A	97	ARG	CZ-NH2	-6.30	1.24	1.33
1	A	343	ARG	CZ-NH2	-6.26	1.25	1.33
1	A	206	TYR	CE1-CZ	6.15	1.46	1.38
1	A	289	ARG	CZ-NH2	-6.06	1.25	1.33
1	A	556	ARG	CZ-NH1	-5.96	1.25	1.33
1	A	94	ARG	CZ-NH2	-5.91	1.25	1.33
1	A	72	ARG	CZ-NH1	-5.75	1.25	1.33
1	A	531	ARG	CZ-NH1	-5.69	1.25	1.33
1	A	285	TYR	CE2-CZ	5.60	1.45	1.38
1	A	235	GLU	CD-OE2	-5.59	1.19	1.25
1	A	532	PHE	CG-CD2	5.53	1.47	1.38
1	A	36	SER	CB-OG	-5.43	1.35	1.42
1	A	137	ARG	CZ-NH1	-5.35	1.26	1.33
1	A	206	TYR	CD2-CE2	5.33	1.47	1.39
1	A	534	GLU	CD-OE2	5.29	1.31	1.25
1	A	443	GLU	CD-OE1	-5.29	1.19	1.25
1	A	334	GLU	CD-OE2	5.25	1.31	1.25
1	A	444	GLU	CD-OE2	-5.20	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	SER	CA-CB	5.20	1.60	1.52
1	A	339	ARG	NE-CZ	-5.15	1.26	1.33
1	A	201	PHE	CE2-CZ	5.09	1.47	1.37
1	A	470	ARG	CZ-NH1	-5.03	1.26	1.33
1	A	97	ARG	NE-CZ	-5.02	1.26	1.33

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH1	30.11	135.35	120.30
1	A	394	ARG	NE-CZ-NH1	27.61	134.10	120.30
1	A	505	ARG	NE-CZ-NH2	-26.92	106.84	120.30
1	A	470	ARG	NE-CZ-NH2	-23.23	108.68	120.30
1	A	72	ARG	NE-CZ-NH2	-20.55	110.02	120.30
1	A	516	ARG	NE-CZ-NH2	20.44	130.52	120.30
1	A	199	ARG	NE-CZ-NH1	20.38	130.49	120.30
1	A	394	ARG	NE-CZ-NH2	-19.62	110.49	120.30
1	A	137	ARG	NE-CZ-NH1	18.62	129.61	120.30
1	A	66	ARG	NE-CZ-NH1	17.51	129.06	120.30
1	A	199	ARG	NE-CZ-NH2	-17.33	111.64	120.30
1	A	453	ARG	NE-CZ-NH2	16.58	128.59	120.30
1	A	378	ARG	CD-NE-CZ	16.02	146.02	123.60
1	A	65	ARG	NE-CZ-NH1	15.97	128.28	120.30
1	A	474	TYR	CG-CD1-CE1	-15.22	109.12	121.30
1	A	321	ASP	CB-CG-OD2	14.90	131.71	118.30
1	A	248	ARG	NE-CZ-NH1	-14.89	112.85	120.30
1	A	47	ARG	NE-CZ-NH1	14.59	127.60	120.30
1	A	346	ARG	NE-CZ-NH1	14.43	127.51	120.30
1	A	489	ARG	CD-NE-CZ	13.96	143.15	123.60
1	A	65	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	508	ARG	CD-NE-CZ	13.66	142.73	123.60
1	A	535	ASP	CB-CG-OD2	13.09	130.08	118.30
1	A	378	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	A	66	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	A	228	GLU	OE1-CD-OE2	12.33	138.10	123.30
1	A	353	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	A	7	TYR	CB-CG-CD1	12.03	128.22	121.00
1	A	299	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	559	ASP	CB-CG-OD1	11.76	128.88	118.30
1	A	505	ARG	NH1-CZ-NH2	11.36	131.89	119.40
1	A	343	ARG	NE-CZ-NH1	-11.07	114.77	120.30
1	A	206	TYR	CG-CD2-CE2	-10.98	112.52	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	ARG	CD-NE-CZ	10.88	138.83	123.60
1	A	248	ARG	CD-NE-CZ	10.83	138.76	123.60
1	A	5	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	A	289	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	334	GLU	OE1-CD-OE2	-10.25	111.00	123.30
1	A	194	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	134	THR	CA-CB-CG2	10.15	126.61	112.40
1	A	453	ARG	CD-NE-CZ	10.05	137.66	123.60
1	A	457	ASP	CB-CG-OD2	-10.04	109.26	118.30
1	A	485	ARG	NE-CZ-NH2	9.83	125.22	120.30
1	A	137	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	474	TYR	CD1-CE1-CZ	9.75	128.58	119.80
1	A	353	ARG	CD-NE-CZ	9.63	137.08	123.60
1	A	39	GLU	OE1-CD-OE2	-9.34	112.09	123.30
1	A	369	GLY	C-N-CA	9.27	144.87	121.70
1	A	63	GLU	OE1-CD-OE2	-9.24	112.21	123.30
1	A	562	GLU	OE1-CD-OE2	-9.12	112.35	123.30
1	A	555	PHE	C-N-CA	9.12	144.50	121.70
1	A	552	PHE	CD1-CE1-CZ	9.06	130.97	120.10
1	A	352	ALA	CB-CA-C	9.05	123.68	110.10
1	A	126	ASP	CB-CG-OD1	8.94	126.35	118.30
1	A	564	PHE	CB-CG-CD1	-8.94	114.54	120.80
1	A	557	GLU	OE1-CD-OE2	-8.94	112.57	123.30
1	A	46	VAL	CA-CB-CG1	8.93	124.29	110.90
1	A	275	VAL	O-C-N	-8.93	108.03	123.20
1	A	7	TYR	CG-CD1-CE1	8.90	128.42	121.30
1	A	339	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	74	PRO	N-CD-CG	8.74	116.31	103.20
1	A	205	GLU	OE1-CD-OE2	-8.73	112.82	123.30
1	A	326	VAL	CA-CB-CG2	8.62	123.83	110.90
1	A	330	GLU	OE1-CD-OE2	8.56	133.57	123.30
1	A	289	ARG	NH1-CZ-NH2	-8.54	110.01	119.40
1	A	488	PHE	CB-CG-CD2	-8.50	114.85	120.80
1	A	133	PHE	CG-CD2-CE2	8.47	130.12	120.80
1	A	357	THR	N-CA-CB	8.43	126.32	110.30
1	A	289	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	A	355	PRO	N-CD-CG	8.38	115.77	103.20
1	A	131	GLU	C-N-CA	8.37	142.63	121.70
1	A	322	VAL	CG1-CB-CG2	-8.34	97.55	110.90
1	A	248	ARG	NH1-CZ-NH2	8.34	128.57	119.40
1	A	83	ASP	CB-CG-OD2	8.34	125.80	118.30
1	A	453	ARG	NH1-CZ-NH2	-8.34	110.23	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	370	ALA	CB-CA-C	8.30	122.56	110.10
1	A	470	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	16	GLU	O-C-N	-8.25	109.50	122.70
1	A	97	ARG	CD-NE-CZ	8.15	135.01	123.60
1	A	42	ASP	CB-CG-OD1	8.11	125.60	118.30
1	A	138	GLN	C-N-CA	8.11	141.97	121.70
1	A	134	THR	N-CA-CB	8.10	125.69	110.30
1	A	4	VAL	CA-CB-CG1	8.09	123.04	110.90
1	A	76	VAL	CA-CB-CG2	8.00	122.90	110.90
1	A	345	ALA	CB-CA-C	7.98	122.07	110.10
1	A	522	TRP	CH2-CZ2-CE2	7.93	125.33	117.40
1	A	54	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	287	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	A	313	PHE	O-C-N	7.88	135.31	122.70
1	A	353	ARG	NH1-CZ-NH2	7.82	128.00	119.40
1	A	162	GLU	OE1-CD-OE2	-7.81	113.92	123.30
1	A	554	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	A	133	PHE	CB-CG-CD2	7.71	126.20	120.80
1	A	102	GLU	O-C-N	-7.69	110.40	122.70
1	A	409	VAL	C-N-CA	7.68	138.43	122.30
1	A	206	TYR	CB-CG-CD1	-7.67	116.40	121.00
1	A	234	ALA	O-C-N	-7.63	110.49	122.70
1	A	104	GLY	CA-C-N	7.63	131.46	116.20
1	A	121	THR	CA-CB-OG1	7.59	124.94	109.00
1	A	202	VAL	CG1-CB-CG2	-7.57	98.79	110.90
1	A	206	TYR	CD1-CG-CD2	7.52	126.17	117.90
1	A	133	PHE	CB-CA-C	7.52	125.43	110.40
1	A	168	ALA	O-C-N	-7.51	110.68	122.70
1	A	481	GLN	C-N-CA	7.50	140.46	121.70
1	A	515	LEU	CB-CG-CD2	7.49	123.73	111.00
1	A	72	ARG	CD-NE-CZ	7.45	134.03	123.60
1	A	75	VAL	CA-CB-CG1	7.42	122.02	110.90
1	A	385	LEU	CB-CG-CD1	7.39	123.56	111.00
1	A	517	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	460	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	409	VAL	CA-CB-CG2	7.37	121.95	110.90
1	A	474	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	A	538	GLU	OE1-CD-OE2	-7.35	114.48	123.30
1	A	133	PHE	C-N-CA	7.33	140.03	121.70
1	A	325	TRP	CZ3-CH2-CZ2	-7.28	112.86	121.60
1	A	295	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	293	ASP	CB-CG-OD1	7.26	124.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ALA	CB-CA-C	7.24	120.96	110.10
1	A	532	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	A	103	ALA	O-C-N	-7.23	110.91	123.20
1	A	325	TRP	CB-CG-CD2	7.21	135.97	126.60
1	A	553	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	A	104	GLY	O-C-N	-7.21	110.95	123.20
1	A	312	GLY	O-C-N	-7.19	111.20	122.70
1	A	378	ARG	NH1-CZ-NH2	-7.18	111.50	119.40
1	A	2	ALA	C-N-CA	7.16	139.60	121.70
1	A	456	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	A	311	LEU	CB-CG-CD2	7.15	123.16	111.00
1	A	91	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	339	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	532	PHE	CD1-CE1-CZ	-7.11	111.57	120.10
1	A	352	ALA	C-N-CA	7.09	139.44	121.70
1	A	330	GLU	O-C-N	-7.08	111.36	122.70
1	A	494	LYS	O-C-N	7.04	133.97	122.70
1	A	532	PHE	CG-CD2-CE2	-7.04	113.05	120.80
1	A	522	TRP	NE1-CE2-CZ2	7.01	138.12	130.40
1	A	7	TYR	CZ-CE2-CD2	7.01	126.11	119.80
1	A	168	ALA	CB-CA-C	6.98	120.56	110.10
1	A	294	ALA	N-CA-CB	-6.97	100.34	110.10
1	A	170	ALA	CB-CA-C	6.97	120.55	110.10
1	A	457	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	243	PRO	C-N-CA	6.96	139.09	121.70
1	A	325	TRP	O-C-N	-6.93	111.61	122.70
1	A	97	ARG	O-C-N	-6.92	111.62	122.70
1	A	537	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	509	ASN	CB-CA-C	6.88	124.17	110.40
1	A	516	ARG	NH1-CZ-NH2	-6.87	111.85	119.40
1	A	485	ARG	NH1-CZ-NH2	-6.86	111.86	119.40
1	A	144	ALA	N-CA-CB	-6.83	100.54	110.10
1	A	139	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	58	GLU	OE1-CD-OE2	-6.81	115.12	123.30
1	A	72	ARG	N-CA-CB	-6.81	98.34	110.60
1	A	470	ARG	NH1-CZ-NH2	6.79	126.86	119.40
1	A	452	PHE	CD1-CE1-CZ	-6.77	111.97	120.10
1	A	290	ALA	N-CA-CB	-6.75	100.64	110.10
1	A	139	ARG	CD-NE-CZ	6.73	133.02	123.60
1	A	552	PHE	CG-CD1-CE1	-6.73	113.40	120.80
1	A	323	VAL	CA-CB-CG2	-6.72	100.82	110.90
1	A	67	LYS	O-C-N	-6.72	111.95	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	LEU	CB-CG-CD1	6.71	122.41	111.00
1	A	553	ASP	CA-C-O	-6.70	106.03	120.10
1	A	145	ASP	C-N-CA	6.69	138.44	121.70
1	A	463	ARG	CD-NE-CZ	6.67	132.93	123.60
1	A	540	ALA	C-N-CA	6.66	138.34	121.70
1	A	356	ALA	N-CA-CB	6.65	119.41	110.10
1	A	565	GLN	O-C-N	-6.65	112.06	122.70
1	A	169	LYS	O-C-N	-6.63	112.09	122.70
1	A	356	ALA	CB-CA-C	6.61	120.02	110.10
1	A	484	VAL	CA-CB-CG1	6.61	120.81	110.90
1	A	47	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	A	274	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	248	ARG	O-C-N	-6.60	111.98	123.20
1	A	379	ALA	CA-C-O	-6.60	106.25	120.10
1	A	124	PHE	CG-CD2-CE2	6.58	128.04	120.80
1	A	264	ALA	CB-CA-C	-6.58	100.23	110.10
1	A	7	TYR	CB-CG-CD2	-6.58	117.06	121.00
1	A	359	ALA	N-CA-CB	-6.57	100.91	110.10
1	A	74	PRO	CA-N-CD	-6.56	102.32	111.50
1	A	139	ARG	O-C-N	-6.56	112.06	123.20
1	A	171	ALA	O-C-N	-6.55	112.06	123.20
1	A	13	LEU	C-N-CA	6.53	136.01	122.30
1	A	46	VAL	CA-CB-CG2	6.53	120.69	110.90
1	A	206	TYR	C-N-CA	6.52	135.99	122.30
1	A	89	LEU	CB-CG-CD1	6.51	122.07	111.00
1	A	131	GLU	OE1-CD-OE2	6.51	131.12	123.30
1	A	71	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	343	ARG	NH1-CZ-NH2	6.51	126.56	119.40
1	A	110	VAL	O-C-N	-6.50	112.14	123.20
1	A	58	GLU	CG-CD-OE2	6.50	131.31	118.30
1	A	206	TYR	CG-CD1-CE1	-6.50	116.10	121.30
1	A	73	PRO	CA-C-N	6.48	135.24	117.10
1	A	517	ASP	OD1-CG-OD2	-6.48	110.99	123.30
1	A	348	GLU	O-C-N	-6.45	112.38	122.70
1	A	362	LEU	C-N-CA	6.45	137.82	121.70
1	A	113	PHE	CB-CG-CD1	-6.42	116.30	120.80
1	A	381	THR	CA-CB-CG2	6.41	121.37	112.40
1	A	517	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	174	LYS	O-C-N	-6.39	112.47	122.70
1	A	325	TRP	CH2-CZ2-CE2	6.38	123.78	117.40
1	A	490	LEU	CB-CA-C	6.38	122.32	110.20
1	A	492	THR	CA-CB-CG2	-6.37	103.48	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	537	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	64	GLU	OE1-CD-OE2	6.36	130.93	123.30
1	A	417	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	A	556	ARG	C-N-CA	6.35	137.57	121.70
1	A	25	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	89	LEU	CB-CG-CD2	6.34	121.78	111.00
1	A	90	LEU	O-C-N	-6.34	112.56	122.70
1	A	74	PRO	N-CA-CB	6.32	110.89	103.30
1	A	505	ARG	O-C-N	-6.32	112.59	122.70
1	A	555	PHE	CD1-CE1-CZ	6.31	127.67	120.10
1	A	325	TRP	C-N-CA	6.31	137.48	121.70
1	A	278	TYR	CD1-CE1-CZ	6.28	125.45	119.80
1	A	442	ALA	CB-CA-C	6.28	119.52	110.10
1	A	7	TYR	CA-CB-CG	6.27	125.31	113.40
1	A	300	LYS	C-N-CA	6.26	137.34	121.70
1	A	491	PRO	N-CD-CG	6.25	112.58	103.20
1	A	91	ASP	O-C-N	6.25	132.70	122.70
1	A	563	ALA	O-C-N	-6.25	112.71	122.70
1	A	278	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	362	LEU	N-CA-CB	-6.22	97.95	110.40
1	A	99	ALA	CB-CA-C	6.21	119.42	110.10
1	A	343	ARG	O-C-N	-6.21	112.77	122.70
1	A	197	MET	O-C-N	-6.18	112.82	122.70
1	A	405	LEU	O-C-N	-6.17	112.83	122.70
1	A	135	THR	CA-CB-OG1	6.17	121.95	109.00
1	A	552	PHE	CB-CG-CD1	6.17	125.12	120.80
1	A	72	ARG	CA-C-O	-6.16	107.16	120.10
1	A	256	LEU	C-N-CA	6.15	137.08	121.70
1	A	507	PRO	N-CD-CG	6.14	112.40	103.20
1	A	386	GLU	OE1-CD-OE2	-6.12	115.96	123.30
1	A	23	LEU	O-C-N	6.11	132.47	122.70
1	A	24	LEU	CB-CG-CD2	6.11	121.38	111.00
1	A	550	ASP	N-CA-CB	-6.07	99.67	110.60
1	A	541	GLN	O-C-N	-6.07	112.89	123.20
1	A	94	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	387	ALA	CB-CA-C	6.06	119.19	110.10
1	A	365	MET	C-N-CA	6.05	136.84	121.70
1	A	310	VAL	C-N-CA	6.04	136.80	121.70
1	A	70	PRO	O-C-N	-6.03	113.05	122.70
1	A	452	PHE	CG-CD1-CE1	6.02	127.42	120.80
1	A	527	ALA	N-CA-CB	-6.02	101.67	110.10
1	A	263	ILE	CB-CA-C	6.01	123.63	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	LYS	O-C-N	6.01	133.41	123.20
1	A	126	ASP	CB-CG-OD2	-6.00	112.91	118.30
1	A	446	GLY	CA-C-O	-6.00	109.81	120.60
1	A	560	VAL	C-N-CA	5.99	136.68	121.70
1	A	543	TYR	CG-CD1-CE1	5.99	126.09	121.30
1	A	11	LYS	C-N-CA	5.96	136.61	121.70
1	A	71	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	206	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	134	THR	C-N-CA	5.95	136.58	121.70
1	A	513	ARG	CG-CD-NE	5.95	124.29	111.80
1	A	245	ALA	N-CA-C	5.95	127.06	111.00
1	A	539	VAL	CA-CB-CG2	5.95	119.82	110.90
1	A	130	HIS	CB-CA-C	5.92	122.24	110.40
1	A	304	PRO	C-N-CA	5.92	134.74	122.30
1	A	34	HIS	CG-CD2-NE2	-5.91	97.96	109.20
1	A	81	HIS	N-CA-CB	-5.91	99.95	110.60
1	A	300	LYS	CA-C-N	5.90	130.18	117.20
1	A	285	TYR	CA-CB-CG	5.89	124.59	113.40
1	A	553	ASP	N-CA-CB	-5.89	100.00	110.60
1	A	149	ILE	N-CA-CB	5.88	124.33	110.80
1	A	124	PHE	CB-CG-CD2	5.88	124.92	120.80
1	A	515	LEU	O-C-N	-5.88	113.30	122.70
1	A	230	ILE	O-C-N	-5.87	113.31	122.70
1	A	426	ALA	N-CA-CB	-5.87	101.88	110.10
1	A	491	PRO	C-N-CA	5.86	136.36	121.70
1	A	517	ASP	CB-CA-C	5.85	122.11	110.40
1	A	69	LEU	CB-CG-CD2	5.85	120.94	111.00
1	A	365	MET	N-CA-CB	-5.84	100.08	110.60
1	A	555	PHE	CB-CG-CD1	5.84	124.89	120.80
1	A	484	VAL	CG1-CB-CG2	-5.84	101.56	110.90
1	A	474	TYR	CD1-CG-CD2	5.83	124.32	117.90
1	A	285	TYR	CA-C-O	-5.83	107.85	120.10
1	A	548	GLY	CA-C-O	-5.83	110.11	120.60
1	A	544	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	A	60	LEU	C-N-CA	5.82	136.26	121.70
1	A	556	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	70	PRO	CA-C-O	5.81	134.14	120.20
1	A	125	ILE	C-N-CA	5.80	136.19	121.70
1	A	400	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	A	307	ALA	CB-CA-C	5.78	118.78	110.10
1	A	3	LYS	C-N-CA	5.77	136.13	121.70
1	A	380	ASP	CB-CG-OD1	5.77	123.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	550	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	566	MET	CA-CB-CG	5.75	123.08	113.30
1	A	234	ALA	N-CA-CB	5.75	118.15	110.10
1	A	164	ALA	N-CA-CB	5.75	118.15	110.10
1	A	339	ARG	CD-NE-CZ	5.74	131.64	123.60
1	A	399	ASP	N-CA-C	5.74	126.49	111.00
1	A	341	GLU	OE1-CD-OE2	5.72	130.17	123.30
1	A	118	PRO	O-C-N	-5.71	113.56	122.70
1	A	295	ASP	O-C-N	-5.71	113.49	123.20
1	A	398	GLU	C-N-CA	5.70	135.95	121.70
1	A	20	LEU	CB-CG-CD1	5.70	120.68	111.00
1	A	480	GLY	C-N-CA	5.69	135.93	121.70
1	A	11	LYS	CD-CE-NZ	5.69	124.78	111.70
1	A	182	ILE	CA-CB-CG1	5.68	121.79	111.00
1	A	97	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	531	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	71	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
1	A	212	VAL	O-C-N	-5.66	113.64	122.70
1	A	399	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	489	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	546	GLY	CA-C-N	5.63	129.59	117.20
1	A	127	THR	CA-C-O	-5.63	108.28	120.10
1	A	243	PRO	N-CA-CB	-5.63	96.41	102.60
1	A	159	PRO	N-CA-CB	5.62	110.05	103.30
1	A	280	VAL	CB-CA-C	5.61	122.06	111.40
1	A	133	PHE	CZ-CE2-CD2	-5.60	113.38	120.10
1	A	497	ALA	N-CA-CB	-5.60	102.26	110.10
1	A	278	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	117	THR	O-C-N	-5.58	110.50	121.10
1	A	239	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	215	ILE	CA-C-O	-5.57	108.41	120.10
1	A	239	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	66	ARG	C-N-CA	5.56	135.61	121.70
1	A	206	TYR	CZ-CE2-CD2	5.56	124.81	119.80
1	A	315	GLU	O-C-N	-5.56	113.81	122.70
1	A	415	SER	N-CA-CB	5.55	118.83	110.50
1	A	117	THR	CA-CB-OG1	5.55	120.65	109.00
1	A	80	GLY	O-C-N	-5.55	113.83	122.70
1	A	277	ASP	CA-CB-CG	5.55	125.60	113.40
1	A	362	LEU	O-C-N	-5.55	113.83	122.70
1	A	513	ARG	CB-CA-C	5.55	121.49	110.40
1	A	360	ALA	C-N-CA	5.54	135.56	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	PHE	CG-CD1-CE1	-5.54	114.71	120.80
1	A	564	PHE	CD1-CG-CD2	5.54	125.50	118.30
1	A	361	LEU	N-CA-CB	5.53	121.46	110.40
1	A	528	SER	CB-CA-C	-5.53	99.59	110.10
1	A	254	SER	O-C-N	-5.52	113.86	122.70
1	A	78	ILE	CA-CB-CG1	-5.52	100.52	111.00
1	A	508	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	385	LEU	CB-CG-CD2	5.50	120.35	111.00
1	A	463	ARG	N-CA-CB	5.50	120.49	110.60
1	A	552	PHE	CG-CD2-CE2	5.50	126.84	120.80
1	A	3	LYS	O-C-N	5.49	131.48	122.70
1	A	454	ILE	CA-CB-CG1	5.49	121.43	111.00
1	A	3	LYS	CA-C-O	-5.49	108.58	120.10
1	A	218	LYS	CB-CA-C	5.48	121.37	110.40
1	A	325	TRP	CE2-CD2-CG	5.47	111.68	107.30
1	A	88	THR	OG1-CB-CG2	-5.46	97.43	110.00
1	A	279	VAL	C-N-CA	5.46	135.36	121.70
1	A	29	VAL	CG1-CB-CG2	-5.46	102.17	110.90
1	A	145	ASP	CA-C-N	5.46	129.20	117.20
1	A	295	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	A	438	VAL	CA-CB-CG2	5.45	119.08	110.90
1	A	447	VAL	CA-CB-CG2	5.45	119.07	110.90
1	A	442	ALA	N-CA-CB	-5.45	102.48	110.10
1	A	93	LEU	O-C-N	-5.44	113.99	122.70
1	A	360	ALA	CB-CA-C	5.44	118.26	110.10
1	A	367	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	A	382	GLN	N-CA-CB	5.43	120.38	110.60
1	A	90	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	118	PRO	N-CA-CB	5.42	109.81	103.30
1	A	373	LEU	CB-CG-CD2	5.42	120.21	111.00
1	A	161	THR	CA-C-O	-5.42	108.72	120.10
1	A	449	LEU	O-C-N	-5.42	114.04	122.70
1	A	557	GLU	N-CA-CB	5.41	120.34	110.60
1	A	4	VAL	O-C-N	-5.40	114.05	122.70
1	A	265	ASN	CB-CG-OD1	5.40	132.40	121.60
1	A	52	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	A	209	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	567	VAL	C-N-CA	5.39	135.16	121.70
1	A	361	LEU	O-C-N	-5.38	114.09	122.70
1	A	370	ALA	C-N-CA	5.38	135.15	121.70
1	A	56	LEU	CB-CG-CD1	5.38	120.14	111.00
1	A	462	VAL	O-C-N	-5.38	114.10	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	GLN	N-CA-CB	5.37	120.27	110.60
1	A	279	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	A	288	ILE	C-N-CA	5.37	135.12	121.70
1	A	373	LEU	CB-CG-CD1	5.37	120.13	111.00
1	A	154	ASP	CB-CA-C	5.34	121.08	110.40
1	A	299	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	516	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	A	231	LEU	C-N-CA	5.33	135.03	121.70
1	A	375	LEU	C-N-CA	5.33	135.02	121.70
1	A	380	ASP	CB-CA-C	5.32	121.04	110.40
1	A	167	HIS	CA-CB-CG	5.32	122.64	113.60
1	A	185	PRO	N-CA-CB	5.31	109.68	103.30
1	A	488	PHE	CG-CD2-CE2	-5.31	114.96	120.80
1	A	537	ARG	N-CA-CB	-5.31	101.05	110.60
1	A	177	PHE	CD1-CE1-CZ	-5.30	113.74	120.10
1	A	334	GLU	O-C-N	-5.28	114.25	122.70
1	A	364	ALA	CB-CA-C	5.27	118.01	110.10
1	A	90	LEU	CB-CG-CD2	5.27	119.95	111.00
1	A	206	TYR	CD1-CE1-CZ	5.26	124.54	119.80
1	A	129	GLY	CA-C-O	-5.26	111.13	120.60
1	A	485	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	331	ALA	O-C-N	-5.25	114.29	122.70
1	A	233	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	43	ALA	O-C-N	5.25	131.09	122.70
1	A	325	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	47	ARG	O-C-N	-5.23	114.33	122.70
1	A	357	THR	CA-CB-CG2	5.23	119.72	112.40
1	A	382	GLN	O-C-N	-5.23	114.31	123.20
1	A	472	PRO	C-N-CA	5.23	134.76	121.70
1	A	97	ARG	N-CA-CB	-5.20	101.24	110.60
1	A	379	ALA	C-N-CA	5.20	134.70	121.70
1	A	219	THR	N-CA-CB	5.20	120.18	110.30
1	A	103	ALA	CA-C-N	5.20	126.59	116.20
1	A	123	VAL	O-C-N	-5.19	114.40	122.70
1	A	167	HIS	O-C-N	-5.19	114.40	122.70
1	A	277	ASP	CA-C-O	5.18	130.98	120.10
1	A	538	GLU	CG-CD-OE2	5.16	128.62	118.30
1	A	103	ALA	N-CA-CB	-5.15	102.89	110.10
1	A	143	VAL	C-N-CA	5.15	134.56	121.70
1	A	443	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	357	THR	C-N-CA	5.14	134.55	121.70
1	A	165	ILE	CB-CA-C	5.14	121.88	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	LEU	CA-C-O	-5.14	109.31	120.10
1	A	242	ASP	O-C-N	5.13	130.85	121.10
1	A	539	VAL	O-C-N	-5.13	114.49	122.70
1	A	353	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	A	213	ILE	N-CA-CB	5.12	122.58	110.80
1	A	137	ARG	CA-C-O	-5.12	109.35	120.10
1	A	118	PRO	CA-C-N	5.12	128.45	117.20
1	A	462	VAL	CB-CA-C	5.11	121.11	111.40
1	A	32	LYS	CB-CA-C	5.11	120.61	110.40
1	A	15	MET	CA-C-N	5.10	128.43	117.20
1	A	347	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	54	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	A	22	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	A	511	GLU	C-N-CA	5.08	134.39	121.70
1	A	244	ASN	C-N-CA	5.06	134.35	121.70
1	A	85	GLY	O-C-N	-5.06	114.61	122.70
1	A	199	ARG	CA-C-N	5.05	126.31	116.20
1	A	534	GLU	N-CA-CB	5.05	119.70	110.60
1	A	1	MET	CG-SD-CE	-5.05	92.12	100.20
1	A	464	ASN	OD1-CG-ND2	-5.04	110.30	121.90
1	A	78	ILE	CA-C-O	-5.04	109.51	120.10
1	A	551	GLY	C-N-CA	5.04	134.31	121.70
1	A	243	PRO	CA-C-N	5.04	128.28	117.20
1	A	134	THR	CA-CB-OG1	5.04	119.58	109.00
1	A	75	VAL	CA-C-O	-5.03	109.53	120.10
1	A	76	VAL	O-C-N	-5.03	114.65	122.70
1	A	347	GLU	CG-CD-OE1	5.03	128.36	118.30
1	A	466	VAL	CA-CB-CG1	5.03	118.45	110.90
1	A	250	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	A	542	GLY	O-C-N	-5.03	114.66	122.70
1	A	260	ALA	N-CA-CB	-5.01	103.09	110.10
1	A	269	GLN	C-N-CA	5.01	134.22	121.70
1	A	516	ARG	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (177) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLU	Peptide
1	A	103	ALA	Mainchain,Peptide
1	A	107	THR	Mainchain
1	A	116	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	117	THR	Mainchain
1	A	122	VAL	Mainchain
1	A	129	GLY	Mainchain
1	A	130	HIS	Peptide
1	A	132	ALA	Mainchain
1	A	134	THR	Mainchain,Peptide
1	A	136	ILE	Mainchain
1	A	137	ARG	Mainchain
1	A	138	GLN	Peptide
1	A	139	ARG	Mainchain
1	A	140	GLY	Mainchain
1	A	141	ALA	Mainchain
1	A	142	LYS	Peptide
1	A	145	ASP	Peptide
1	A	146	ILE	Mainchain
1	A	147	ALA	Mainchain
1	A	154	ASP	Mainchain
1	A	155	ASP	Mainchain
1	A	156	GLY	Mainchain
1	A	157	ILE	Mainchain
1	A	161	THR	Mainchain
1	A	166	ALA	Mainchain
1	A	167	HIS	Mainchain
1	A	169	LYS	Mainchain
1	A	170	ALA	Mainchain
1	A	171	ALA	Mainchain
1	A	172	GLY	Mainchain
1	A	173	ALA	Peptide
1	A	174	LYS	Mainchain
1	A	175	LEU	Mainchain
1	A	179	ILE	Mainchain
1	A	186	GLN	Mainchain
1	A	204	GLU	Mainchain
1	A	212	VAL	Mainchain
1	A	216	SER	Mainchain
1	A	217	ALA	Mainchain
1	A	219	THR	Mainchain,Peptide
1	A	231	LEU	Mainchain
1	A	233	LEU	Mainchain
1	A	234	ALA	Mainchain
1	A	239	TYR	Sidechain
1	A	244	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	245	ALA	Mainchain
1	A	248	ARG	Mainchain
1	A	252	LEU	Mainchain
1	A	254	SER	Mainchain
1	A	259	GLN	Mainchain
1	A	260	ALA	Mainchain
1	A	269	GLN	Mainchain
1	A	271	GLY	Mainchain
1	A	275	VAL	Mainchain
1	A	281	ALA	Mainchain
1	A	282	GLY	Mainchain
1	A	285	TYR	Mainchain
1	A	287	ARG	Mainchain
1	A	293	ASP	Mainchain
1	A	294	ALA	Mainchain
1	A	297	ASN	Mainchain
1	A	298	GLN	Mainchain
1	A	303	GLY	Mainchain
1	A	312	GLY	Mainchain
1	A	315	GLU	Mainchain
1	A	316	LEU	Mainchain
1	A	320	GLY	Mainchain
1	A	325	TRP	Mainchain
1	A	330	GLU	Mainchain
1	A	331	ALA	Mainchain
1	A	332	ALA	Mainchain
1	A	337	GLU	Mainchain
1	A	345	ALA	Mainchain
1	A	346	ARG	Mainchain
1	A	348	GLU	Mainchain,Peptide
1	A	349	GLU	Mainchain
1	A	350	GLU	Mainchain
1	A	355	PRO	Mainchain
1	A	356	ALA	Mainchain
1	A	358	MET	Mainchain
1	A	359	ALA	Mainchain,Peptide
1	A	36	SER	Mainchain
1	A	361	LEU	Mainchain,Peptide
1	A	362	LEU	Peptide
1	A	363	ALA	Mainchain
1	A	369	GLY	Mainchain,Peptide
1	A	370	ALA	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	374	ASN	Mainchain
1	A	375	LEU	Peptide
1	A	376	ILE	Mainchain
1	A	378	ARG	Mainchain
1	A	379	ALA	Mainchain,Peptide
1	A	380	ASP	Mainchain
1	A	382	GLN	Mainchain,Peptide
1	A	383	GLY	Mainchain,Peptide
1	A	391	ILE	Mainchain
1	A	40	GLU	Mainchain
1	A	404	ILE	Mainchain
1	A	409	VAL	Mainchain
1	A	422	THR	Mainchain
1	A	435	PRO	Mainchain
1	A	438	VAL	Mainchain
1	A	443	GLU	Mainchain
1	A	446	GLY	Mainchain
1	A	448	LEU	Mainchain
1	A	450	LYS	Mainchain
1	A	453	ARG	Mainchain
1	A	456	TYR	Mainchain
1	A	463	ARG	Mainchain
1	A	464	ASN	Mainchain
1	A	465	MET	Mainchain
1	A	469	ALA	Mainchain
1	A	47	ARG	Mainchain
1	A	470	ARG	Mainchain
1	A	476	GLU	Peptide
1	A	479	LEU	Peptide
1	A	480	GLY	Mainchain,Peptide
1	A	485	ARG	Mainchain
1	A	486	ALA	Mainchain
1	A	488	PHE	Peptide
1	A	493	GLY	Mainchain
1	A	495	GLN	Mainchain
1	A	499	CYS	Mainchain
1	A	50	VAL	Mainchain
1	A	502	THR	Mainchain
1	A	510	ALA	Mainchain
1	A	513	ARG	Mainchain
1	A	515	LEU	Mainchain
1	A	516	ARG	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	521	ILE	Mainchain
1	A	532	PHE	Mainchain
1	A	537	ARG	Mainchain
1	A	541	GLN	Mainchain
1	A	542	GLY	Mainchain
1	A	545	CYS	Mainchain
1	A	547	ILE	Mainchain
1	A	548	GLY	Mainchain
1	A	550	ASP	Peptide
1	A	551	GLY	Mainchain
1	A	553	ASP	Mainchain
1	A	555	PHE	Mainchain
1	A	557	GLU	Mainchain
1	A	558	GLY	Mainchain
1	A	563	ALA	Mainchain
1	A	565	GLN	Mainchain
1	A	568	GLU	Mainchain,Peptide
1	A	61	ALA	Mainchain
1	A	67	LYS	Mainchain
1	A	69	LEU	Mainchain
1	A	71	ARG	Mainchain
1	A	72	ARG	Peptide
1	A	74	PRO	Mainchain,Peptide
1	A	75	VAL	Mainchain
1	A	76	VAL	Mainchain
1	A	78	ILE	Mainchain
1	A	80	GLY	Mainchain
1	A	81	HIS	Mainchain
1	A	83	ASP	Mainchain
1	A	85	GLY	Mainchain
1	A	90	LEU	Mainchain
1	A	96	SER	Mainchain
1	A	99	ALA	Mainchain,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	4383	0	4462	364	0
All	All	4383	0	4462	364	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 41.

All (364) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ARG:CG	1:A:556:ARG:HH11	1.40	1.30
1:A:134:THR:HG23	1:A:382:GLN:CG	1.72	1.19
1:A:79:MET:HB2	1:A:164:ALA:CB	1.72	1.18
1:A:75:VAL:HB	1:A:144:ALA:CA	1.74	1.17
1:A:493:GLY:HA2	1:A:530:LYS:HE3	1.24	1.16
1:A:373:LEU:HD12	1:A:465:MET:HE3	1.26	1.16
1:A:382:GLN:HG2	1:A:409:VAL:HG11	1.27	1.15
1:A:134:THR:HG23	1:A:382:GLN:CB	1.78	1.14
1:A:481:GLN:HG3	1:A:562:GLU:HG3	1.26	1.14
1:A:371:LYS:HB3	1:A:468:GLY:HA2	1.34	1.09
1:A:79:MET:HB2	1:A:164:ALA:HB2	1.31	1.09
1:A:72:ARG:HD2	1:A:74:PRO:HD3	1.35	1.07
1:A:75:VAL:CB	1:A:144:ALA:HA	1.85	1.06
1:A:371:LYS:HD3	1:A:468:GLY:HA3	1.31	1.06
1:A:488:PHE:HZ	1:A:532:PHE:HB2	1.13	1.06
1:A:92:TYR:CE2	1:A:223:VAL:HG21	1.90	1.06
1:A:76:VAL:HG13	1:A:147:ALA:HA	1.28	1.06
1:A:496:VAL:HG21	1:A:530:LYS:HB2	1.28	1.05
1:A:496:VAL:HG11	1:A:530:LYS:CG	1.87	1.05
1:A:371:LYS:CD	1:A:468:GLY:HA3	1.86	1.04
1:A:496:VAL:HG11	1:A:530:LYS:HG3	1.40	1.03
1:A:373:LEU:HD12	1:A:465:MET:CE	1.88	1.02
1:A:496:VAL:HG11	1:A:530:LYS:CB	1.87	1.02
1:A:143:VAL:HG13	1:A:250:VAL:HG11	1.36	1.01
1:A:481:GLN:CG	1:A:562:GLU:HG3	1.91	1.01
1:A:76:VAL:HG11	1:A:148:VAL:HG13	1.44	1.00
1:A:263:ILE:HD12	1:A:309:GLN:NE2	1.77	1.00
1:A:382:GLN:CG	1:A:409:VAL:HG11	1.92	0.99
1:A:75:VAL:HB	1:A:144:ALA:HA	1.03	0.99
1:A:363:ALA:HB1	1:A:403:ASN:HA	1.45	0.99
1:A:380:ASP:HB2	1:A:432:VAL:HG13	1.44	0.99
1:A:453:ARG:O	1:A:453:ARG:HG3	1.58	0.98
1:A:375:LEU:HD23	1:A:426:ALA:HB3	1.44	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HB2	1:A:294:ALA:C	1.82	0.98
1:A:556:ARG:HG3	1:A:556:ARG:NH1	1.34	0.97
1:A:124:PHE:HE1	1:A:148:VAL:HG11	1.27	0.97
1:A:496:VAL:HB	1:A:546:GLY:HA3	1.46	0.97
1:A:487:ILE:CG2	1:A:556:ARG:HD3	1.94	0.97
1:A:488:PHE:CZ	1:A:532:PHE:HB2	2.00	0.97
1:A:382:GLN:HG2	1:A:409:VAL:CG1	1.95	0.96
1:A:493:GLY:CA	1:A:530:LYS:HE3	1.95	0.95
1:A:92:TYR:HE2	1:A:223:VAL:HG21	1.31	0.94
1:A:496:VAL:CG2	1:A:530:LYS:HB2	1.97	0.94
1:A:92:TYR:CG	1:A:217:ALA:HA	2.03	0.94
1:A:134:THR:HA	1:A:382:GLN:C	1.87	0.94
1:A:487:ILE:HG22	1:A:556:ARG:HD3	1.50	0.93
1:A:275:VAL:O	1:A:275:VAL:HG12	1.64	0.93
1:A:76:VAL:HG13	1:A:147:ALA:CA	1.97	0.93
1:A:92:TYR:CD2	1:A:217:ALA:HA	2.04	0.93
1:A:380:ASP:HB2	1:A:432:VAL:CG1	1.98	0.92
1:A:82:VAL:HG11	1:A:430:PHE:CZ	2.03	0.92
1:A:78:ILE:HD13	1:A:89:LEU:HD13	1.52	0.92
1:A:380:ASP:CB	1:A:432:VAL:HG13	1.98	0.92
1:A:80:GLY:HA2	1:A:160:GLN:HB2	1.52	0.91
1:A:496:VAL:HG11	1:A:530:LYS:HB2	1.51	0.90
1:A:80:GLY:HA2	1:A:160:GLN:CB	2.02	0.90
1:A:134:THR:HG23	1:A:382:GLN:HB2	1.52	0.90
1:A:398:GLU:HB2	1:A:466:VAL:HG12	1.55	0.88
1:A:263:ILE:HB	1:A:309:GLN:CD	1.95	0.87
1:A:371:LYS:CB	1:A:468:GLY:HA2	2.04	0.87
1:A:134:THR:HG23	1:A:382:GLN:HG3	1.53	0.87
1:A:76:VAL:CG1	1:A:148:VAL:H	1.88	0.87
1:A:79:MET:HB2	1:A:164:ALA:HB1	1.55	0.86
1:A:481:GLN:HA	1:A:562:GLU:HA	1.54	0.86
1:A:72:ARG:HG3	1:A:72:ARG:O	1.73	0.86
1:A:92:TYR:HE2	1:A:223:VAL:CG2	1.88	0.85
1:A:124:PHE:CE1	1:A:148:VAL:HG11	2.11	0.84
1:A:82:VAL:HG21	1:A:430:PHE:CZ	2.13	0.84
1:A:80:GLY:O	1:A:86:LYS:HE2	1.78	0.84
1:A:263:ILE:HB	1:A:309:GLN:OE1	1.78	0.83
1:A:82:VAL:HG22	1:A:130:HIS:CD2	2.13	0.83
1:A:134:THR:C	1:A:382:GLN:HB2	1.99	0.83
1:A:79:MET:CB	1:A:164:ALA:HB2	2.10	0.82
1:A:82:VAL:HG11	1:A:430:PHE:CE1	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HB2	1:A:294:ALA:O	1.80	0.81
1:A:376:ILE:HG22	1:A:405:LEU:HB2	1.61	0.81
1:A:76:VAL:CG1	1:A:147:ALA:HA	2.10	0.80
1:A:92:TYR:CE2	1:A:223:VAL:CG2	2.64	0.80
1:A:72:ARG:HD2	1:A:74:PRO:CD	2.10	0.80
1:A:380:ASP:CG	1:A:432:VAL:HG13	2.02	0.80
1:A:124:PHE:HE1	1:A:148:VAL:CG1	1.94	0.80
1:A:248:ARG:O	1:A:269:GLN:HB2	1.82	0.79
1:A:134:THR:HA	1:A:383:GLY:CA	2.13	0.78
1:A:72:ARG:CD	1:A:74:PRO:HG3	2.13	0.78
1:A:380:ASP:HB2	1:A:432:VAL:HG22	1.66	0.77
1:A:483:GLU:HA	1:A:560:VAL:HA	1.66	0.77
1:A:134:THR:CG2	1:A:382:GLN:HB2	2.15	0.76
1:A:496:VAL:CG1	1:A:530:LYS:HB2	2.15	0.76
1:A:375:LEU:CD2	1:A:426:ALA:HB3	2.14	0.76
1:A:82:VAL:HG22	1:A:130:HIS:HD2	1.50	0.75
1:A:380:ASP:HB2	1:A:432:VAL:CG2	2.16	0.75
1:A:92:TYR:CG	1:A:217:ALA:CA	2.69	0.75
1:A:76:VAL:N	1:A:144:ALA:HB1	2.01	0.75
1:A:78:ILE:CD1	1:A:89:LEU:HD13	2.17	0.75
1:A:165:ILE:HG21	1:A:201:PHE:CZ	2.22	0.75
1:A:496:VAL:CG1	1:A:530:LYS:HG3	2.16	0.74
1:A:82:VAL:CG1	1:A:430:PHE:CZ	2.70	0.74
1:A:496:VAL:HG21	1:A:530:LYS:CB	2.12	0.74
1:A:75:VAL:HB	1:A:144:ALA:CB	2.17	0.74
1:A:92:TYR:HB2	1:A:217:ALA:O	1.87	0.74
1:A:78:ILE:HD13	1:A:89:LEU:CD1	2.18	0.73
1:A:453:ARG:O	1:A:453:ARG:CG	2.37	0.73
1:A:72:ARG:CG	1:A:72:ARG:O	2.37	0.73
1:A:512:VAL:HG12	1:A:563:ALA:HB2	1.70	0.72
1:A:487:ILE:HG22	1:A:556:ARG:CD	2.18	0.71
1:A:86:LYS:HB3	1:A:86:LYS:HZ2	1.55	0.71
1:A:92:TYR:CB	1:A:217:ALA:HB1	2.21	0.70
1:A:82:VAL:CG2	1:A:430:PHE:CZ	2.73	0.70
1:A:260:ALA:O	1:A:311:LEU:HD11	1.92	0.70
1:A:380:ASP:H	1:A:432:VAL:HG22	1.57	0.70
1:A:263:ILE:HD12	1:A:309:GLN:CD	2.11	0.70
1:A:134:THR:HA	1:A:383:GLY:N	2.07	0.69
1:A:481:GLN:HG3	1:A:562:GLU:CG	2.15	0.69
1:A:487:ILE:HG23	1:A:556:ARG:HD3	1.73	0.69
1:A:71:ARG:CZ	1:A:71:ARG:HB3	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:CG	1:A:82:VAL:H	2.11	0.68
1:A:373:LEU:HD23	1:A:465:MET:O	1.93	0.68
1:A:211:ILE:HG13	1:A:233:LEU:HD22	1.74	0.68
1:A:371:LYS:HD3	1:A:468:GLY:CA	2.18	0.68
1:A:82:VAL:HG21	1:A:430:PHE:CE2	2.30	0.67
1:A:398:GLU:HB2	1:A:466:VAL:CG1	2.23	0.67
1:A:134:THR:CG2	1:A:382:GLN:CG	2.63	0.67
1:A:76:VAL:HA	1:A:146:ILE:O	1.96	0.66
1:A:134:THR:CA	1:A:382:GLN:C	2.63	0.66
1:A:132:ALA:HB1	1:A:383:GLY:C	2.17	0.65
1:A:496:VAL:HB	1:A:546:GLY:CA	2.25	0.65
1:A:289:ARG:NH2	1:A:311:LEU:HD22	2.11	0.65
1:A:371:LYS:HB3	1:A:468:GLY:CA	2.20	0.65
1:A:79:MET:SD	1:A:164:ALA:HB1	2.37	0.65
1:A:82:VAL:CG1	1:A:430:PHE:HZ	2.07	0.65
1:A:92:TYR:HB2	1:A:217:ALA:HB1	1.79	0.65
1:A:80:GLY:HA2	1:A:160:GLN:HB3	1.77	0.64
1:A:86:LYS:HB3	1:A:86:LYS:NZ	2.11	0.64
1:A:371:LYS:CB	1:A:468:GLY:CA	2.76	0.64
1:A:137:ARG:HH11	1:A:167:HIS:CD2	2.17	0.63
1:A:488:PHE:HZ	1:A:532:PHE:CB	2.02	0.63
1:A:522:TRP:CZ2	1:A:550:ASP:HB2	2.33	0.63
1:A:92:TYR:CD1	1:A:217:ALA:HA	2.34	0.63
1:A:75:VAL:HG21	1:A:143:VAL:O	1.98	0.62
1:A:490:LEU:HD12	1:A:491:PRO:CD	2.29	0.62
1:A:371:LYS:CE	1:A:468:GLY:HA3	2.29	0.62
1:A:134:THR:CG2	1:A:382:GLN:CB	2.66	0.62
1:A:365:MET:HB2	1:A:403:ASN:HD22	1.64	0.62
1:A:132:ALA:HB3	1:A:383:GLY:HA3	1.80	0.61
1:A:493:GLY:HA2	1:A:530:LYS:CE	2.16	0.61
1:A:266:MET:O	1:A:307:ALA:HA	2.01	0.61
1:A:496:VAL:CB	1:A:530:LYS:HB2	2.30	0.61
1:A:522:TRP:CH2	1:A:550:ASP:HB2	2.36	0.61
1:A:134:THR:O	1:A:382:GLN:HB2	2.01	0.60
1:A:92:TYR:CE2	1:A:217:ALA:HA	2.36	0.60
1:A:376:ILE:HD11	1:A:420:ALA:HB2	1.82	0.60
1:A:278:TYR:CE1	1:A:287:ARG:HD2	2.37	0.60
1:A:384:SER:HA	1:A:455:ILE:HD11	1.84	0.59
1:A:363:ALA:O	1:A:403:ASN:HB2	2.02	0.59
1:A:111:GLY:HA3	1:A:252:LEU:HD13	1.84	0.59
1:A:488:PHE:CE2	1:A:532:PHE:HA	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLY:HA3	1:A:312:GLY:C	2.23	0.59
1:A:263:ILE:HB	1:A:309:GLN:CG	2.32	0.59
1:A:134:THR:CG2	1:A:382:GLN:HG3	2.31	0.59
1:A:375:LEU:HD23	1:A:426:ALA:CB	2.27	0.58
1:A:487:ILE:CG2	1:A:556:ARG:CD	2.77	0.58
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.67	0.58
1:A:380:ASP:HB2	1:A:432:VAL:CB	2.33	0.58
1:A:275:VAL:O	1:A:275:VAL:CG1	2.32	0.58
1:A:77:VAL:HG23	1:A:125:ILE:HG21	1.85	0.58
1:A:133:PHE:HZ	1:A:160:GLN:O	1.86	0.58
1:A:79:MET:CB	1:A:164:ALA:CB	2.64	0.58
1:A:70:PRO:HG2	1:A:243:PRO:HG3	1.84	0.58
1:A:82:VAL:CG2	1:A:130:HIS:HD2	2.16	0.57
1:A:81:HIS:CG	1:A:82:VAL:N	2.71	0.57
1:A:72:ARG:HD2	1:A:74:PRO:CG	2.34	0.57
1:A:211:ILE:HD12	1:A:229:MET:CE	2.34	0.57
1:A:143:VAL:HA	1:A:269:GLN:NE2	2.18	0.57
1:A:27:MET:SD	1:A:46:VAL:HG22	2.44	0.57
1:A:146:ILE:CG2	1:A:176:ILE:HD12	2.34	0.57
1:A:76:VAL:CA	1:A:144:ALA:HB1	2.34	0.57
1:A:76:VAL:HG22	1:A:146:ILE:HB	1.85	0.57
1:A:80:GLY:CA	1:A:160:GLN:HB2	2.31	0.57
1:A:132:ALA:HB1	1:A:384:SER:N	2.20	0.57
1:A:496:VAL:CG1	1:A:530:LYS:CG	2.73	0.56
1:A:380:ASP:CB	1:A:432:VAL:CG1	2.71	0.56
1:A:522:TRP:CZ2	1:A:550:ASP:CB	2.88	0.56
1:A:70:PRO:HG2	1:A:243:PRO:CG	2.34	0.56
1:A:503:GLN:HG3	1:A:504:GLY:H	1.70	0.56
1:A:75:VAL:CG2	1:A:144:ALA:HA	2.35	0.56
1:A:76:VAL:HG11	1:A:148:VAL:H	1.70	0.56
1:A:488:PHE:CZ	1:A:532:PHE:CB	2.82	0.56
1:A:77:VAL:HG13	1:A:79:MET:HE2	1.88	0.56
1:A:92:TYR:CD1	1:A:217:ALA:C	2.80	0.56
1:A:70:PRO:HG2	1:A:243:PRO:CD	2.36	0.56
1:A:134:THR:HG23	1:A:382:GLN:CD	2.24	0.55
1:A:376:ILE:O	1:A:427:ILE:HA	2.06	0.55
1:A:132:ALA:CB	1:A:383:GLY:C	2.74	0.55
1:A:90:LEU:O	1:A:94:ARG:HB2	2.07	0.55
1:A:174:LYS:HG2	1:A:237:GLU:OE1	2.06	0.55
1:A:86:LYS:HZ1	1:A:130:HIS:HB3	1.71	0.55
1:A:131:GLU:C	1:A:133:PHE:H	2.11	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:CG	1:A:468:GLY:HA3	2.38	0.54
1:A:72:ARG:CD	1:A:74:PRO:CG	2.85	0.54
1:A:288:ILE:HA	1:A:311:LEU:O	2.08	0.54
1:A:143:VAL:CG1	1:A:250:VAL:HG11	2.24	0.54
1:A:92:TYR:CD2	1:A:217:ALA:CA	2.86	0.54
1:A:380:ASP:H	1:A:432:VAL:CG2	2.20	0.54
1:A:484:VAL:HB	1:A:561:ILE:HD11	1.90	0.54
1:A:481:GLN:CG	1:A:562:GLU:CG	2.78	0.54
1:A:72:ARG:HD3	1:A:74:PRO:HG3	1.89	0.54
1:A:515:LEU:HD11	1:A:562:GLU:OE1	2.07	0.53
1:A:133:PHE:HB3	1:A:136:ILE:HG12	1.90	0.53
1:A:371:LYS:O	1:A:400:VAL:HG22	2.08	0.53
1:A:483:GLU:HG2	1:A:560:VAL:CG2	2.38	0.53
1:A:168:ALA:HB1	1:A:175:LEU:CD2	2.38	0.53
1:A:278:TYR:CZ	1:A:287:ARG:HD2	2.44	0.53
1:A:252:LEU:HD11	1:A:267:LEU:HB2	1.91	0.52
1:A:286:GLY:HA3	1:A:312:GLY:O	2.09	0.52
1:A:483:GLU:HG2	1:A:560:VAL:HG13	1.91	0.52
1:A:77:VAL:HG13	1:A:79:MET:CE	2.40	0.52
1:A:75:VAL:HG12	1:A:144:ALA:HB2	1.92	0.52
1:A:556:ARG:HH11	1:A:556:ARG:HG3	0.49	0.52
1:A:143:VAL:HG13	1:A:250:VAL:CG1	2.24	0.52
1:A:76:VAL:CG1	1:A:148:VAL:N	2.67	0.52
1:A:380:ASP:CG	1:A:432:VAL:CG1	2.77	0.52
1:A:289:ARG:NH2	1:A:311:LEU:CD2	2.72	0.52
1:A:289:ARG:CZ	1:A:311:LEU:HD22	2.40	0.51
1:A:249:GLY:HA2	1:A:269:GLN:CG	2.40	0.51
1:A:249:GLY:HA2	1:A:269:GLN:HB2	1.93	0.51
1:A:483:GLU:HG2	1:A:560:VAL:CG1	2.41	0.51
1:A:80:GLY:O	1:A:130:HIS:HB2	2.11	0.51
1:A:81:HIS:CD2	1:A:82:VAL:H	2.28	0.51
1:A:148:VAL:CG2	1:A:148:VAL:O	2.59	0.51
1:A:254:SER:HA	1:A:264:ALA:HA	1.93	0.51
1:A:371:LYS:O	1:A:400:VAL:CG2	2.59	0.50
1:A:285:TYR:O	1:A:285:TYR:CG	2.64	0.50
1:A:483:GLU:HG2	1:A:560:VAL:HG22	1.93	0.50
1:A:146:ILE:HG21	1:A:176:ILE:HD12	1.94	0.50
1:A:377:LEU:CD2	1:A:428:LEU:HB2	2.42	0.50
1:A:471:GLU:HB3	1:A:472:PRO:HD3	1.94	0.50
1:A:211:ILE:HD12	1:A:229:MET:HE2	1.93	0.50
1:A:70:PRO:CG	1:A:243:PRO:HG3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CE1	1:A:163:GLU:OE1	2.65	0.49
1:A:365:MET:HB2	1:A:403:ASN:ND2	2.27	0.49
1:A:75:VAL:C	1:A:76:VAL:CG2	2.80	0.49
1:A:371:LYS:CD	1:A:468:GLY:CA	2.76	0.49
1:A:81:HIS:HB2	1:A:160:GLN:HG2	1.93	0.49
1:A:483:GLU:HA	1:A:560:VAL:CA	2.40	0.49
1:A:134:THR:CG2	1:A:382:GLN:CD	2.80	0.49
1:A:378:ARG:HB2	1:A:427:ILE:HG22	1.95	0.49
1:A:471:GLU:O	1:A:474:TYR:CD2	2.65	0.49
1:A:265:ASN:HA	1:A:308:VAL:O	2.12	0.49
1:A:76:VAL:HG13	1:A:147:ALA:N	2.26	0.49
1:A:483:GLU:CG	1:A:560:VAL:HG22	2.43	0.49
1:A:374:ASN:O	1:A:375:LEU:HD23	2.12	0.49
1:A:371:LYS:CG	1:A:468:GLY:CA	2.90	0.49
1:A:262:ILE:C	1:A:263:ILE:HG23	2.33	0.49
1:A:260:ALA:O	1:A:311:LEU:CD1	2.59	0.49
1:A:128:PRO:HB2	1:A:130:HIS:CE1	2.47	0.48
1:A:80:GLY:O	1:A:130:HIS:CB	2.61	0.48
1:A:428:LEU:HD13	1:A:458:LEU:HD21	1.95	0.48
1:A:482:ALA:O	1:A:561:ILE:HB	2.12	0.48
1:A:165:ILE:CG2	1:A:201:PHE:CZ	2.95	0.48
1:A:132:ALA:HB3	1:A:383:GLY:CA	2.44	0.48
1:A:176:ILE:HD13	1:A:230:ILE:HG12	1.95	0.48
1:A:513:ARG:HB2	1:A:564:PHE:CE1	2.49	0.48
1:A:79:MET:CB	1:A:164:ALA:HB1	2.38	0.47
1:A:75:VAL:HG12	1:A:76:VAL:H	1.79	0.47
1:A:387:ALA:O	1:A:391:ILE:HD12	2.14	0.47
1:A:75:VAL:C	1:A:76:VAL:HG23	2.34	0.47
1:A:82:VAL:CG2	1:A:130:HIS:CD2	2.93	0.47
1:A:373:LEU:HD12	1:A:465:MET:HE2	1.85	0.47
1:A:83:ASP:OD2	1:A:453:ARG:HG2	2.15	0.47
1:A:513:ARG:HD2	1:A:564:PHE:HE1	1.79	0.47
1:A:363:ALA:HB1	1:A:403:ASN:CA	2.31	0.47
1:A:380:ASP:CB	1:A:432:VAL:HG22	2.41	0.47
1:A:367:GLU:C	1:A:369:GLY:H	2.18	0.47
1:A:481:GLN:HG2	1:A:562:GLU:HG3	1.91	0.47
1:A:82:VAL:HG12	1:A:83:ASP:N	2.30	0.47
1:A:75:VAL:C	1:A:144:ALA:HB1	2.35	0.47
1:A:475:LYS:HG2	1:A:475:LYS:HZ2	1.66	0.46
1:A:378:ARG:HD2	1:A:412:PRO:HA	1.96	0.46
1:A:484:VAL:HG12	1:A:559:ASP:CA	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLY:HA2	1:A:269:GLN:HG3	1.97	0.46
1:A:363:ALA:HB3	1:A:403:ASN:OD1	2.16	0.46
1:A:568:GLU:H	1:A:569:VAL:HG13	1.80	0.46
1:A:481:GLN:N	1:A:562:GLU:HA	2.31	0.46
1:A:233:LEU:HG	1:A:233:LEU:O	2.16	0.46
1:A:259:GLN:HA	1:A:259:GLN:OE1	2.16	0.46
1:A:522:TRP:HZ2	1:A:550:ASP:CG	2.19	0.45
1:A:133:PHE:C	1:A:383:GLY:HA2	2.36	0.45
1:A:79:MET:SD	1:A:164:ALA:CB	3.03	0.45
1:A:508:ARG:HB2	1:A:537:ARG:O	2.16	0.45
1:A:373:LEU:HD23	1:A:465:MET:C	2.35	0.45
1:A:490:LEU:HD12	1:A:491:PRO:HD3	1.99	0.45
1:A:285:TYR:C	1:A:313:PHE:HA	2.37	0.45
1:A:148:VAL:HG23	1:A:148:VAL:O	2.17	0.45
1:A:559:ASP:OD1	1:A:560:VAL:HG23	2.17	0.45
1:A:130:HIS:H	1:A:130:HIS:HD1	1.66	0.44
1:A:134:THR:CG2	1:A:382:GLN:NE2	2.81	0.44
1:A:505:ARG:HH21	1:A:569:VAL:C	2.21	0.44
1:A:501:VAL:HG22	1:A:506:ILE:HG12	2.00	0.44
1:A:86:LYS:NZ	1:A:130:HIS:HB3	2.31	0.44
1:A:78:ILE:C	1:A:79:MET:HG3	2.37	0.44
1:A:92:TYR:CD1	1:A:217:ALA:CA	3.00	0.44
1:A:251:ILE:HG12	1:A:323:VAL:CG2	2.48	0.44
1:A:483:GLU:CB	1:A:560:VAL:HG22	2.48	0.43
1:A:211:ILE:HD12	1:A:229:MET:HE3	2.00	0.43
1:A:501:VAL:HG12	1:A:502:THR:N	2.33	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.18	0.43
1:A:257:ASP:HB3	1:A:260:ALA:HB3	2.00	0.43
1:A:79:MET:C	1:A:86:LYS:HD3	2.39	0.43
1:A:75:VAL:CG1	1:A:144:ALA:HB2	2.49	0.43
1:A:490:LEU:HD12	1:A:491:PRO:HD2	2.00	0.43
1:A:119:GLN:N	1:A:119:GLN:OE1	2.50	0.43
1:A:484:VAL:HB	1:A:561:ILE:CD1	2.47	0.43
1:A:46:VAL:O	1:A:50:VAL:HG23	2.18	0.43
1:A:353:ARG:NH1	1:A:356:ALA:HB3	2.33	0.43
1:A:412:PRO:HG2	1:A:434:PRO:HA	2.01	0.43
1:A:360:ALA:HB1	1:A:364:ALA:HB2	2.01	0.43
1:A:143:VAL:HA	1:A:269:GLN:HE22	1.80	0.43
1:A:373:LEU:HB2	1:A:465:MET:O	2.19	0.43
1:A:513:ARG:HB3	1:A:562:GLU:O	2.18	0.43
1:A:6:ILE:HG13	1:A:34:HIS:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HD21	1:A:217:ALA:HB3	1.84	0.43
1:A:92:TYR:CB	1:A:217:ALA:O	2.62	0.43
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.70	0.43
1:A:458:LEU:HD23	1:A:458:LEU:C	2.38	0.43
1:A:371:LYS:HE2	1:A:468:GLY:O	2.19	0.42
1:A:90:LEU:HD22	1:A:125:ILE:O	2.19	0.42
1:A:505:ARG:HE	1:A:569:VAL:HG23	1.84	0.42
1:A:247:PRO:HG3	1:A:271:GLY:HA3	2.01	0.42
1:A:134:THR:CB	1:A:382:GLN:HB2	2.50	0.42
1:A:110:VAL:HB	1:A:307:ALA:CB	2.50	0.42
1:A:139:ARG:N	1:A:140:GLY:HA2	2.34	0.42
1:A:131:GLU:C	1:A:133:PHE:N	2.71	0.42
1:A:108:GLN:HB2	1:A:294:ALA:CA	2.48	0.42
1:A:567:VAL:HG13	1:A:567:VAL:O	2.19	0.42
1:A:79:MET:HE1	1:A:167:HIS:ND1	2.34	0.42
1:A:86:LYS:HD2	1:A:129:GLY:O	2.19	0.42
1:A:378:ARG:HD2	1:A:412:PRO:CA	2.50	0.42
1:A:513:ARG:HB2	1:A:564:PHE:HE1	1.85	0.41
1:A:357:THR:C	1:A:359:ALA:H	2.24	0.41
1:A:82:VAL:CG2	1:A:430:PHE:CE2	3.00	0.41
1:A:92:TYR:CG	1:A:217:ALA:CB	3.04	0.41
1:A:484:VAL:HG11	1:A:559:ASP:N	2.35	0.41
1:A:388:ILE:CD1	1:A:458:LEU:HD13	2.50	0.41
1:A:281:ALA:CB	1:A:313:PHE:CE1	3.03	0.41
1:A:132:ALA:CB	1:A:384:SER:N	2.83	0.41
1:A:79:MET:CE	1:A:131:GLU:CD	2.89	0.41
1:A:143:VAL:HG22	1:A:250:VAL:HG21	2.02	0.41
1:A:481:GLN:CA	1:A:562:GLU:HA	2.38	0.41
1:A:281:ALA:HB3	1:A:313:PHE:CE1	2.56	0.41
1:A:388:ILE:HD11	1:A:458:LEU:HD13	2.03	0.41
1:A:249:GLY:HA2	1:A:269:GLN:CB	2.51	0.41
1:A:484:VAL:HG12	1:A:559:ASP:C	2.40	0.41
1:A:287:ARG:O	1:A:312:GLY:HA2	2.20	0.41
1:A:69:LEU:HA	1:A:70:PRO:HD2	1.73	0.41
1:A:238:ASP:OD1	1:A:240:ARG:NH2	2.54	0.40
1:A:76:VAL:HG13	1:A:146:ILE:C	2.41	0.40
1:A:180:ASN:ND2	1:A:217:ALA:HB3	2.36	0.40
1:A:458:LEU:O	1:A:462:VAL:HG23	2.21	0.40
1:A:128:PRO:HB2	1:A:130:HIS:HE1	1.86	0.40
1:A:134:THR:CA	1:A:382:GLN:HB2	2.52	0.40
1:A:263:ILE:HB	1:A:309:GLN:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG13	1:A:430:PHE:HZ	1.84	0.40
1:A:488:PHE:HE2	1:A:532:PHE:HA	1.84	0.40
1:A:110:VAL:HB	1:A:307:ALA:HB3	2.04	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	567/569 (100%)	436 (77%)	92 (16%)	39 (7%)	1 23

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	73	PRO
1	A	131	GLU
1	A	132	ALA
1	A	243	PRO
1	A	358	MET
1	A	363	ALA
1	A	369	GLY
1	A	370	ALA
1	A	382	GLN
1	A	399	ASP
1	A	464	ASN
1	A	474	TYR
1	A	481	GLN
1	A	555	PHE
1	A	556	ARG
1	A	75	VAL
1	A	157	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	ALA
1	A	349	GLU
1	A	359	ALA
1	A	396	THR
1	A	517	ASP
1	A	99	ALA
1	A	141	ALA
1	A	507	PRO
1	A	541	GLN
1	A	557	GLU
1	A	567	VAL
1	A	74	PRO
1	A	169	LYS
1	A	350	GLU
1	A	478	VAL
1	A	542	GLY
1	A	71	ARG
1	A	463	ARG
1	A	357	THR
1	A	383	GLY
1	A	436	GLY

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	450/450 (100%)	392 (87%)	58 (13%)	5 28

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	VAL
1	A	6	ILE
1	A	7	TYR
1	A	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	ARG
1	A	73	PRO
1	A	79	MET
1	A	86	LYS
1	A	88	THR
1	A	89	LEU
1	A	106	ILE
1	A	117	THR
1	A	121	THR
1	A	130	HIS
1	A	135	THR
1	A	137	ARG
1	A	139	ARG
1	A	148	VAL
1	A	176	ILE
1	A	183	ASP
1	A	211	ILE
1	A	213	ILE
1	A	218	LYS
1	A	256	LEU
1	A	295	ASP
1	A	306	SER
1	A	311	LEU
1	A	314	GLN
1	A	321	ASP
1	A	346	ARG
1	A	349	GLU
1	A	361	LEU
1	A	371	LYS
1	A	373	LEU
1	A	378	ARG
1	A	385	LEU
1	A	399	ASP
1	A	409	VAL
1	A	417	VAL
1	A	422	THR
1	A	430	PHE
1	A	437	SER
1	A	451	THR
1	A	454	ILE
1	A	464	ASN
1	A	475	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	477	GLU
1	A	489	ARG
1	A	492	THR
1	A	495	GLN
1	A	529	LEU
1	A	537	ARG
1	A	538	GLU
1	A	550	ASP
1	A	556	ARG
1	A	565	GLN
1	A	568	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.