



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 17, 2018 – 01:09 am GMT

PDB ID : 4A7F
EMDB ID: : EMD-1987
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 3)
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;
Raunser, S.
Deposited on : 2011-11-14
Resolution : 7.70 Å(reported)
Based on PDB ID : 3MFP, 1LKK

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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 ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

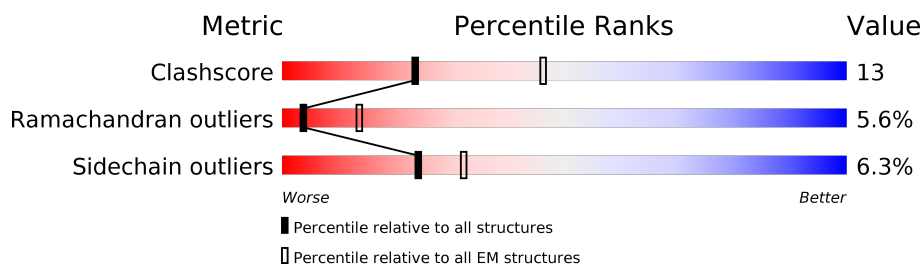
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	375	
1	D	375	
1	E	375	
1	F	375	
1	I	375	
2	B	136	
2	H	136	
3	C	697	
3	G	697	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	697	<div><div></div><div>74%</div><div>22%</div><div>••</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33500 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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1 ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		
2	H	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		

- Molecule 3 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	G	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	J	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		

There are 9 discrepancies between the modelled and reference sequences:

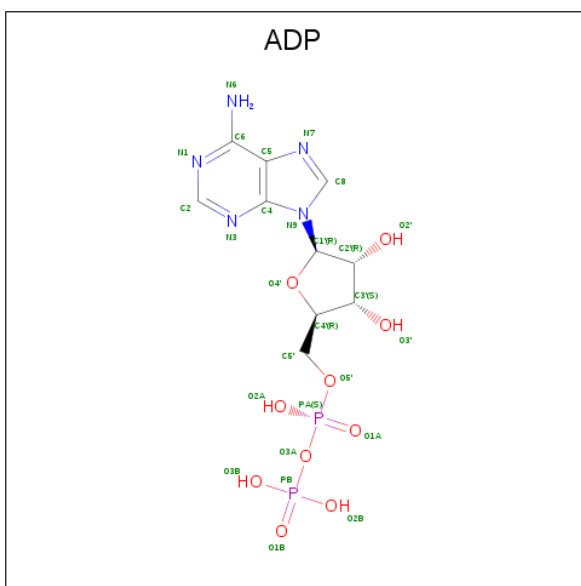
Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	conflict	UNP Q03479

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	conflict	UNP Q03479
C	334	GLU	SER	engineered mutation	UNP Q03479
G	77	MET	ILE	conflict	UNP Q03479
G	215	ASP	ASN	conflict	UNP Q03479
G	334	GLU	SER	engineered mutation	UNP Q03479
J	77	MET	ILE	conflict	UNP Q03479
J	215	ASP	ASN	conflict	UNP Q03479
J	334	GLU	SER	engineered mutation	UNP Q03479

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

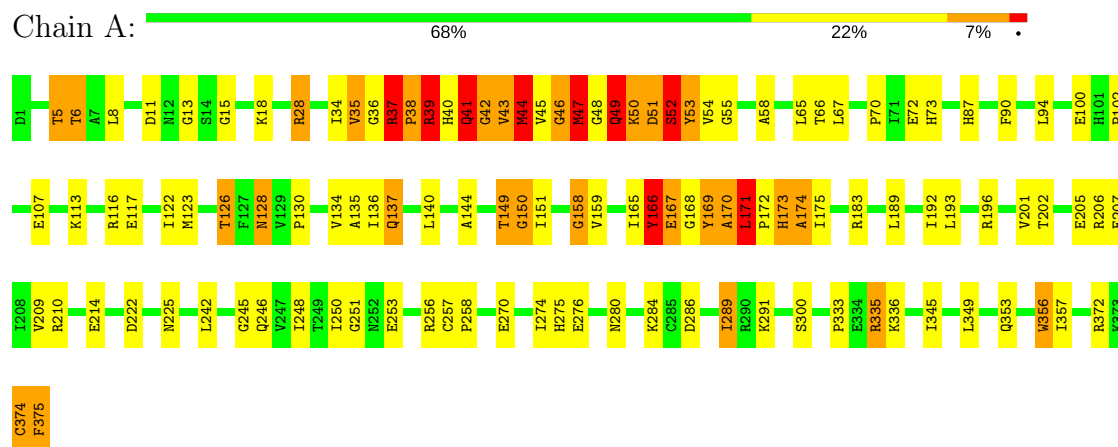
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	I	1	Total 1	Ca 1	0
5	A	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0
5	F	1	Total 1	Ca 1	0
5	E	1	Total 1	Ca 1	0

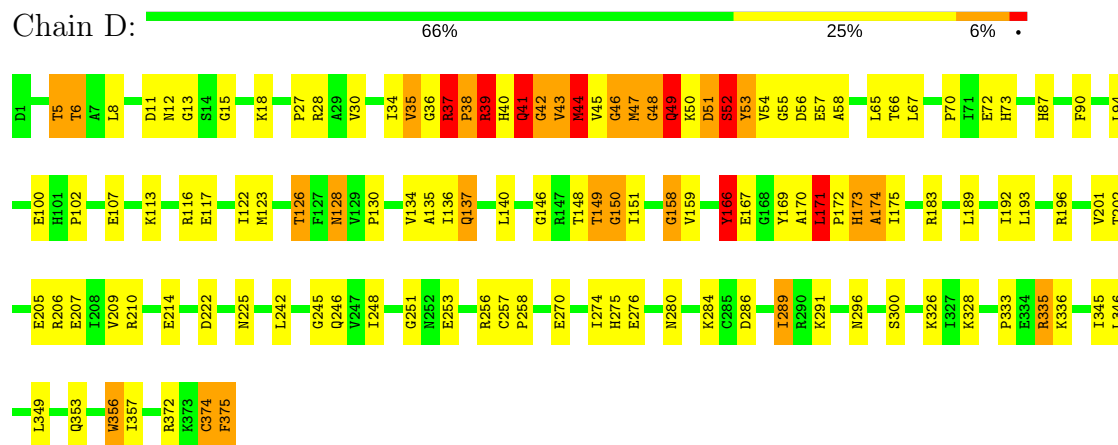
3 Residue-property plots

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

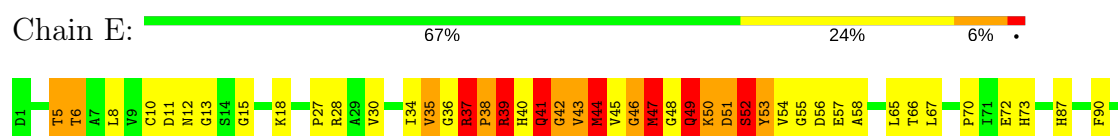
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



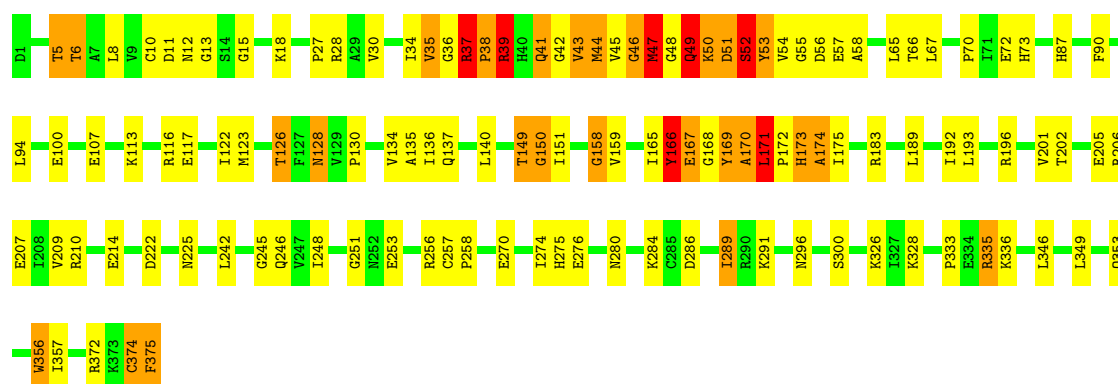
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





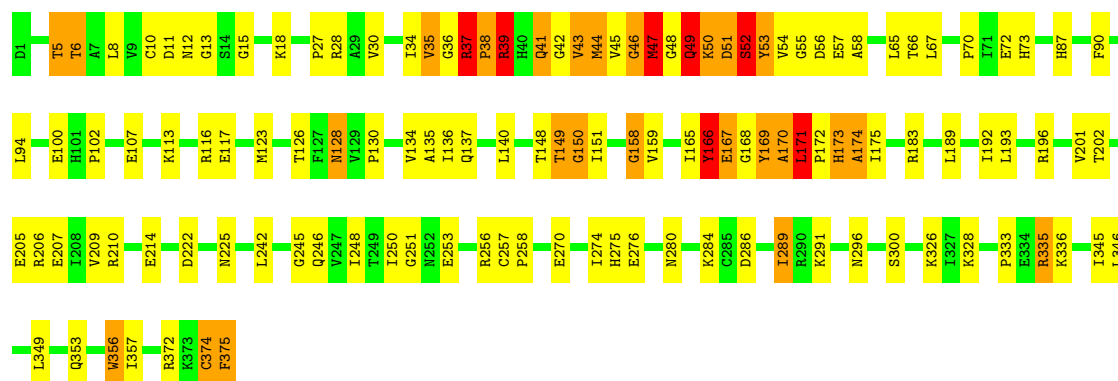
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain F: 67% 24% 7%



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain I: 66% 25% 7%



• Molecule 2: TROPOMYOSIN 1 ALPHA

Chain B: 98%



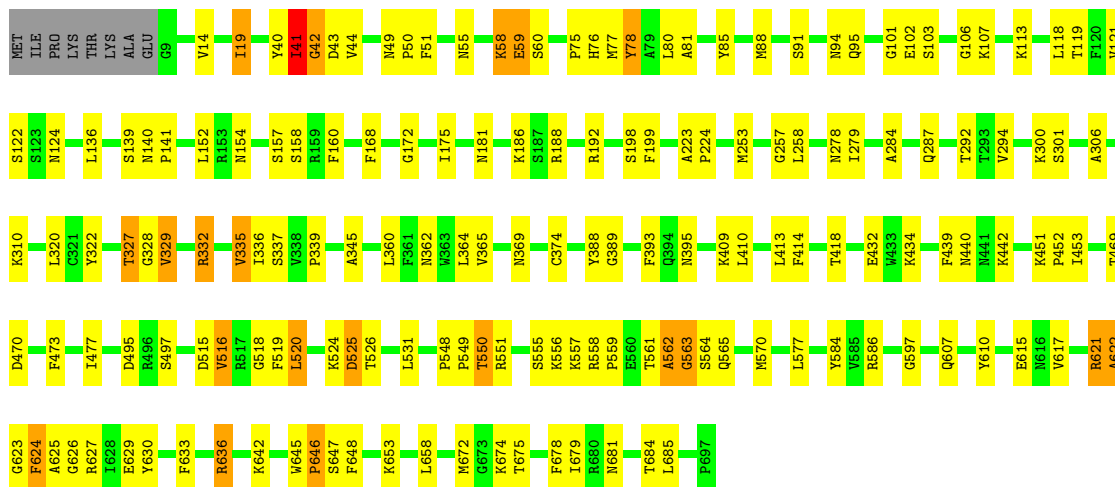
• Molecule 2: TROPOMYOSIN 1 ALPHA

Chain H: 99%



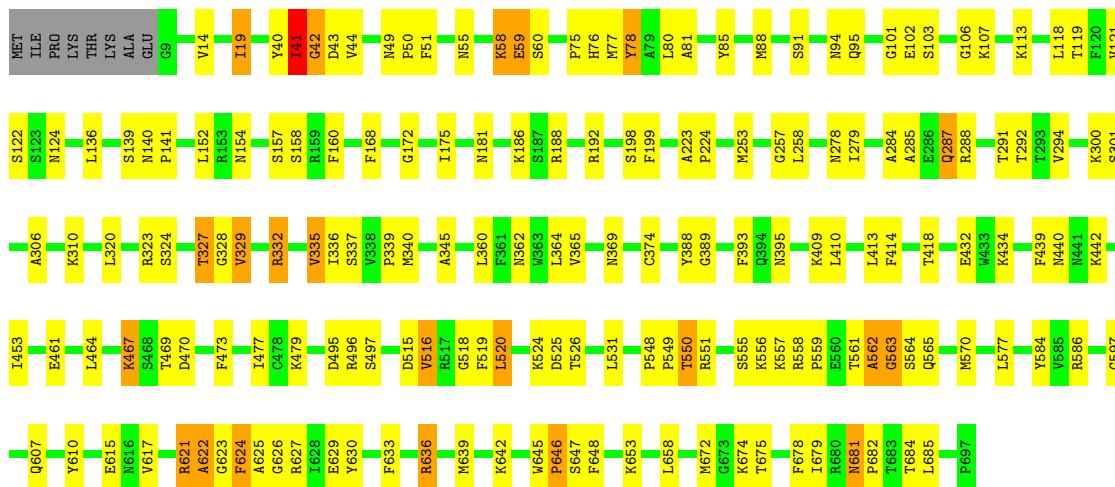
• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain C: 75% 21% ..



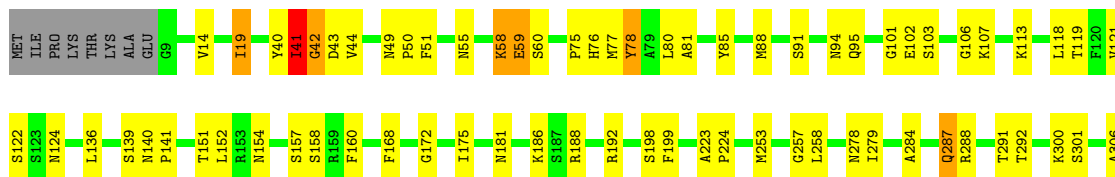
• Molecule 3: MYOSIN IE HEAVY CHAIN

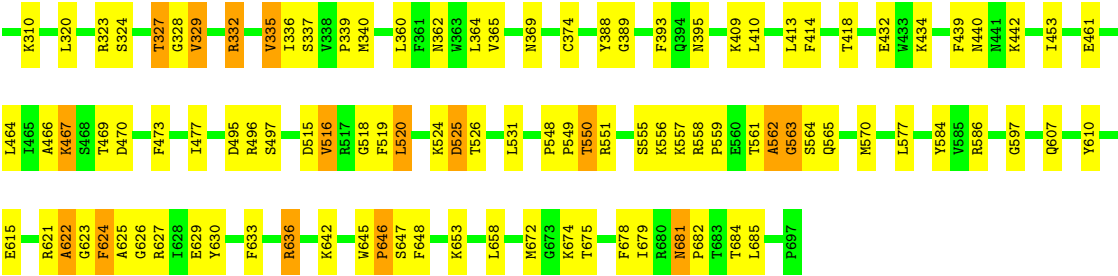
Chain G: 73% 22% ..



• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J: 74% 22% ..





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	5481	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	169644	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.91	10/2984 (0.3%)	0.65	8/4040 (0.2%)
1	D	0.89	9/2984 (0.3%)	0.63	8/4040 (0.2%)
1	E	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
1	F	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
1	I	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
2	B	0.31	0/1107	0.31	0/1471
2	H	0.22	0/1107	0.35	0/1471
3	C	0.26	0/5592	0.39	0/7533
3	G	0.22	0/5592	0.37	0/7533
3	J	0.22	0/5592	0.37	0/7533
All	All	0.62	49/33910 (0.1%)	0.51	40/45741 (0.1%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	166	TYR	CD2-CE2	19.81	1.69	1.39
1	D	166	TYR	CD2-CE2	19.81	1.69	1.39
1	A	166	TYR	CD2-CE2	19.79	1.69	1.39
1	I	166	TYR	CD2-CE2	19.77	1.69	1.39
1	F	166	TYR	CD2-CE2	19.73	1.69	1.39
1	E	166	TYR	CD1-CE1	18.68	1.67	1.39
1	D	166	TYR	CD1-CE1	18.68	1.67	1.39
1	A	166	TYR	CD1-CE1	18.66	1.67	1.39
1	F	166	TYR	CD1-CE1	18.64	1.67	1.39
1	I	166	TYR	CD1-CE1	18.63	1.67	1.39
1	I	166	TYR	CE2-CZ	17.94	1.61	1.38
1	A	166	TYR	CE2-CZ	17.92	1.61	1.38
1	F	166	TYR	CE2-CZ	17.91	1.61	1.38
1	E	166	TYR	CE2-CZ	17.90	1.61	1.38
1	D	166	TYR	CE2-CZ	17.88	1.61	1.38
1	I	166	TYR	CE1-CZ	14.97	1.58	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	TYR	CE1-CZ	14.96	1.57	1.38
1	A	166	TYR	CE1-CZ	14.95	1.57	1.38
1	D	166	TYR	CE1-CZ	14.92	1.57	1.38
1	E	166	TYR	CE1-CZ	14.90	1.57	1.38
1	D	166	TYR	CG-CD1	12.33	1.55	1.39
1	I	166	TYR	CG-CD1	12.29	1.55	1.39
1	E	166	TYR	CG-CD1	12.28	1.55	1.39
1	A	166	TYR	CG-CD1	12.26	1.55	1.39
1	F	166	TYR	CG-CD1	12.22	1.55	1.39
1	I	166	TYR	CG-CD2	11.50	1.54	1.39
1	F	166	TYR	CG-CD2	11.47	1.54	1.39
1	D	166	TYR	CG-CD2	11.45	1.54	1.39
1	A	166	TYR	CG-CD2	11.44	1.54	1.39
1	E	166	TYR	CG-CD2	11.44	1.54	1.39
1	D	150	GLY	N-CA	9.99	1.61	1.46
1	I	150	GLY	N-CA	9.96	1.60	1.46
1	A	150	GLY	N-CA	9.96	1.60	1.46
1	E	150	GLY	N-CA	9.95	1.60	1.46
1	F	150	GLY	N-CA	9.92	1.60	1.46
1	E	43	VAL	CA-CB	7.13	1.69	1.54
1	F	43	VAL	CA-CB	7.10	1.69	1.54
1	I	43	VAL	CA-CB	7.08	1.69	1.54
1	A	43	VAL	CA-CB	7.08	1.69	1.54
1	D	43	VAL	CA-CB	7.07	1.69	1.54
1	F	149	THR	C-N	6.83	1.45	1.33
1	D	149	THR	C-N	6.80	1.45	1.33
1	A	149	THR	C-N	6.79	1.45	1.33
1	E	149	THR	C-N	6.79	1.45	1.33
1	I	149	THR	C-N	6.78	1.45	1.33
1	E	47	MET	C-N	5.04	1.42	1.33
1	A	47	MET	C-N	5.02	1.42	1.33
1	F	47	MET	C-N	5.01	1.42	1.33
1	I	47	MET	C-N	5.01	1.42	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	39	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	39	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	F	39	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	E	39	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	D	39	ARG	NE-CZ-NH2	-9.96	115.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	THR	C-N-CA	9.73	142.73	122.30
1	I	149	THR	C-N-CA	9.73	142.72	122.30
1	A	149	THR	C-N-CA	9.72	142.70	122.30
1	D	149	THR	C-N-CA	9.71	142.70	122.30
1	F	149	THR	C-N-CA	9.71	142.69	122.30
1	A	39	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	39	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	I	39	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	F	39	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	D	39	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	43	VAL	CG1-CB-CG2	-6.70	100.18	110.90
1	F	43	VAL	CG1-CB-CG2	-6.68	100.21	110.90
1	A	43	VAL	CG1-CB-CG2	-6.68	100.22	110.90
1	E	43	VAL	CG1-CB-CG2	-6.66	100.25	110.90
1	I	43	VAL	CG1-CB-CG2	-6.65	100.25	110.90
1	D	43	VAL	CA-CB-CG1	6.20	120.20	110.90
1	A	43	VAL	CA-CB-CG1	6.19	120.18	110.90
1	I	43	VAL	CA-CB-CG1	6.18	120.17	110.90
1	F	43	VAL	CA-CB-CG1	6.18	120.17	110.90
1	E	43	VAL	CA-CB-CG1	6.17	120.16	110.90
1	F	46	GLY	C-N-CA	5.75	136.07	121.70
1	E	46	GLY	C-N-CA	5.74	136.05	121.70
1	A	46	GLY	C-N-CA	5.74	136.04	121.70
1	I	46	GLY	C-N-CA	5.74	136.04	121.70
1	D	46	GLY	C-N-CA	5.72	136.00	121.70
1	D	171	LEU	C-N-CD	5.45	139.84	128.40
1	E	171	LEU	C-N-CD	5.44	139.83	128.40
1	A	171	LEU	C-N-CD	5.44	139.82	128.40
1	I	171	LEU	C-N-CD	5.43	139.79	128.40
1	F	171	LEU	C-N-CD	5.42	139.79	128.40
1	F	41	GLN	N-CA-CB	5.05	119.70	110.60
1	E	41	GLN	N-CA-CB	5.05	119.69	110.60
1	A	41	GLN	N-CA-CB	5.03	119.66	110.60
1	D	41	GLN	N-CA-CB	5.02	119.64	110.60
1	I	41	GLN	N-CA-CB	5.02	119.63	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2934	0	2895	160	0
1	D	2934	0	2895	139	0
1	E	2934	0	2895	125	0
1	F	2934	0	2895	127	0
1	I	2934	0	2895	138	0
2	B	1104	0	1104	2	0
2	H	1104	0	1104	4	0
3	C	5494	0	5490	88	0
3	G	5494	0	5490	98	0
3	J	5494	0	5490	93	0
4	A	27	0	12	7	0
4	D	27	0	12	7	0
4	E	27	0	12	7	0
4	F	27	0	12	7	0
4	I	27	0	12	7	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	33500	0	33213	877	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 13.

All (877) 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:44:MET:SD	1:I:169:TYR:HE1	1.32	1.51
1:A:169:TYR:HE1	1:D:44:MET:SD	1.39	1.46
1:E:44:MET:SD	1:F:169:TYR:HE1	1.44	1.38
1:A:44:MET:SD	1:I:169:TYR:CE1	2.14	1.38
1:I:53:TYR:O	1:I:58:ALA:CB	1.75	1.35
1:E:53:TYR:O	1:E:58:ALA:CB	1.75	1.35
1:D:53:TYR:O	1:D:58:ALA:CB	1.75	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:TYR:O	1:F:58:ALA:CB	1.75	1.34
1:A:53:TYR:O	1:A:58:ALA:CB	1.75	1.33
1:E:53:TYR:O	1:E:58:ALA:HB2	1.17	1.32
1:A:169:TYR:CE1	1:D:44:MET:SD	2.21	1.32
1:I:53:TYR:O	1:I:58:ALA:HB2	1.17	1.31
1:F:53:TYR:O	1:F:58:ALA:HB2	1.17	1.29
1:A:41:GLN:OE1	1:I:171:LEU:HB3	1.29	1.29
1:D:53:TYR:O	1:D:58:ALA:HB2	1.17	1.28
1:A:53:TYR:O	1:A:58:ALA:HB2	1.17	1.27
1:E:44:MET:SD	1:F:169:TYR:CE1	2.26	1.27
1:F:149:THR:O	1:F:166:TYR:CZ	1.87	1.23
1:E:41:GLN:OE1	1:F:171:LEU:HB3	1.33	1.23
1:A:40:HIS:O	1:I:171:LEU:HD23	1.34	1.22
1:A:171:LEU:HB3	1:D:41:GLN:OE1	1.37	1.20
1:E:40:HIS:O	1:F:171:LEU:HD23	1.42	1.20
1:A:171:LEU:HD23	1:D:40:HIS:O	1.43	1.17
1:I:149:THR:O	1:I:166:TYR:CZ	1.88	1.17
1:A:36:GLY:O	1:A:52:SER:CA	1.94	1.16
1:I:36:GLY:O	1:I:52:SER:CA	1.94	1.16
1:D:36:GLY:O	1:D:52:SER:CA	1.94	1.16
1:D:149:THR:O	1:D:166:TYR:CZ	1.88	1.16
1:A:149:THR:O	1:A:166:TYR:CZ	1.88	1.16
1:F:36:GLY:O	1:F:52:SER:CA	1.94	1.14
1:F:149:THR:O	1:F:166:TYR:CE2	1.97	1.14
1:E:36:GLY:O	1:E:52:SER:CA	1.94	1.13
1:A:149:THR:O	1:A:166:TYR:CE2	1.98	1.09
1:D:149:THR:O	1:D:166:TYR:CE2	1.97	1.09
1:I:149:THR:O	1:I:166:TYR:CE2	1.98	1.08
1:F:37:ARG:HB3	1:F:38:PRO:CD	1.85	1.06
1:E:149:THR:O	1:E:166:TYR:CZ	1.88	1.05
1:A:37:ARG:HB3	1:A:38:PRO:CD	1.85	1.05
1:A:34:ILE:O	1:A:35:VAL:HG23	1.56	1.04
1:E:37:ARG:HB3	1:E:38:PRO:CD	1.85	1.04
1:I:34:ILE:O	1:I:35:VAL:HG23	1.56	1.04
1:D:34:ILE:O	1:D:35:VAL:HG23	1.56	1.03
1:F:34:ILE:O	1:F:35:VAL:HG23	1.56	1.03
1:D:37:ARG:HB3	1:D:38:PRO:CD	1.85	1.03
1:E:34:ILE:O	1:E:35:VAL:HG23	1.56	1.03
1:I:37:ARG:HB3	1:I:38:PRO:CD	1.85	1.03
1:E:36:GLY:O	1:E:52:SER:HA	1.58	1.02
1:D:36:GLY:O	1:D:52:SER:HA	1.58	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:O	1:A:52:SER:HA	1.58	1.02
1:F:36:GLY:O	1:F:52:SER:HA	1.58	1.00
1:I:36:GLY:O	1:I:52:SER:HA	1.58	1.00
1:D:53:TYR:C	1:D:58:ALA:HB2	1.82	1.00
1:A:53:TYR:C	1:A:58:ALA:HB2	1.82	0.99
1:F:53:TYR:C	1:F:58:ALA:HB2	1.82	0.99
1:I:53:TYR:C	1:I:58:ALA:HB2	1.82	0.99
1:E:53:TYR:C	1:E:58:ALA:HB2	1.82	0.98
1:F:37:ARG:HH11	1:F:37:ARG:CG	1.79	0.95
1:A:43:VAL:HG12	1:I:165:ILE:HD11	1.47	0.95
1:I:37:ARG:HH11	1:I:37:ARG:CG	1.79	0.95
1:A:41:GLN:NE2	1:I:169:TYR:O	1.99	0.95
1:E:37:ARG:CG	1:E:37:ARG:HH11	1.79	0.94
1:D:37:ARG:HH11	1:D:37:ARG:CG	1.79	0.94
1:A:37:ARG:CG	1:A:37:ARG:HH11	1.79	0.93
1:E:53:TYR:O	1:E:58:ALA:HB1	1.69	0.93
1:E:43:VAL:HG12	1:F:165:ILE:HD11	1.51	0.92
1:I:53:TYR:O	1:I:58:ALA:HB1	1.69	0.92
1:F:53:TYR:O	1:F:58:ALA:HB1	1.69	0.91
1:D:53:TYR:O	1:D:58:ALA:HB1	1.69	0.90
1:A:53:TYR:O	1:A:58:ALA:HB1	1.69	0.90
1:A:165:ILE:HD11	1:D:43:VAL:HG12	1.54	0.89
1:A:169:TYR:O	1:D:41:GLN:NE2	2.05	0.89
1:E:36:GLY:O	1:E:52:SER:C	2.14	0.86
1:D:36:GLY:O	1:D:52:SER:C	2.14	0.86
1:A:28:ARG:O	1:A:28:ARG:NE	2.07	0.86
1:F:36:GLY:O	1:F:52:SER:C	2.14	0.86
1:I:36:GLY:O	1:I:52:SER:C	2.14	0.86
1:A:43:VAL:H	1:I:168:GLY:HA2	1.41	0.85
3:G:285:ALA:O	2:H:142:GLU:CD	2.14	0.85
1:F:36:GLY:O	1:F:52:SER:O	1.94	0.85
1:A:36:GLY:O	1:A:52:SER:C	2.14	0.85
3:G:285:ALA:O	2:H:142:GLU:OE2	1.93	0.85
1:E:41:GLN:NE2	1:F:169:TYR:O	2.10	0.84
1:I:36:GLY:O	1:I:52:SER:O	1.94	0.84
1:D:36:GLY:O	1:D:52:SER:O	1.94	0.84
1:E:36:GLY:O	1:E:52:SER:O	1.94	0.84
1:A:37:ARG:CB	1:A:38:PRO:CD	2.55	0.84
1:A:42:GLY:HA2	1:I:167:GLU:O	1.78	0.84
1:A:36:GLY:O	1:A:52:SER:O	1.94	0.84
1:D:37:ARG:CB	1:D:38:PRO:CD	2.55	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:ARG:CB	1:I:38:PRO:CD	2.55	0.82
3:G:327:THR:HG22	3:G:328:GLY:N	1.95	0.82
3:J:327:THR:HG22	3:J:328:GLY:N	1.95	0.82
1:A:41:GLN:OE1	1:I:171:LEU:CB	2.21	0.81
1:A:47:MET:HE3	3:G:479:LYS:HE2	1.63	0.80
3:C:327:THR:HG22	3:C:328:GLY:N	1.95	0.80
1:F:37:ARG:CB	1:F:38:PRO:CD	2.55	0.80
1:D:171:LEU:HB2	1:D:172:PRO:HD2	1.64	0.80
3:G:285:ALA:O	2:H:142:GLU:OE1	1.99	0.80
1:I:171:LEU:HB2	1:I:172:PRO:HD2	1.64	0.80
1:A:171:LEU:HB2	1:A:172:PRO:HD2	1.64	0.79
1:A:41:GLN:NE2	1:I:170:ALA:O	2.15	0.79
1:E:37:ARG:CB	1:E:38:PRO:CD	2.55	0.79
1:A:37:ARG:CB	1:A:38:PRO:HD3	2.14	0.78
1:E:171:LEU:HB2	1:E:172:PRO:HD2	1.64	0.78
1:F:171:LEU:HB2	1:F:172:PRO:HD2	1.64	0.78
1:I:35:VAL:HG22	1:I:54:VAL:HB	1.66	0.78
1:I:37:ARG:CB	1:I:38:PRO:HD3	2.13	0.78
1:D:37:ARG:CB	1:D:38:PRO:HD3	2.14	0.78
1:E:37:ARG:HG3	1:E:37:ARG:HH11	1.47	0.78
1:A:167:GLU:O	1:D:42:GLY:HA2	1.84	0.78
1:I:37:ARG:HH11	1:I:37:ARG:HG3	1.47	0.78
1:D:35:VAL:HG22	1:D:54:VAL:HB	1.66	0.77
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.47	0.77
1:D:37:ARG:HH11	1:D:37:ARG:HG3	1.47	0.77
1:A:167:GLU:HB3	1:D:40:HIS:CD2	2.19	0.77
1:A:35:VAL:HG22	1:A:54:VAL:HB	1.66	0.77
1:E:37:ARG:CB	1:E:38:PRO:HD3	2.14	0.77
1:E:35:VAL:HG22	1:E:54:VAL:HB	1.66	0.77
1:A:168:GLY:HA2	1:D:43:VAL:H	1.49	0.76
1:F:37:ARG:HH11	1:F:37:ARG:HG3	1.47	0.76
1:F:35:VAL:HG22	1:F:54:VAL:HB	1.66	0.76
1:E:41:GLN:NE2	1:F:170:ALA:O	2.18	0.76
1:E:43:VAL:H	1:F:168:GLY:HA2	1.49	0.76
3:J:327:THR:CG2	3:J:328:GLY:N	2.50	0.75
1:F:37:ARG:CB	1:F:38:PRO:HD3	2.13	0.75
3:G:327:THR:CG2	3:G:328:GLY:N	2.49	0.75
3:G:58:LYS:O	3:G:60:SER:N	2.19	0.75
1:F:52:SER:O	1:F:53:TYR:HB2	1.87	0.75
3:J:58:LYS:O	3:J:60:SER:N	2.19	0.75
1:A:52:SER:O	1:A:53:TYR:HB2	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LYS:O	3:C:60:SER:N	2.19	0.75
1:D:52:SER:O	1:D:53:TYR:HB2	1.87	0.74
1:E:52:SER:O	1:E:53:TYR:HB2	1.87	0.74
1:I:52:SER:O	1:I:53:TYR:HB2	1.87	0.74
3:C:562:ALA:O	3:C:564:SER:N	2.21	0.74
3:G:562:ALA:O	3:G:564:SER:N	2.21	0.73
1:A:41:GLN:CD	1:I:170:ALA:O	2.27	0.73
1:E:36:GLY:O	1:E:52:SER:CB	2.36	0.73
1:E:42:GLY:HA2	1:F:167:GLU:O	1.87	0.73
1:F:36:GLY:O	1:F:52:SER:CB	2.36	0.73
1:A:40:HIS:O	1:I:171:LEU:CD2	2.28	0.73
1:A:40:HIS:CD2	1:I:167:GLU:HB3	2.23	0.73
1:D:36:GLY:O	1:D:52:SER:CB	2.36	0.73
1:A:171:LEU:CB	1:D:41:GLN:OE1	2.30	0.73
1:F:51:ASP:O	1:F:53:TYR:N	2.17	0.73
3:J:278:ASN:O	3:J:301:SER:OG	2.07	0.73
1:A:36:GLY:O	1:A:52:SER:CB	2.36	0.73
3:C:327:THR:CG2	3:C:328:GLY:N	2.52	0.73
3:C:278:ASN:O	3:C:301:SER:OG	2.07	0.73
1:D:39:ARG:HB3	1:D:66:THR:OG1	1.89	0.73
3:J:562:ALA:O	3:J:564:SER:N	2.21	0.72
1:F:39:ARG:HB3	1:F:66:THR:OG1	1.89	0.72
1:A:39:ARG:HB3	1:A:66:THR:OG1	1.89	0.72
3:G:278:ASN:O	3:G:301:SER:OG	2.07	0.72
1:I:37:ARG:NH1	1:I:37:ARG:CG	2.47	0.72
1:F:37:ARG:CG	1:F:37:ARG:NH1	2.47	0.72
1:I:36:GLY:O	1:I:52:SER:CB	2.36	0.72
1:I:39:ARG:HB3	1:I:66:THR:OG1	1.89	0.72
1:D:349:LEU:HD22	3:J:461:GLU:HA	1.71	0.71
1:A:170:ALA:O	1:D:41:GLN:NE2	2.24	0.71
1:F:45:VAL:C	1:F:47:MET:H	1.94	0.71
1:E:51:ASP:O	1:E:53:TYR:N	2.16	0.71
1:E:39:ARG:HB3	1:E:66:THR:OG1	1.89	0.71
3:J:548:PRO:O	3:J:550:THR:N	2.24	0.71
1:A:51:ASP:O	1:A:53:TYR:N	2.16	0.70
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.57	0.70
1:D:37:ARG:HH11	1:D:37:ARG:HG2	1.57	0.70
1:A:49:GLN:HG3	1:A:50:LYS:N	2.07	0.70
3:C:548:PRO:O	3:C:550:THR:N	2.24	0.70
3:G:548:PRO:O	3:G:550:THR:N	2.24	0.70
1:E:45:VAL:C	1:E:47:MET:H	1.94	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLN:HG3	1:D:50:LYS:N	2.07	0.70
1:E:41:GLN:OE1	1:F:171:LEU:CB	2.26	0.70
1:I:37:ARG:HH11	1:I:37:ARG:HG2	1.57	0.70
1:D:51:ASP:O	1:D:53:TYR:N	2.16	0.70
3:J:625:ALA:O	3:J:627:ARG:NH1	2.25	0.70
3:C:625:ALA:O	3:C:627:ARG:NH1	2.25	0.69
3:G:625:ALA:O	3:G:627:ARG:NH1	2.25	0.69
1:F:49:GLN:HG3	1:F:50:LYS:N	2.07	0.69
1:A:45:VAL:C	1:A:47:MET:H	1.94	0.69
1:I:45:VAL:C	1:I:47:MET:H	1.94	0.69
1:D:45:VAL:C	1:D:47:MET:H	1.94	0.69
1:I:49:GLN:HG3	1:I:50:LYS:N	2.07	0.69
1:E:40:HIS:CD2	1:F:167:GLU:HB3	2.28	0.69
1:E:49:GLN:HG3	1:E:50:LYS:N	2.07	0.69
1:E:41:GLN:CD	1:F:170:ALA:O	2.31	0.68
1:A:43:VAL:N	1:I:168:GLY:HA2	2.08	0.68
1:I:51:ASP:O	1:I:53:TYR:N	2.16	0.68
3:C:365:VAL:O	3:C:369:ASN:ND2	2.26	0.68
1:F:37:ARG:HB3	1:F:38:PRO:HD2	1.74	0.68
3:G:365:VAL:O	3:G:369:ASN:ND2	2.26	0.68
3:C:102:GLU:OE2	3:C:607:GLN:NE2	2.27	0.68
1:F:37:ARG:HH11	1:F:37:ARG:HG2	1.57	0.68
3:J:102:GLU:OE2	3:J:607:GLN:NE2	2.27	0.68
3:G:327:THR:CG2	3:G:328:GLY:H	2.07	0.68
1:A:37:ARG:HG2	1:A:37:ARG:NH1	2.09	0.68
1:D:38:PRO:HG3	1:D:49:GLN:CG	2.23	0.68
1:E:38:PRO:HG3	1:E:49:GLN:CG	2.23	0.68
1:I:38:PRO:HG3	1:I:49:GLN:CG	2.23	0.68
1:A:38:PRO:HG3	1:A:49:GLN:CG	2.23	0.67
1:D:37:ARG:NH1	1:D:37:ARG:HG2	2.09	0.67
1:A:167:GLU:C	1:D:40:HIS:NE2	2.47	0.67
3:J:365:VAL:O	3:J:369:ASN:ND2	2.26	0.67
1:D:37:ARG:HB3	1:D:38:PRO:HD2	1.74	0.67
1:F:38:PRO:HG3	1:F:49:GLN:CG	2.23	0.67
1:D:37:ARG:NH1	1:D:37:ARG:CG	2.47	0.67
3:G:102:GLU:OE2	3:G:607:GLN:NE2	2.27	0.67
1:E:37:ARG:HG2	1:E:37:ARG:HH11	1.57	0.67
3:J:327:THR:CG2	3:J:328:GLY:H	2.07	0.67
1:E:37:ARG:NH1	1:E:37:ARG:HG2	2.09	0.66
1:I:37:ARG:HB3	1:I:38:PRO:HD2	1.74	0.66
3:G:461:GLU:HA	1:I:349:LEU:HD22	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TYR:HB3	1:D:65:LEU:HD21	1.78	0.66
1:D:34:ILE:O	1:D:35:VAL:CG2	2.41	0.66
1:F:37:ARG:HG2	1:F:37:ARG:NH1	2.09	0.66
1:A:171:LEU:HB2	1:A:172:PRO:CD	2.26	0.66
1:A:53:TYR:HB3	1:A:65:LEU:HD21	1.78	0.66
1:D:171:LEU:HB2	1:D:172:PRO:CD	2.26	0.66
1:I:171:LEU:HB2	1:I:172:PRO:CD	2.26	0.66
3:J:327:THR:H	3:J:332:ARG:HA	1.61	0.66
3:C:327:THR:CG2	3:C:328:GLY:H	2.08	0.66
1:I:34:ILE:O	1:I:35:VAL:CG2	2.41	0.66
1:I:53:TYR:HB3	1:I:65:LEU:HD21	1.78	0.65
1:I:35:VAL:CG2	1:I:54:VAL:HB	2.26	0.65
1:E:35:VAL:CG2	1:E:54:VAL:HB	2.26	0.65
1:F:53:TYR:HB3	1:F:65:LEU:HD21	1.77	0.65
1:A:35:VAL:CG2	1:A:54:VAL:HB	2.26	0.65
1:E:53:TYR:HB3	1:E:65:LEU:HD21	1.78	0.65
1:F:35:VAL:CG2	1:F:54:VAL:HB	2.26	0.65
1:A:170:ALA:O	1:D:41:GLN:CD	2.34	0.65
1:D:35:VAL:CG2	1:D:54:VAL:HB	2.26	0.65
1:E:34:ILE:O	1:E:35:VAL:CG2	2.41	0.65
1:F:171:LEU:HB2	1:F:172:PRO:CD	2.26	0.65
1:E:171:LEU:HB2	1:E:172:PRO:CD	2.26	0.64
1:F:173:HIS:CG	1:F:174:ALA:N	2.66	0.64
3:C:327:THR:H	3:C:332:ARG:HA	1.62	0.64
3:G:88:MET:SD	3:G:91:SER:OG	2.55	0.64
1:I:37:ARG:HG2	1:I:37:ARG:NH1	2.09	0.64
1:I:43:VAL:HG23	1:I:46:GLY:HA3	1.79	0.64
3:J:88:MET:SD	3:J:91:SER:OG	2.55	0.64
1:D:173:HIS:CG	1:D:174:ALA:N	2.66	0.64
1:E:173:HIS:CG	1:E:174:ALA:N	2.66	0.64
1:A:43:VAL:HG23	1:A:46:GLY:HA3	1.79	0.64
3:C:88:MET:SD	3:C:91:SER:OG	2.55	0.64
3:G:327:THR:H	3:G:332:ARG:HA	1.61	0.64
1:D:43:VAL:HG23	1:D:46:GLY:HA3	1.80	0.64
1:A:37:ARG:HB3	1:A:38:PRO:HD2	1.75	0.63
1:F:34:ILE:O	1:F:35:VAL:CG2	2.41	0.63
1:I:173:HIS:CG	1:I:174:ALA:N	2.66	0.63
1:A:202:THR:OG1	1:A:205:GLU:OE1	2.15	0.63
1:E:38:PRO:HG3	1:E:49:GLN:HG2	1.80	0.63
1:E:40:HIS:NE2	1:F:167:GLU:C	2.52	0.63
1:E:202:THR:OG1	1:E:205:GLU:OE1	2.16	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLU:OE1	1:E:270:GLU:N	2.32	0.63
1:F:36:GLY:O	1:F:52:SER:HB3	1.99	0.63
1:F:38:PRO:HG3	1:F:49:GLN:HG2	1.80	0.63
1:D:270:GLU:OE1	1:D:270:GLU:N	2.32	0.63
1:D:38:PRO:HG3	1:D:49:GLN:CD	2.19	0.63
1:E:37:ARG:HB3	1:E:38:PRO:HD2	1.74	0.63
1:I:202:THR:OG1	1:I:205:GLU:OE1	2.16	0.63
1:D:202:THR:OG1	1:D:205:GLU:OE1	2.15	0.63
1:F:49:GLN:NE2	1:F:53:TYR:CZ	2.67	0.63
1:I:38:PRO:HG3	1:I:49:GLN:CD	2.19	0.63
1:I:36:GLY:O	1:I:52:SER:HB3	1.99	0.63
1:A:270:GLU:N	1:A:270:GLU:OE1	2.32	0.63
1:A:38:PRO:HG3	1:A:49:GLN:CD	2.19	0.63
1:E:49:GLN:NE2	1:E:53:TYR:CZ	2.67	0.63
1:I:270:GLU:N	1:I:270:GLU:OE1	2.32	0.62
1:E:43:VAL:N	1:F:168:GLY:HA2	2.14	0.62
1:D:189:LEU:HD22	1:D:209:VAL:HG13	1.81	0.62
1:F:202:THR:OG1	1:F:205:GLU:OE1	2.15	0.62
1:F:38:PRO:HG3	1:F:49:GLN:CD	2.19	0.62
3:G:59:GLU:OE1	3:G:59:GLU:N	2.33	0.62
1:A:173:HIS:CG	1:A:174:ALA:N	2.66	0.62
1:A:189:LEU:HD22	1:A:209:VAL:HG13	1.81	0.62
1:A:47:MET:CE	3:G:479:LYS:HE2	2.29	0.62
1:E:36:GLY:O	1:E:52:SER:HB3	1.99	0.62
1:F:43:VAL:HG23	1:F:46:GLY:HA3	1.79	0.62
3:C:59:GLU:N	3:C:59:GLU:OE1	2.33	0.62
1:F:270:GLU:N	1:F:270:GLU:OE1	2.32	0.62
1:I:49:GLN:NE2	1:I:53:TYR:CZ	2.67	0.62
1:E:43:VAL:HG23	1:E:46:GLY:HA3	1.80	0.62
3:J:59:GLU:N	3:J:59:GLU:OE1	2.33	0.62
1:D:36:GLY:O	1:D:52:SER:HB3	1.99	0.62
1:E:189:LEU:HD22	1:E:209:VAL:HG13	1.81	0.62
1:E:38:PRO:HG3	1:E:49:GLN:CD	2.19	0.62
1:I:189:LEU:HD22	1:I:209:VAL:HG13	1.81	0.62
3:J:122:SER:OG	3:J:172:GLY:O	2.17	0.62
1:A:36:GLY:O	1:A:52:SER:HB3	1.99	0.62
1:F:189:LEU:HD22	1:F:209:VAL:HG13	1.81	0.62
1:A:38:PRO:HG3	1:A:49:GLN:HG2	1.80	0.62
1:I:38:PRO:HG3	1:I:49:GLN:HG2	1.80	0.62
1:D:49:GLN:NE2	1:D:53:TYR:CZ	2.67	0.61
1:E:43:VAL:HG23	1:E:46:GLY:CA	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:VAL:HG23	1:F:46:GLY:CA	2.31	0.61
1:D:38:PRO:HG3	1:D:49:GLN:HG2	1.80	0.61
3:G:555:SER:O	3:G:557:LYS:N	2.34	0.61
1:A:49:GLN:NE2	1:A:53:TYR:CZ	2.67	0.61
1:A:52:SER:O	1:A:53:TYR:CB	2.48	0.61
1:A:40:HIS:NE2	1:I:167:GLU:C	2.54	0.61
3:G:122:SER:OG	3:G:172:GLY:O	2.17	0.61
1:A:34:ILE:O	1:A:35:VAL:CG2	2.41	0.61
3:C:555:SER:O	3:C:557:LYS:N	2.34	0.60
1:A:43:VAL:HG23	1:A:46:GLY:CA	2.30	0.60
3:C:122:SER:OG	3:C:172:GLY:O	2.17	0.60
1:E:52:SER:O	1:E:53:TYR:CB	2.48	0.60
1:F:56:ASP:OD1	1:F:57:GLU:N	2.34	0.60
3:J:555:SER:O	3:J:557:LYS:N	2.34	0.60
3:G:327:THR:HA	3:G:332:ARG:H	1.66	0.60
1:D:43:VAL:HG23	1:D:46:GLY:CA	2.31	0.60
1:I:43:VAL:HG23	1:I:46:GLY:CA	2.30	0.60
1:D:56:ASP:OD1	1:D:57:GLU:N	2.34	0.60
1:I:56:ASP:OD1	1:I:57:GLU:N	2.34	0.60
1:F:52:SER:O	1:F:53:TYR:CB	2.48	0.60
1:E:40:HIS:HD1	1:F:171:LEU:CD2	2.14	0.60
1:A:168:GLY:HA2	1:D:43:VAL:N	2.17	0.60
1:D:52:SER:O	1:D:53:TYR:CB	2.48	0.60
1:E:56:ASP:OD1	1:E:57:GLU:N	2.34	0.60
1:A:42:GLY:CA	1:I:167:GLU:O	2.50	0.59
3:J:327:THR:HA	3:J:332:ARG:H	1.67	0.59
3:C:327:THR:HA	3:C:332:ARG:H	1.68	0.59
1:I:52:SER:O	1:I:53:TYR:CB	2.48	0.59
1:I:207:GLU:OE2	1:I:210:ARG:NH1	2.36	0.59
1:A:207:GLU:OE2	1:A:210:ARG:NH1	2.36	0.58
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.85	0.58
1:I:107:GLU:HB2	1:I:134:VAL:HG22	1.85	0.58
1:D:207:GLU:OE2	1:D:210:ARG:NH1	2.36	0.58
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.85	0.58
1:A:167:GLU:CB	1:D:40:HIS:NE2	2.66	0.58
1:I:43:VAL:O	1:I:45:VAL:N	2.37	0.58
1:D:150:GLY:O	1:D:166:TYR:CG	2.57	0.58
1:I:150:GLY:O	1:I:166:TYR:CG	2.57	0.58
3:C:328:GLY:O	3:C:329:VAL:HB	2.03	0.58
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.85	0.58
1:A:43:VAL:O	1:A:45:VAL:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:O	1:D:45:VAL:N	2.37	0.58
1:E:150:GLY:O	1:E:166:TYR:CG	2.57	0.58
1:E:207:GLU:OE2	1:E:210:ARG:NH1	2.36	0.58
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.86	0.58
1:F:207:GLU:OE2	1:F:210:ARG:NH1	2.36	0.58
1:E:38:PRO:CG	1:E:49:GLN:HG2	2.34	0.57
1:E:43:VAL:O	1:E:45:VAL:N	2.37	0.57
3:G:339:PRO:HD2	1:I:333:PRO:HG2	1.85	0.57
1:A:150:GLY:O	1:A:166:TYR:CG	2.57	0.57
1:A:38:PRO:CG	1:A:49:GLN:HG2	2.34	0.57
1:I:38:PRO:CG	1:I:49:GLN:HG2	2.34	0.57
1:F:38:PRO:CG	1:F:49:GLN:HG2	2.34	0.57
1:D:38:PRO:CG	1:D:49:GLN:HG2	2.34	0.57
1:E:40:HIS:O	1:F:171:LEU:CD2	2.35	0.57
1:F:150:GLY:O	1:F:166:TYR:CG	2.57	0.57
1:F:43:VAL:O	1:F:45:VAL:N	2.37	0.57
1:D:51:ASP:C	1:D:53:TYR:H	2.06	0.56
1:A:167:GLU:HB3	1:D:40:HIS:NE2	2.19	0.56
3:G:323:ARG:NH1	3:G:340:MET:SD	2.79	0.56
3:J:136:LEU:O	3:J:139:SER:OG	2.22	0.56
1:D:333:PRO:HG2	3:J:339:PRO:HD2	1.88	0.55
3:J:49:ASN:OD1	3:J:51:PHE:N	2.39	0.55
1:A:51:ASP:C	1:A:53:TYR:H	2.06	0.55
1:I:374:CYS:SG	1:I:375:PHE:N	2.80	0.55
3:J:323:ARG:NH1	3:J:340:MET:SD	2.79	0.55
1:F:51:ASP:C	1:F:53:TYR:H	2.06	0.55
3:G:136:LEU:O	3:G:139:SER:OG	2.22	0.55
3:J:629:GLU:O	3:J:633:PHE:N	2.39	0.55
3:G:629:GLU:O	3:G:633:PHE:N	2.39	0.55
3:G:645:TRP:O	3:G:647:SER:N	2.40	0.55
1:A:11:ASP:N	1:A:18:LYS:O	2.40	0.55
3:C:629:GLU:O	3:C:633:PHE:N	2.39	0.55
1:D:11:ASP:N	1:D:18:LYS:O	2.40	0.55
1:F:11:ASP:N	1:F:18:LYS:O	2.40	0.55
1:A:374:CYS:SG	1:A:375:PHE:N	2.80	0.55
1:D:374:CYS:SG	1:D:375:PHE:N	2.80	0.55
3:G:49:ASN:OD1	3:G:51:PHE:N	2.39	0.55
1:A:40:HIS:HD1	1:I:171:LEU:CD2	2.20	0.55
1:A:173:HIS:O	1:A:175:ILE:N	2.41	0.55
3:C:49:ASN:OD1	3:C:51:PHE:N	2.39	0.55
1:E:11:ASP:N	1:E:18:LYS:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:CYS:SG	1:F:375:PHE:N	2.80	0.55
3:J:645:TRP:O	3:J:647:SER:N	2.40	0.55
1:D:173:HIS:O	1:D:175:ILE:N	2.41	0.54
1:E:173:HIS:O	1:E:175:ILE:N	2.41	0.54
1:I:173:HIS:O	1:I:175:ILE:N	2.40	0.54
1:A:171:LEU:CD2	1:D:40:HIS:HD1	2.19	0.54
1:E:374:CYS:SG	1:E:375:PHE:N	2.80	0.54
1:E:37:ARG:NH1	1:E:37:ARG:CG	2.47	0.54
1:F:173:HIS:O	1:F:175:ILE:N	2.41	0.54
1:D:48:GLY:O	1:D:50:LYS:HG3	2.08	0.54
1:I:51:ASP:C	1:I:53:TYR:H	2.06	0.54
3:C:645:TRP:O	3:C:647:SER:N	2.40	0.54
1:D:55:GLY:O	1:D:58:ALA:N	2.40	0.54
1:D:37:ARG:CG	1:D:38:PRO:HD3	2.38	0.54
1:E:43:VAL:CG2	1:E:46:GLY:HA3	2.38	0.54
1:I:11:ASP:N	1:I:18:LYS:O	2.40	0.54
1:E:50:LYS:HE3	1:E:51:ASP:N	2.23	0.53
1:E:55:GLY:O	1:E:58:ALA:N	2.40	0.53
1:F:50:LYS:HE3	1:F:51:ASP:N	2.23	0.53
3:G:624:PHE:O	3:G:627:ARG:NH1	2.41	0.53
1:I:336:LYS:HE3	4:I:376:ADP:H5'2	1.90	0.53
1:A:336:LYS:HE3	4:A:376:ADP:H5'2	1.90	0.53
1:A:37:ARG:CG	1:A:38:PRO:HD3	2.38	0.53
3:C:624:PHE:O	3:C:627:ARG:NH1	2.41	0.53
1:F:37:ARG:CG	1:F:38:PRO:HD3	2.38	0.53
1:I:296:ASN:OD1	1:I:328:LYS:NZ	2.41	0.53
3:J:624:PHE:O	3:J:627:ARG:NH1	2.41	0.53
1:F:43:VAL:CG2	1:F:46:GLY:HA3	2.38	0.53
1:A:43:VAL:HG12	1:I:165:ILE:CD1	2.32	0.53
1:D:296:ASN:OD1	1:D:328:LYS:NZ	2.41	0.53
1:A:333:PRO:O	1:A:335:ARG:NH2	2.42	0.53
1:A:55:GLY:O	1:A:58:ALA:N	2.40	0.53
1:F:296:ASN:OD1	1:F:328:LYS:NZ	2.41	0.53
1:F:333:PRO:O	1:F:335:ARG:NH2	2.42	0.53
1:I:50:LYS:HE3	1:I:51:ASP:N	2.23	0.53
3:J:40:TYR:O	3:J:41:ILE:HG13	2.08	0.53
1:E:296:ASN:OD1	1:E:328:LYS:NZ	2.41	0.53
1:E:37:ARG:CG	1:E:38:PRO:HD3	2.38	0.53
1:E:40:HIS:NE2	1:F:167:GLU:HB3	2.24	0.53
1:F:336:LYS:HE3	4:F:376:ADP:H5'2	1.90	0.53
1:F:55:GLY:O	1:F:58:ALA:N	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:40:TYR:O	3:G:41:ILE:HG13	2.08	0.53
1:A:40:HIS:NE2	1:I:167:GLU:CB	2.72	0.53
1:I:37:ARG:CG	1:I:38:PRO:HD3	2.38	0.53
1:D:336:LYS:HE3	4:D:376:ADP:H5'2	1.90	0.53
1:I:43:VAL:CG2	1:I:46:GLY:HA3	2.38	0.53
1:I:53:TYR:CB	1:I:65:LEU:HD21	2.39	0.53
1:I:333:PRO:O	1:I:335:ARG:NH2	2.42	0.53
1:I:55:GLY:O	1:I:58:ALA:N	2.40	0.53
1:A:167:GLU:O	1:D:42:GLY:CA	2.56	0.52
1:A:43:VAL:CG2	1:A:46:GLY:HA3	2.38	0.52
1:A:50:LYS:HE3	1:A:51:ASP:N	2.23	0.52
1:A:53:TYR:CB	1:A:65:LEU:HD21	2.39	0.52
3:C:40:TYR:O	3:C:41:ILE:HG13	2.08	0.52
1:D:333:PRO:O	1:D:335:ARG:NH2	2.42	0.52
3:C:679:ILE:HG21	3:C:684:THR:HG21	1.91	0.52
1:I:214:GLU:HB2	4:I:376:ADP:C2	2.44	0.52
1:D:122:ILE:O	1:D:126:THR:OG1	2.27	0.52
1:D:242:LEU:HD12	1:D:248:ILE:HD11	1.92	0.52
1:E:333:PRO:O	1:E:335:ARG:NH2	2.42	0.52
1:E:336:LYS:HE3	4:E:376:ADP:H5'2	1.90	0.52
1:E:214:GLU:HB2	4:E:376:ADP:C2	2.44	0.52
3:J:679:ILE:HG21	3:J:684:THR:HG21	1.91	0.52
1:A:214:GLU:HB2	4:A:376:ADP:C2	2.44	0.52
1:A:49:GLN:NE2	1:A:53:TYR:CE2	2.77	0.52
1:D:49:GLN:NE2	1:D:53:TYR:CE2	2.77	0.52
1:E:53:TYR:CB	1:E:65:LEU:HD21	2.39	0.52
1:F:214:GLU:HB2	4:F:376:ADP:C2	2.44	0.52
1:I:49:GLN:NE2	1:I:53:TYR:CE2	2.77	0.52
1:A:242:LEU:HD12	1:A:248:ILE:HD11	1.92	0.52
1:D:214:GLU:HB2	4:D:376:ADP:C2	2.44	0.52
1:D:53:TYR:CB	1:D:65:LEU:HD21	2.39	0.52
3:G:679:ILE:HG21	3:G:684:THR:HG21	1.91	0.52
1:D:43:VAL:CG2	1:D:46:GLY:HA3	2.38	0.52
3:G:328:GLY:O	3:G:329:VAL:HB	2.10	0.52
1:I:242:LEU:HD12	1:I:248:ILE:HD11	1.92	0.52
1:F:49:GLN:NE2	1:F:53:TYR:CE2	2.77	0.51
3:G:103:SER:OG	3:G:158:SER:N	2.43	0.51
1:A:40:HIS:NE2	1:I:167:GLU:HB3	2.25	0.51
1:E:40:HIS:NE2	1:F:167:GLU:CB	2.74	0.51
3:J:103:SER:OG	3:J:158:SER:N	2.43	0.51
3:C:322:TYR:HB3	3:C:337:SER:OG	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:LYS:HD2	4:F:376:ADP:C8	2.46	0.51
1:E:49:GLN:NE2	1:E:53:TYR:CE2	2.77	0.51
3:J:674:LYS:HD3	3:J:675:THR:HG23	1.93	0.51
1:A:345:ILE:O	1:A:349:LEU:HD13	2.10	0.51
3:C:470:ASP:HB3	3:C:516:VAL:HG22	1.93	0.51
1:E:242:LEU:HD12	1:E:248:ILE:HD11	1.92	0.51
1:F:53:TYR:CB	1:F:65:LEU:HD21	2.39	0.51
3:G:674:LYS:HD3	3:G:675:THR:HG23	1.93	0.51
1:I:336:LYS:HD2	4:I:376:ADP:C8	2.46	0.51
3:J:328:GLY:O	3:J:329:VAL:HB	2.10	0.51
3:J:470:ASP:HB3	3:J:516:VAL:HG22	1.93	0.51
3:G:119:THR:O	3:G:121:VAL:N	2.42	0.51
3:G:470:ASP:HB3	3:G:516:VAL:HG22	1.93	0.51
3:C:103:SER:OG	3:C:158:SER:N	2.44	0.50
3:C:140:ASN:HB2	3:C:141:PRO:HD3	1.92	0.50
3:C:674:LYS:HD3	3:C:675:THR:HG23	1.93	0.50
1:D:50:LYS:O	1:D:52:SER:N	2.45	0.50
1:E:122:ILE:O	1:E:126:THR:OG1	2.27	0.50
1:D:117:GLU:OE1	1:D:117:GLU:N	2.45	0.50
3:J:140:ASN:HB2	3:J:141:PRO:HD3	1.92	0.50
1:A:144:ALA:HA	1:A:345:ILE:HD11	1.92	0.50
1:E:117:GLU:N	1:E:117:GLU:OE1	2.45	0.50
1:E:336:LYS:HD2	4:E:376:ADP:C8	2.46	0.50
3:G:140:ASN:HB2	3:G:141:PRO:HD3	1.92	0.50
3:J:561:THR:O	3:J:562:ALA:C	2.50	0.50
1:A:117:GLU:OE1	1:A:117:GLU:N	2.45	0.50
1:A:336:LYS:HD2	4:A:376:ADP:C8	2.46	0.50
1:A:50:LYS:O	1:A:52:SER:N	2.45	0.50
3:C:561:THR:O	3:C:562:ALA:C	2.50	0.50
1:F:242:LEU:HD12	1:F:248:ILE:HD11	1.92	0.50
3:C:136:LEU:O	3:C:139:SER:OG	2.22	0.50
1:D:336:LYS:HD2	4:D:376:ADP:C8	2.46	0.50
1:A:167:GLU:C	1:D:40:HIS:CD2	2.85	0.50
1:E:50:LYS:O	1:E:52:SER:N	2.44	0.50
3:C:43:ASP:HB3	3:C:80:LEU:HD22	1.93	0.50
3:J:119:THR:O	3:J:121:VAL:N	2.43	0.50
3:G:561:THR:O	3:G:562:ALA:C	2.50	0.50
3:J:43:ASP:HB3	3:J:80:LEU:HD22	1.93	0.50
1:F:90:PHE:HA	1:F:94:LEU:HD12	1.94	0.50
3:G:43:ASP:HB3	3:G:80:LEU:HD22	1.93	0.50
3:C:495:ASP:OD2	3:C:497:SER:OG	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:626:GLY:HA3	3:C:685:LEU:HD11	1.94	0.50
1:D:5:THR:O	1:D:6:THR:OG1	2.30	0.50
1:I:5:THR:O	1:I:6:THR:OG1	2.30	0.50
3:G:284:ALA:O	3:G:292:THR:OG1	2.30	0.49
3:C:562:ALA:O	3:C:565:GLN:N	2.43	0.49
1:E:40:HIS:ND1	1:F:171:LEU:CD2	2.75	0.49
1:E:51:ASP:C	1:E:53:TYR:H	2.06	0.49
3:G:467:LYS:HB3	1:I:148:THR:HG23	1.94	0.49
1:I:50:LYS:O	1:I:52:SER:N	2.45	0.49
3:C:515:ASP:OD1	3:C:516:VAL:N	2.42	0.49
1:F:50:LYS:O	1:F:52:SER:N	2.45	0.49
1:F:5:THR:O	1:F:6:THR:OG1	2.30	0.49
3:J:562:ALA:O	3:J:565:GLN:N	2.43	0.49
1:A:90:PHE:HA	1:A:94:LEU:HD12	1.94	0.49
1:F:122:ILE:O	1:F:126:THR:OG1	2.27	0.49
1:I:90:PHE:HA	1:I:94:LEU:HD12	1.94	0.49
1:A:122:ILE:O	1:A:126:THR:OG1	2.27	0.49
3:G:626:GLY:HA3	3:G:685:LEU:HD11	1.94	0.49
1:I:117:GLU:OE1	1:I:117:GLU:N	2.45	0.49
1:D:150:GLY:O	1:D:166:TYR:CD1	2.66	0.49
3:G:518:GLY:O	3:G:520:LEU:N	2.46	0.49
3:G:562:ALA:O	3:G:565:GLN:N	2.43	0.49
3:J:518:GLY:O	3:J:520:LEU:N	2.46	0.49
3:J:55:ASN:ND2	3:J:55:ASN:O	2.46	0.49
1:F:117:GLU:N	1:F:117:GLU:OE1	2.45	0.49
3:J:645:TRP:HB3	3:J:646:PRO:HD2	1.94	0.49
1:E:5:THR:O	1:E:6:THR:OG1	2.30	0.49
1:A:150:GLY:O	1:A:166:TYR:CD1	2.66	0.49
3:C:284:ALA:O	3:C:292:THR:OG1	2.30	0.49
3:J:626:GLY:HA3	3:J:685:LEU:HD11	1.94	0.49
1:F:8:LEU:HD21	1:F:94:LEU:HD13	1.95	0.48
1:D:336:LYS:HD2	4:D:376:ADP:H8	1.79	0.48
1:E:90:PHE:HA	1:E:94:LEU:HD12	1.94	0.48
1:A:336:LYS:HD2	4:A:376:ADP:H8	1.79	0.48
1:F:150:GLY:O	1:F:166:TYR:CD1	2.66	0.48
3:J:41:ILE:HG22	3:J:41:ILE:O	2.13	0.48
3:C:119:THR:O	3:C:121:VAL:N	2.43	0.48
3:C:55:ASN:ND2	3:C:55:ASN:O	2.46	0.48
1:E:150:GLY:O	1:E:166:TYR:CD1	2.66	0.48
1:E:8:LEU:HD21	1:E:94:LEU:HD13	1.95	0.48
1:F:336:LYS:HD2	4:F:376:ADP:H8	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:GLY:O	1:I:166:TYR:CD1	2.66	0.48
1:I:336:LYS:HD2	4:I:376:ADP:H8	1.79	0.48
3:J:495:ASP:OD2	3:J:497:SER:OG	2.30	0.48
3:C:645:TRP:HB3	3:C:646:PRO:HD2	1.94	0.48
1:A:171:LEU:CD2	1:D:40:HIS:O	2.36	0.48
3:G:645:TRP:HB3	3:G:646:PRO:HD2	1.94	0.48
3:G:495:ASP:OD2	3:G:497:SER:OG	2.30	0.48
3:G:55:ASN:O	3:G:55:ASN:ND2	2.46	0.48
1:D:345:ILE:HG23	3:J:464:LEU:HB3	1.94	0.48
1:D:276:GLU:N	1:D:276:GLU:OE1	2.47	0.48
3:G:41:ILE:O	3:G:41:ILE:HG22	2.13	0.48
3:G:464:LEU:HB3	1:I:345:ILE:HG23	1.95	0.48
3:C:518:GLY:O	3:C:520:LEU:N	2.46	0.47
3:C:607:GLN:HA	3:C:610:TYR:CE2	2.48	0.47
1:D:90:PHE:HA	1:D:94:LEU:HD12	1.94	0.47
1:A:276:GLU:OE1	1:A:276:GLU:N	2.47	0.47
3:C:562:ALA:O	3:C:563:GLY:C	2.53	0.47
1:E:276:GLU:OE1	1:E:276:GLU:N	2.47	0.47
1:E:336:LYS:HD2	4:E:376:ADP:H8	1.79	0.47
3:G:607:GLN:HA	3:G:610:TYR:CE2	2.48	0.47
3:J:284:ALA:O	3:J:292:THR:OG1	2.30	0.47
3:J:562:ALA:O	3:J:563:GLY:C	2.53	0.47
3:J:607:GLN:HA	3:J:610:TYR:CE2	2.48	0.47
1:F:276:GLU:N	1:F:276:GLU:OE1	2.47	0.47
1:A:28:ARG:O	1:A:28:ARG:CZ	2.61	0.47
1:A:5:THR:O	1:A:6:THR:OG1	2.30	0.47
3:J:41:ILE:O	3:J:42:GLY:C	2.52	0.47
1:D:8:LEU:HD21	1:D:94:LEU:HD13	1.95	0.47
1:A:8:LEU:HD21	1:A:94:LEU:HD13	1.95	0.47
1:F:27:PRO:O	1:F:28:ARG:NH1	2.48	0.47
3:C:41:ILE:HG22	3:C:41:ILE:O	2.13	0.47
1:D:13:GLY:HA3	4:D:376:ADP:O2B	2.15	0.47
3:G:562:ALA:O	3:G:563:GLY:C	2.53	0.47
1:I:276:GLU:OE1	1:I:276:GLU:N	2.47	0.47
3:J:434:LYS:NZ	3:J:672:MET:O	2.48	0.47
1:E:280:ASN:O	1:E:284:LYS:NZ	2.48	0.47
3:J:515:ASP:OD1	3:J:516:VAL:N	2.42	0.47
3:J:630:TYR:OH	3:J:672:MET:HA	2.15	0.47
3:C:327:THR:HG22	3:C:328:GLY:H	1.69	0.47
1:F:222:ASP:OD2	1:F:225:ASN:ND2	2.48	0.47
1:E:42:GLY:CA	1:F:167:GLU:O	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:ASP:O	1:I:18:LYS:N	2.48	0.46
1:I:8:LEU:HD21	1:I:94:LEU:HD13	1.95	0.46
1:D:135:ALA:HB1	1:D:140:LEU:HD11	1.97	0.46
1:A:167:GLU:CA	1:D:40:HIS:NE2	2.78	0.46
3:G:515:ASP:OD1	3:G:516:VAL:N	2.42	0.46
3:G:434:LYS:NZ	3:G:672:MET:O	2.47	0.46
1:I:222:ASP:OD2	1:I:225:ASN:ND2	2.48	0.46
1:I:158:GLY:N	4:I:376:ADP:O3B	2.47	0.46
3:C:630:TYR:OH	3:C:672:MET:HA	2.15	0.46
3:G:41:ILE:O	3:G:42:GLY:C	2.52	0.46
1:I:13:GLY:HA3	4:I:376:ADP:O2B	2.15	0.46
1:I:37:ARG:HG3	1:I:38:PRO:HD3	1.98	0.46
3:C:413:LEU:HD13	3:C:577:LEU:HD13	1.96	0.46
1:D:222:ASP:OD2	1:D:225:ASN:ND2	2.48	0.46
1:F:72:GLU:O	1:F:73:HIC:C	2.64	0.46
3:J:473:PHE:CZ	3:J:477:ILE:HD11	2.50	0.46
1:E:11:ASP:O	1:E:18:LYS:N	2.48	0.46
3:G:413:LEU:HD13	3:G:577:LEU:HD13	1.96	0.46
3:J:327:THR:HG23	3:J:328:GLY:H	1.78	0.46
1:D:11:ASP:O	1:D:18:LYS:N	2.48	0.46
1:D:148:THR:HG23	3:J:467:LYS:HB3	1.97	0.46
1:D:37:ARG:HG3	1:D:38:PRO:HD3	1.98	0.46
1:E:13:GLY:HA3	4:E:376:ADP:O2B	2.15	0.46
1:E:27:PRO:O	1:E:28:ARG:NH1	2.48	0.46
3:G:630:TYR:OH	3:G:672:MET:HA	2.15	0.46
3:J:413:LEU:HD13	3:J:577:LEU:HD13	1.96	0.46
1:A:158:GLY:N	4:A:376:ADP:O3B	2.47	0.46
1:A:37:ARG:HG3	1:A:38:PRO:HD3	1.98	0.46
3:C:41:ILE:O	3:C:42:GLY:C	2.52	0.46
3:C:615:GLU:OE1	3:C:615:GLU:N	2.48	0.46
1:E:37:ARG:HG3	1:E:38:PRO:HD3	1.98	0.46
1:F:37:ARG:HG3	1:F:38:PRO:HD3	1.98	0.46
3:G:360:LEU:O	3:G:364:LEU:N	2.49	0.46
1:A:40:HIS:HA	1:I:171:LEU:HD22	1.98	0.46
1:A:11:ASP:O	1:A:18:LYS:N	2.48	0.46
1:A:222:ASP:OD2	1:A:225:ASN:ND2	2.48	0.46
1:E:49:GLN:CG	1:E:50:LYS:N	2.78	0.46
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.97	0.46
3:C:473:PHE:CZ	3:C:477:ILE:HD11	2.50	0.46
1:E:222:ASP:OD2	1:E:225:ASN:ND2	2.48	0.46
1:E:72:GLU:O	1:E:73:HIC:C	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:GLY:HA3	4:F:376:ADP:O2B	2.15	0.46
1:F:11:ASP:O	1:F:18:LYS:N	2.48	0.46
1:A:41:GLN:OE1	1:I:170:ALA:O	2.34	0.46
3:G:328:GLY:CA	1:I:30:VAL:HG22	2.45	0.46
3:J:558:ARG:HB2	3:J:559:PRO:HD3	1.98	0.46
3:J:615:GLU:OE1	3:J:615:GLU:N	2.48	0.46
1:D:158:GLY:N	4:D:376:ADP:O3B	2.47	0.45
1:A:40:HIS:CD2	1:I:167:GLU:C	2.89	0.45
1:A:72:GLU:O	1:A:73:HIC:C	2.64	0.45
3:C:558:ARG:HB2	3:C:559:PRO:HD3	1.98	0.45
1:E:41:GLN:OE1	1:F:170:ALA:O	2.34	0.45
1:A:13:GLY:HA3	4:A:376:ADP:O2B	2.15	0.45
1:D:72:GLU:O	1:D:73:HIC:C	2.64	0.45
3:G:473:PHE:CZ	3:G:477:ILE:HD11	2.50	0.45
3:G:558:ARG:HB2	3:G:559:PRO:HD3	1.98	0.45
1:A:274:ILE:HD12	1:A:275:HIS:N	2.32	0.45
1:D:49:GLN:CG	1:D:50:LYS:N	2.78	0.45
1:F:274:ILE:HD12	1:F:275:HIS:N	2.32	0.45
1:I:49:GLN:CG	1:I:50:LYS:N	2.78	0.45
1:E:135:ALA:HB1	1:E:140:LEU:HD11	1.97	0.45
1:E:274:ILE:HD12	1:E:275:HIS:N	2.32	0.45
1:F:135:ALA:HB1	1:F:140:LEU:HD11	1.97	0.45
3:G:327:THR:HG23	3:G:328:GLY:H	1.78	0.45
1:I:135:ALA:HB1	1:I:140:LEU:HD11	1.97	0.45
1:I:72:GLU:O	1:I:73:HIC:C	2.64	0.45
1:D:27:PRO:O	1:D:28:ARG:NH1	2.48	0.45
1:I:27:PRO:O	1:I:28:ARG:NH1	2.48	0.45
1:A:40:HIS:ND1	1:I:171:LEU:CD2	2.80	0.45
1:E:40:HIS:HD1	1:F:171:LEU:HD21	1.82	0.45
3:G:118:LEU:HD21	3:G:168:PHE:HE2	1.82	0.45
1:I:274:ILE:HD12	1:I:275:HIS:N	2.32	0.45
3:J:306:ALA:O	3:J:310:LYS:N	2.50	0.45
1:A:353:GLN:HA	1:A:356:TRP:CE2	2.52	0.45
1:D:353:GLN:HA	1:D:356:TRP:CE2	2.52	0.45
1:E:353:GLN:HA	1:E:356:TRP:CE2	2.52	0.45
3:G:615:GLU:OE1	3:G:615:GLU:N	2.48	0.45
3:J:77:MET:O	3:J:78:TYR:O	2.35	0.45
1:F:286:ASP:O	1:F:289:ILE:HG22	2.17	0.45
1:A:37:ARG:CG	1:A:37:ARG:NH1	2.47	0.44
1:F:353:GLN:HA	1:F:356:TRP:CE2	2.52	0.44
3:J:223:ALA:HB3	3:J:224:PRO:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:OE1	1:A:256:ARG:NH1	2.51	0.44
3:C:118:LEU:HD21	3:C:168:PHE:HE2	1.82	0.44
3:C:19:ILE:O	3:C:19:ILE:HG23	2.18	0.44
3:C:306:ALA:O	3:C:310:LYS:N	2.50	0.44
1:F:280:ASN:O	1:F:284:LYS:NZ	2.48	0.44
3:G:77:MET:O	3:G:78:TYR:O	2.35	0.44
1:D:253:GLU:OE1	1:D:256:ARG:NH1	2.51	0.44
3:G:639:MET:SD	3:G:639:MET:N	2.81	0.44
3:C:223:ALA:HB3	3:C:224:PRO:HD3	1.99	0.44
1:D:274:ILE:HD12	1:D:275:HIS:N	2.32	0.44
3:G:19:ILE:O	3:G:19:ILE:HG23	2.18	0.44
2:B:199:THR:O	2:B:203:ASN:ND2	2.48	0.44
3:C:622:ALA:HB3	3:C:678:PHE:CE1	2.53	0.44
3:C:94:ASN:O	3:C:95:GLN:NE2	2.51	0.44
3:G:306:ALA:O	3:G:310:LYS:N	2.50	0.44
3:G:622:ALA:HB3	3:G:678:PHE:CE1	2.53	0.44
3:J:118:LEU:HD21	3:J:168:PHE:HE2	1.82	0.44
3:J:94:ASN:O	3:J:95:GLN:NE2	2.51	0.44
1:A:171:LEU:CD2	1:D:40:HIS:ND1	2.81	0.44
3:C:434:LYS:NZ	3:C:672:MET:O	2.48	0.44
1:D:136:ILE:N	1:D:136:ILE:HD12	2.32	0.44
1:F:253:GLU:OE1	1:F:256:ARG:NH1	2.51	0.44
1:I:136:ILE:HD12	1:I:136:ILE:N	2.32	0.44
1:I:353:GLN:HA	1:I:356:TRP:CE2	2.52	0.44
3:J:622:ALA:HB3	3:J:678:PHE:CE1	2.53	0.44
1:D:286:ASP:O	1:D:289:ILE:HG22	2.17	0.44
1:F:136:ILE:HD12	1:F:136:ILE:N	2.32	0.44
1:F:49:GLN:CG	1:F:50:LYS:N	2.78	0.44
3:G:223:ALA:HB3	3:G:224:PRO:HD3	1.99	0.44
1:I:253:GLU:OE1	1:I:256:ARG:NH1	2.51	0.44
1:E:136:ILE:N	1:E:136:ILE:HD12	2.32	0.43
1:E:253:GLU:OE1	1:E:256:ARG:NH1	2.51	0.43
1:E:286:ASP:O	1:E:289:ILE:HG22	2.17	0.43
1:E:158:GLY:N	4:E:376:ADP:O3B	2.47	0.43
1:E:40:HIS:CD2	1:F:167:GLU:C	2.91	0.43
3:J:19:ILE:O	3:J:19:ILE:HG23	2.18	0.43
1:A:49:GLN:CG	1:A:50:LYS:N	2.78	0.43
1:D:257:CYS:HB3	1:D:258:PRO:HD3	2.00	0.43
3:G:81:ALA:O	3:G:85:TYR:N	2.52	0.43
3:J:287:GLN:HG3	3:J:291:THR:HG23	2.00	0.43
3:J:360:LEU:O	3:J:364:LEU:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:81:ALA:O	3:J:85:TYR:N	2.52	0.43
1:A:167:GLU:O	1:D:40:HIS:CD2	2.71	0.43
1:F:346:LEU:HA	1:F:349:LEU:HG	2.01	0.43
1:D:146:GLY:HA2	3:J:466:ALA:HB3	2.01	0.43
1:A:286:ASP:O	1:A:289:ILE:HG22	2.17	0.43
3:C:451:LYS:HB3	3:C:452:PRO:HD2	2.00	0.43
1:D:280:ASN:O	1:D:284:LYS:NZ	2.48	0.43
1:E:346:LEU:HA	1:E:349:LEU:HG	2.01	0.43
1:F:257:CYS:HB3	1:F:258:PRO:HD3	2.00	0.43
3:J:320:LEU:HA	3:J:531:LEU:HD22	2.00	0.43
3:G:287:GLN:HG3	3:G:291:THR:HG23	2.00	0.43
3:G:94:ASN:O	3:G:95:GLN:NE2	2.51	0.43
1:I:286:ASP:O	1:I:289:ILE:HG22	2.17	0.43
3:J:393:PHE:HB2	3:J:395:ASN:O	2.19	0.43
1:D:345:ILE:HD12	3:J:464:LEU:HB3	2.00	0.43
1:A:136:ILE:N	1:A:136:ILE:HD12	2.33	0.43
1:A:257:CYS:HB3	1:A:258:PRO:HD3	2.00	0.43
3:C:175:ILE:HB	3:C:374:CYS:HB3	2.01	0.43
3:C:393:PHE:HB2	3:C:395:ASN:O	2.19	0.43
3:C:77:MET:O	3:C:78:TYR:O	2.35	0.43
1:D:346:LEU:HA	1:D:349:LEU:HG	2.01	0.43
1:F:35:VAL:HG13	1:F:52:SER:CB	2.49	0.43
1:I:35:VAL:HG13	1:I:52:SER:CB	2.49	0.43
1:E:35:VAL:HG13	1:E:52:SER:CB	2.49	0.43
1:A:35:VAL:HG13	1:A:52:SER:CB	2.49	0.42
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.00	0.42
1:F:123:MET:O	1:F:128:ASN:N	2.52	0.42
3:J:151:THR:OG1	3:J:154:ASN:O	2.29	0.42
1:A:170:ALA:O	1:D:41:GLN:OE1	2.37	0.42
1:A:189:LEU:HG	1:A:193:LEU:HD13	2.01	0.42
3:G:393:PHE:HB2	3:G:395:ASN:O	2.19	0.42
1:I:123:MET:O	1:I:128:ASN:N	2.52	0.42
3:C:181:ASN:OD1	3:C:362:ASN:ND2	2.47	0.42
1:D:123:MET:O	1:D:128:ASN:N	2.52	0.42
1:D:357:ILE:HD12	1:D:357:ILE:N	2.34	0.42
1:I:189:LEU:HG	1:I:193:LEU:HD13	2.01	0.42
1:I:280:ASN:O	1:I:284:LYS:NZ	2.48	0.42
1:I:53:TYR:HB2	1:I:65:LEU:HG	2.02	0.42
1:D:210:ARG:HD2	4:D:376:ADP:O3'	2.19	0.42
1:D:53:TYR:HB2	1:D:65:LEU:HG	2.01	0.42
1:F:210:ARG:HD2	4:F:376:ADP:O3'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LEU:HA	1:I:349:LEU:HG	2.01	0.42
3:J:175:ILE:HB	3:J:374:CYS:HB3	2.01	0.42
3:J:681:ASN:HA	3:J:682:PRO:HD3	1.92	0.42
1:A:53:TYR:HB2	1:A:65:LEU:HG	2.02	0.42
3:C:81:ALA:O	3:C:85:TYR:N	2.52	0.42
3:G:181:ASN:OD1	3:G:362:ASN:ND2	2.47	0.42
3:G:327:THR:HA	3:G:332:ARG:N	2.34	0.42
1:I:257:CYS:HB3	1:I:258:PRO:HD3	2.00	0.42
3:C:320:LEU:HA	3:C:531:LEU:HD22	2.00	0.42
1:D:189:LEU:HG	1:D:193:LEU:HD13	2.01	0.42
1:F:357:ILE:N	1:F:357:ILE:HD12	2.34	0.42
3:G:320:LEU:HA	3:G:531:LEU:HD22	2.00	0.42
2:B:169:LEU:HD22	2:H:165:VAL:HG13	2.02	0.42
3:C:409:LYS:NZ	3:C:570:MET:O	2.53	0.42
1:A:171:LEU:HD21	1:D:40:HIS:HD1	1.84	0.42
1:E:210:ARG:HD2	4:E:376:ADP:O3'	2.19	0.42
3:G:681:ASN:HA	3:G:682:PRO:HD3	1.92	0.42
1:A:357:ILE:N	1:A:357:ILE:HD12	2.34	0.42
1:A:210:ARG:HD2	4:A:376:ADP:O3'	2.19	0.42
3:C:154:ASN:HB3	3:C:157:SER:HB2	2.02	0.42
1:D:30:VAL:HG22	3:J:328:GLY:CA	2.50	0.42
1:D:35:VAL:HG13	1:D:52:SER:CB	2.49	0.42
1:E:40:HIS:HD1	1:F:171:LEU:HD22	1.83	0.42
1:F:158:GLY:N	4:F:376:ADP:O3B	2.47	0.42
1:D:18:LYS:HA	1:D:30:VAL:HG12	2.02	0.42
1:F:53:TYR:HB2	1:F:65:LEU:HG	2.02	0.42
3:G:175:ILE:HB	3:G:374:CYS:HB3	2.01	0.42
3:J:409:LYS:NZ	3:J:570:MET:O	2.53	0.42
1:A:123:MET:O	1:A:128:ASN:N	2.52	0.42
1:E:123:MET:O	1:E:128:ASN:N	2.52	0.42
1:E:357:ILE:HD12	1:E:357:ILE:N	2.34	0.42
1:E:53:TYR:HB2	1:E:65:LEU:HG	2.01	0.42
3:G:550:THR:HG22	3:G:551:ARG:HG3	2.02	0.42
1:I:210:ARG:HD2	4:I:376:ADP:O3'	2.19	0.42
3:J:107:LYS:N	3:J:107:LYS:HD3	2.35	0.42
1:D:166:TYR:HD1	1:D:166:TYR:HA	1.83	0.41
1:A:40:HIS:HD1	1:I:171:LEU:HD21	1.84	0.41
3:G:50:PRO:O	3:G:51:PHE:HB2	2.21	0.41
3:G:409:LYS:NZ	3:G:570:MET:O	2.53	0.41
3:J:50:PRO:O	3:J:51:PHE:HB2	2.21	0.41
3:J:645:TRP:O	3:J:648:PHE:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:LYS:N	3:C:107:LYS:HD3	2.35	0.41
3:C:414:PHE:O	3:C:418:THR:N	2.53	0.41
3:C:41:ILE:O	3:C:44:VAL:N	2.53	0.41
3:G:107:LYS:HD3	3:G:107:LYS:N	2.35	0.41
3:C:550:THR:HG22	3:C:551:ARG:HG3	2.02	0.41
3:C:645:TRP:O	3:C:648:PHE:N	2.54	0.41
1:D:328:LYS:HB3	1:D:328:LYS:HZ3	1.85	0.41
1:E:189:LEU:HG	1:E:193:LEU:HD13	2.01	0.41
3:G:335:VAL:HG13	3:G:336:ILE:N	2.36	0.41
3:G:630:TYR:CD2	3:G:675:THR:HA	2.56	0.41
1:I:357:ILE:HD12	1:I:357:ILE:N	2.34	0.41
3:C:50:PRO:O	3:C:51:PHE:HB2	2.21	0.41
1:F:189:LEU:HG	1:F:193:LEU:HD13	2.01	0.41
3:G:328:GLY:HA2	1:I:30:VAL:HG22	2.02	0.41
3:G:414:PHE:O	3:G:418:THR:N	2.53	0.41
3:J:335:VAL:HG13	3:J:336:ILE:N	2.36	0.41
3:J:414:PHE:O	3:J:418:THR:N	2.53	0.41
1:A:333:PRO:HG2	3:C:339:PRO:HD2	2.03	0.41
3:C:630:TYR:CD2	3:C:675:THR:HA	2.56	0.41
1:F:18:LYS:HA	1:F:30:VAL:HG12	2.02	0.41
1:F:300:SER:HA	1:F:335:ARG:HB2	2.02	0.41
3:G:188:ARG:O	3:G:192:ARG:NH1	2.54	0.41
3:G:198:SER:OG	3:G:199:PHE:N	2.54	0.41
3:G:41:ILE:O	3:G:44:VAL:N	2.53	0.41
3:G:645:TRP:O	3:G:648:PHE:N	2.54	0.41
1:I:300:SER:HA	1:I:335:ARG:HB2	2.02	0.41
3:J:154:ASN:HB3	3:J:157:SER:HB2	2.02	0.41
3:J:181:ASN:OD1	3:J:362:ASN:ND2	2.47	0.41
3:J:41:ILE:O	3:J:44:VAL:N	2.53	0.41
3:G:103:SER:HB2	3:G:389:GLY:N	2.36	0.41
3:J:103:SER:HB2	3:J:389:GLY:N	2.36	0.41
3:J:188:ARG:O	3:J:192:ARG:NH1	2.54	0.41
3:J:198:SER:OG	3:J:199:PHE:N	2.54	0.41
3:C:103:SER:HB2	3:C:389:GLY:N	2.36	0.41
3:C:360:LEU:O	3:C:364:LEU:N	2.49	0.41
3:C:40:TYR:CZ	3:C:75:PRO:HA	2.56	0.41
3:G:154:ASN:HB3	3:G:157:SER:HB2	2.02	0.41
3:G:324:SER:HB3	3:G:337:SER:HB3	2.03	0.41
3:G:40:TYR:CZ	3:G:75:PRO:HA	2.56	0.41
1:I:6:THR:HB	1:I:102:PRO:HD3	2.03	0.41
1:A:6:THR:HB	1:A:102:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ARG:O	3:C:192:ARG:NH1	2.54	0.41
1:A:171:LEU:HD22	1:D:40:HIS:HA	2.03	0.41
1:E:10:CYS:SG	1:E:11:ASP:N	2.94	0.41
1:E:300:SER:HA	1:E:335:ARG:HB2	2.02	0.41
3:J:327:THR:HA	3:J:332:ARG:N	2.35	0.41
3:J:40:TYR:CZ	3:J:75:PRO:HA	2.56	0.41
1:A:280:ASN:O	1:A:284:LYS:NZ	2.48	0.41
3:C:327:THR:HA	3:C:332:ARG:N	2.36	0.41
3:C:294:VAL:HG21	3:C:345:ALA:HB1	2.02	0.41
3:G:253:MET:HB3	3:G:258:LEU:HB2	2.02	0.41
3:J:253:MET:HB3	3:J:258:LEU:HB2	2.02	0.41
3:J:630:TYR:CD2	3:J:675:THR:HA	2.56	0.41
3:C:617:VAL:HG13	3:C:621:ARG:NH1	2.36	0.41
1:D:6:THR:HB	1:D:102:PRO:HD3	2.03	0.41
3:G:294:VAL:HG21	3:G:345:ALA:HB1	2.02	0.41
1:A:40:HIS:NE2	1:I:167:GLU:CA	2.83	0.41
3:J:525:ASP:O	3:J:525:ASP:CG	2.59	0.41
3:J:550:THR:HG22	3:J:551:ARG:HG3	2.02	0.41
1:A:300:SER:HA	1:A:335:ARG:HB2	2.02	0.40
3:C:327:THR:HG23	3:C:328:GLY:H	1.85	0.40
1:I:10:CYS:SG	1:I:11:ASP:N	2.94	0.40
3:J:629:GLU:HA	3:J:675:THR:O	2.21	0.40
1:A:136:ILE:O	1:A:137:GLN:C	2.60	0.40
3:C:629:GLU:HA	3:C:675:THR:O	2.22	0.40
1:F:12:ASN:OD1	1:F:13:GLY:N	2.54	0.40
3:G:617:VAL:HG13	3:G:621:ARG:NH1	2.36	0.40
1:I:18:LYS:HA	1:I:30:VAL:HG12	2.02	0.40
3:J:324:SER:HB3	3:J:337:SER:HB3	2.03	0.40
1:A:44:MET:SD	1:I:169:TYR:CD1	2.98	0.40
3:C:198:SER:OG	3:C:199:PHE:N	2.54	0.40
3:C:253:MET:HB3	3:C:258:LEU:HB2	2.02	0.40
3:C:335:VAL:HG13	3:C:336:ILE:N	2.36	0.40
1:D:12:ASN:OD1	1:D:13:GLY:N	2.55	0.40
1:D:300:SER:HA	1:D:335:ARG:HB2	2.02	0.40
3:G:629:GLU:HA	3:G:675:THR:O	2.21	0.40
1:I:12:ASN:OD1	1:I:13:GLY:N	2.54	0.40
1:A:248:ILE:HG22	1:A:250:ILE:HG23	2.04	0.40
3:C:409:LYS:O	3:C:413:LEU:N	2.54	0.40
1:E:12:ASN:OD1	1:E:13:GLY:N	2.55	0.40
1:E:18:LYS:HA	1:E:30:VAL:HG12	2.02	0.40
1:I:372:ARG:CZ	1:I:372:ARG:HA	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HA	1:A:335:ARG:HG3	2.04	0.40
1:A:372:ARG:HA	1:A:372:ARG:CZ	2.52	0.40
3:C:525:ASP:CG	3:C:525:ASP:O	2.59	0.40
1:D:136:ILE:O	1:D:137:GLN:C	2.60	0.40
1:D:372:ARG:CZ	1:D:372:ARG:HA	2.52	0.40
1:F:10:CYS:SG	1:F:11:ASP:N	2.94	0.40
1:F:372:ARG:HA	1:F:372:ARG:CZ	2.52	0.40
1:I:166:TYR:HA	1:I:166:TYR:HD1	1.83	0.40
1:I:248:ILE:HG22	1:I:250:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	18
1	D	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	18
1	E	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	18
1	F	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	18
1	I	372/375 (99%)	293 (79%)	52 (14%)	27 (7%)	1	18
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	2	26
3	G	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	2	26
3	J	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	2	26
All	All	4177/4238 (99%)	3382 (81%)	561 (13%)	234 (6%)	4	24

All (234) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	37	ARG
1	A	38	PRO
1	A	44	MET
1	A	47	MET
1	A	49	GLN
1	A	51	ASP
1	A	52	SER
1	A	53	TYR
1	A	137	GLN
1	A	171	LEU
1	A	174	ALA
3	C	59	GLU
3	C	78	TYR
3	C	335	VAL
3	C	549	PRO
3	C	550	THR
3	C	562	ALA
3	C	563	GLY
1	D	35	VAL
1	D	37	ARG
1	D	38	PRO
1	D	44	MET
1	D	47	MET
1	D	49	GLN
1	D	51	ASP
1	D	52	SER
1	D	53	TYR
1	D	137	GLN
1	D	171	LEU
1	D	174	ALA
1	E	35	VAL
1	E	37	ARG
1	E	38	PRO
1	E	44	MET
1	E	47	MET
1	E	49	GLN
1	E	51	ASP
1	E	52	SER
1	E	53	TYR
1	E	137	GLN
1	E	171	LEU
1	E	174	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	35	VAL
1	F	37	ARG
1	F	38	PRO
1	F	44	MET
1	F	47	MET
1	F	49	GLN
1	F	51	ASP
1	F	52	SER
1	F	53	TYR
1	F	137	GLN
1	F	171	LEU
1	F	174	ALA
3	G	59	GLU
3	G	78	TYR
3	G	335	VAL
3	G	549	PRO
3	G	550	THR
3	G	562	ALA
3	G	563	GLY
1	I	35	VAL
1	I	37	ARG
1	I	38	PRO
1	I	44	MET
1	I	47	MET
1	I	49	GLN
1	I	51	ASP
1	I	52	SER
1	I	53	TYR
1	I	137	GLN
1	I	171	LEU
1	I	174	ALA
3	J	59	GLU
3	J	78	TYR
3	J	335	VAL
3	J	549	PRO
3	J	550	THR
3	J	562	ALA
3	J	563	GLY
1	A	15	GLY
1	A	42	GLY
1	A	289	ILE
3	C	41	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	76	HIS
3	C	432	GLU
3	C	440	ASN
3	C	520	LEU
3	C	622	ALA
1	D	15	GLY
1	D	42	GLY
1	D	289	ILE
1	E	15	GLY
1	E	42	GLY
1	E	289	ILE
1	F	15	GLY
1	F	42	GLY
1	F	289	ILE
3	G	41	ILE
3	G	76	HIS
3	G	432	GLU
3	G	440	ASN
3	G	520	LEU
3	G	622	ALA
1	I	15	GLY
1	I	42	GLY
1	I	289	ILE
3	J	41	ILE
3	J	76	HIS
3	J	432	GLU
3	J	440	ASN
3	J	520	LEU
3	J	622	ALA
1	A	128	ASN
1	A	167	GLU
3	C	106	GLY
3	C	257	GLY
3	C	524	LYS
3	C	556	LYS
1	D	128	ASN
1	D	167	GLU
1	E	128	ASN
1	E	167	GLU
1	F	128	ASN
1	F	167	GLU
3	G	106	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	257	GLY
3	G	524	LYS
3	G	556	LYS
1	I	128	ASN
1	I	167	GLU
3	J	106	GLY
3	J	257	GLY
3	J	524	LYS
3	J	556	LYS
1	A	67	LEU
1	A	158	GLY
1	A	245	GLY
1	A	251	GLY
3	C	327	THR
3	C	329	VAL
3	C	519	PHE
3	C	597	GLY
3	C	636	ARG
1	D	67	LEU
1	D	158	GLY
1	D	245	GLY
1	D	251	GLY
1	E	67	LEU
1	E	158	GLY
1	E	245	GLY
1	E	251	GLY
1	F	67	LEU
1	F	158	GLY
1	F	245	GLY
1	F	251	GLY
3	G	327	THR
3	G	329	VAL
3	G	519	PHE
3	G	597	GLY
3	G	636	ARG
1	I	67	LEU
1	I	158	GLY
1	I	245	GLY
1	I	251	GLY
3	J	327	THR
3	J	329	VAL
3	J	519	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	597	GLY
3	J	636	ARG
1	A	70	PRO
1	A	100	GLU
3	C	279	ILE
3	C	646	PRO
1	D	70	PRO
1	D	100	GLU
1	E	70	PRO
1	E	100	GLU
1	F	70	PRO
1	F	100	GLU
3	G	279	ILE
3	G	646	PRO
1	I	70	PRO
1	I	100	GLU
3	J	279	ILE
3	J	646	PRO
1	A	6	THR
1	A	170	ALA
3	C	124	ASN
3	C	287	GLN
1	D	6	THR
1	D	170	ALA
1	E	6	THR
1	E	170	ALA
1	F	6	THR
1	F	170	ALA
3	G	124	ASN
3	G	287	GLN
1	I	6	THR
1	I	170	ALA
3	J	124	ASN
3	J	287	GLN
1	A	48	GLY
1	A	201	VAL
3	C	101	GLY
1	D	48	GLY
1	D	201	VAL
1	E	48	GLY
1	E	201	VAL
1	F	48	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	201	VAL
3	G	101	GLY
1	I	48	GLY
1	I	201	VAL
3	J	101	GLY
3	C	14	VAL
3	C	42	GLY
3	C	453	ILE
3	C	623	GLY
3	G	14	VAL
3	G	42	GLY
3	G	453	ILE
3	G	623	GLY
3	J	14	VAL
3	J	42	GLY
3	J	453	ILE
3	J	623	GLY
3	C	19	ILE
3	C	681	ASN
3	G	19	ILE
3	G	681	ASN
3	J	19	ILE
3	J	681	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	317/317 (100%)	286 (90%)	31 (10%)	9	32
1	D	317/317 (100%)	288 (91%)	29 (9%)	10	35
1	E	317/317 (100%)	286 (90%)	31 (10%)	9	32
1	F	317/317 (100%)	286 (90%)	31 (10%)	9	32
1	I	317/317 (100%)	286 (90%)	31 (10%)	9	32
2	B	118/118 (100%)	118 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	585 (96%)	24 (4%)	35	63
3	G	609/616 (99%)	582 (96%)	27 (4%)	31	60
3	J	609/616 (99%)	582 (96%)	27 (4%)	31	60
All	All	3648/3669 (99%)	3417 (94%)	231 (6%)	24	50

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	28	ARG
1	A	37	ARG
1	A	39	ARG
1	A	41	GLN
1	A	44	MET
1	A	47	MET
1	A	49	GLN
1	A	50	LYS
1	A	52	SER
1	A	87	HIS
1	A	113	LYS
1	A	116	ARG
1	A	126	THR
1	A	130	PRO
1	A	151	ILE
1	A	159	VAL
1	A	166	TYR
1	A	169	TYR
1	A	171	LEU
1	A	173	HIS
1	A	183	ARG
1	A	192	ILE
1	A	196	ARG
1	A	206	ARG
1	A	246	GLN
1	A	291	LYS
1	A	335	ARG
1	A	356	TRP
1	A	374	CYS
1	A	375	PHE
3	C	41	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	58	LYS
3	C	113	LYS
3	C	152	LEU
3	C	160	PHE
3	C	186	LYS
3	C	300	LYS
3	C	332	ARG
3	C	388	TYR
3	C	410	LEU
3	C	439	PHE
3	C	442	LYS
3	C	469	THR
3	C	516	VAL
3	C	525	ASP
3	C	526	THR
3	C	584	TYR
3	C	586	ARG
3	C	621	ARG
3	C	624	PHE
3	C	636	ARG
3	C	642	LYS
3	C	653	LYS
3	C	658	LEU
1	D	5	THR
1	D	37	ARG
1	D	39	ARG
1	D	41	GLN
1	D	44	MET
1	D	49	GLN
1	D	52	SER
1	D	87	HIS
1	D	113	LYS
1	D	116	ARG
1	D	126	THR
1	D	130	PRO
1	D	151	ILE
1	D	159	VAL
1	D	166	TYR
1	D	169	TYR
1	D	171	LEU
1	D	173	HIS
1	D	183	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	192	ILE
1	D	196	ARG
1	D	206	ARG
1	D	246	GLN
1	D	291	LYS
1	D	326	LYS
1	D	335	ARG
1	D	356	TRP
1	D	374	CYS
1	D	375	PHE
1	E	5	THR
1	E	37	ARG
1	E	39	ARG
1	E	41	GLN
1	E	44	MET
1	E	47	MET
1	E	49	GLN
1	E	50	LYS
1	E	52	SER
1	E	87	HIS
1	E	113	LYS
1	E	116	ARG
1	E	126	THR
1	E	130	PRO
1	E	151	ILE
1	E	159	VAL
1	E	166	TYR
1	E	169	TYR
1	E	171	LEU
1	E	173	HIS
1	E	183	ARG
1	E	192	ILE
1	E	196	ARG
1	E	206	ARG
1	E	246	GLN
1	E	291	LYS
1	E	326	LYS
1	E	335	ARG
1	E	356	TRP
1	E	374	CYS
1	E	375	PHE
1	F	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	37	ARG
1	F	39	ARG
1	F	41	GLN
1	F	44	MET
1	F	47	MET
1	F	49	GLN
1	F	50	LYS
1	F	52	SER
1	F	87	HIS
1	F	113	LYS
1	F	116	ARG
1	F	126	THR
1	F	130	PRO
1	F	151	ILE
1	F	159	VAL
1	F	166	TYR
1	F	169	TYR
1	F	171	LEU
1	F	173	HIS
1	F	183	ARG
1	F	192	ILE
1	F	196	ARG
1	F	206	ARG
1	F	246	GLN
1	F	291	LYS
1	F	326	LYS
1	F	335	ARG
1	F	356	TRP
1	F	374	CYS
1	F	375	PHE
3	G	41	ILE
3	G	58	LYS
3	G	113	LYS
3	G	152	LEU
3	G	160	PHE
3	G	186	LYS
3	G	288	ARG
3	G	300	LYS
3	G	332	ARG
3	G	388	TYR
3	G	410	LEU
3	G	439	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	442	LYS
3	G	467	LYS
3	G	469	THR
3	G	496	ARG
3	G	516	VAL
3	G	525	ASP
3	G	526	THR
3	G	584	TYR
3	G	586	ARG
3	G	621	ARG
3	G	624	PHE
3	G	636	ARG
3	G	642	LYS
3	G	653	LYS
3	G	658	LEU
1	I	5	THR
1	I	37	ARG
1	I	39	ARG
1	I	41	GLN
1	I	44	MET
1	I	47	MET
1	I	49	GLN
1	I	50	LYS
1	I	52	SER
1	I	87	HIS
1	I	113	LYS
1	I	116	ARG
1	I	126	THR
1	I	130	PRO
1	I	151	ILE
1	I	159	VAL
1	I	166	TYR
1	I	169	TYR
1	I	171	LEU
1	I	173	HIS
1	I	183	ARG
1	I	192	ILE
1	I	196	ARG
1	I	206	ARG
1	I	246	GLN
1	I	291	LYS
1	I	326	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	335	ARG
1	I	356	TRP
1	I	374	CYS
1	I	375	PHE
3	J	41	ILE
3	J	58	LYS
3	J	113	LYS
3	J	152	LEU
3	J	160	PHE
3	J	186	LYS
3	J	288	ARG
3	J	300	LYS
3	J	332	ARG
3	J	388	TYR
3	J	410	LEU
3	J	439	PHE
3	J	442	LYS
3	J	467	LYS
3	J	469	THR
3	J	496	ARG
3	J	516	VAL
3	J	525	ASP
3	J	526	THR
3	J	584	TYR
3	J	586	ARG
3	J	621	ARG
3	J	624	PHE
3	J	636	ARG
3	J	642	LYS
3	J	653	LYS
3	J	658	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	161	HIS
1	A	252	ASN
3	C	125	GLN
3	C	167	GLN
3	C	313	GLN
3	C	402	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	607	GLN
1	D	137	GLN
1	D	161	HIS
1	D	252	ASN
1	D	353	GLN
1	E	137	GLN
1	E	161	HIS
1	E	252	ASN
1	E	354	GLN
1	F	137	GLN
1	F	161	HIS
1	F	252	ASN
1	F	354	GLN
3	G	125	GLN
3	G	167	GLN
3	G	313	GLN
3	G	402	ASN
3	G	607	GLN
1	I	137	GLN
1	I	161	HIS
1	I	252	ASN
1	I	353	GLN
1	I	354	GLN
3	J	125	GLN
3	J	167	GLN
3	J	313	GLN
3	J	402	ASN
3	J	607	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	HIC	A	73	1	10,11,12	2.99	4 (40%)	7,14,16	1.94	3 (42%)
1	HIC	D	73	1	10,11,12	2.98	4 (40%)	7,14,16	1.94	3 (42%)
1	HIC	E	73	1	10,11,12	3.01	4 (40%)	7,14,16	1.94	3 (42%)
1	HIC	F	73	1	10,11,12	2.99	4 (40%)	7,14,16	1.95	3 (42%)
1	HIC	I	73	1	10,11,12	2.99	4 (40%)	7,14,16	1.93	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	HIC	D	73	1	-	0/4/6/8	0/1/1/1
1	HIC	E	73	1	-	0/4/6/8	0/1/1/1
1	HIC	F	73	1	-	0/4/6/8	0/1/1/1
1	HIC	I	73	1	-	0/4/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	73	HIC	CD2-CG	2.15	1.39	1.36
1	A	73	HIC	CD2-CG	2.19	1.39	1.36
1	D	73	HIC	CD2-CG	2.19	1.39	1.36
1	E	73	HIC	CD2-CG	2.20	1.39	1.36
1	F	73	HIC	CD2-CG	2.20	1.39	1.36
1	F	73	HIC	CA-N	2.96	1.57	1.47
1	A	73	HIC	CA-N	2.98	1.57	1.47
1	D	73	HIC	CA-N	2.99	1.57	1.47
1	I	73	HIC	CA-N	2.99	1.57	1.47
1	E	73	HIC	CA-N	2.99	1.57	1.47
1	A	73	HIC	CE1-NE2	3.28	1.40	1.36
1	I	73	HIC	CE1-NE2	3.30	1.40	1.36
1	F	73	HIC	CE1-NE2	3.30	1.40	1.36
1	D	73	HIC	CE1-NE2	3.31	1.40	1.36
1	E	73	HIC	CE1-NE2	3.32	1.40	1.36
1	D	73	HIC	CA-C	7.40	1.60	1.50
1	F	73	HIC	CA-C	7.43	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CA-C	7.43	1.60	1.50
1	I	73	HIC	CA-C	7.44	1.60	1.50
1	E	73	HIC	CA-C	7.47	1.60	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	HIC	CB-CA-C	-3.76	104.16	111.41
1	F	73	HIC	CB-CA-C	-3.76	104.17	111.41
1	A	73	HIC	CB-CA-C	-3.75	104.18	111.41
1	D	73	HIC	CB-CA-C	-3.75	104.19	111.41
1	I	73	HIC	CB-CA-C	-3.73	104.22	111.41
1	F	73	HIC	O-C-CA	-2.64	117.72	124.96
1	I	73	HIC	O-C-CA	-2.63	117.73	124.96
1	E	73	HIC	O-C-CA	-2.63	117.75	124.96
1	A	73	HIC	O-C-CA	-2.62	117.76	124.96
1	D	73	HIC	O-C-CA	-2.61	117.79	124.96
1	D	73	HIC	CG-CD2-NE2	-2.23	105.36	107.78
1	E	73	HIC	CG-CD2-NE2	-2.22	105.37	107.78
1	F	73	HIC	CG-CD2-NE2	-2.22	105.37	107.78
1	A	73	HIC	CG-CD2-NE2	-2.22	105.37	107.78
1	I	73	HIC	CG-CD2-NE2	-2.18	105.42	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	1	0
1	D	73	HIC	1	0
1	E	73	HIC	1	0
1	F	73	HIC	1	0
1	I	73	HIC	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	376	-	25,29,29	1.08	1 (4%)	25,45,45	1.62	4 (16%)
4	ADP	D	376	-	25,29,29	1.09	1 (4%)	25,45,45	1.62	4 (16%)
4	ADP	E	376	-	25,29,29	1.08	1 (4%)	25,45,45	1.62	4 (16%)
4	ADP	F	376	-	25,29,29	1.08	1 (4%)	25,45,45	1.61	4 (16%)
4	ADP	I	376	-	25,29,29	1.09	1 (4%)	25,45,45	1.62	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	376	-	-	0/12/32/32	0/3/3/3
4	ADP	D	376	-	-	0/12/32/32	0/3/3/3
4	ADP	E	376	-	-	0/12/32/32	0/3/3/3
4	ADP	F	376	-	-	0/12/32/32	0/3/3/3
4	ADP	I	376	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	376	ADP	C2-N1	2.94	1.39	1.33
4	A	376	ADP	C2-N1	2.94	1.39	1.33
4	F	376	ADP	C2-N1	2.95	1.39	1.33
4	I	376	ADP	C2-N1	2.95	1.39	1.33
4	D	376	ADP	C2-N1	2.99	1.39	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	376	ADP	N3-C2-N1	-4.28	125.20	128.86
4	D	376	ADP	N3-C2-N1	-4.25	125.22	128.86
4	I	376	ADP	N3-C2-N1	-4.25	125.22	128.86
4	A	376	ADP	N3-C2-N1	-4.24	125.23	128.86
4	F	376	ADP	N3-C2-N1	-4.17	125.30	128.86
4	A	376	ADP	O3B-PB-O2B	2.03	115.62	107.59
4	E	376	ADP	O3B-PB-O2B	2.03	115.63	107.59
4	D	376	ADP	O3B-PB-O2B	2.03	115.64	107.59
4	I	376	ADP	O3B-PB-O2B	2.04	115.65	107.59
4	F	376	ADP	O3B-PB-O2B	2.04	115.67	107.59
4	F	376	ADP	C2-N1-C6	2.17	122.44	118.75
4	D	376	ADP	C2-N1-C6	2.20	122.49	118.75
4	I	376	ADP	C2-N1-C6	2.22	122.52	118.75
4	A	376	ADP	C2-N1-C6	2.22	122.52	118.75
4	E	376	ADP	C2-N1-C6	2.24	122.55	118.75
4	E	376	ADP	C4-C5-N7	4.20	113.47	109.41
4	A	376	ADP	C4-C5-N7	4.21	113.48	109.41
4	F	376	ADP	C4-C5-N7	4.21	113.48	109.41
4	D	376	ADP	C4-C5-N7	4.22	113.49	109.41
4	I	376	ADP	C4-C5-N7	4.24	113.51	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	376	ADP	7	0
4	D	376	ADP	7	0
4	E	376	ADP	7	0
4	F	376	ADP	7	0
4	I	376	ADP	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	2
3	J	2
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	107:LYS	C	108:THR	N	3.75
1	G	107:LYS	C	108:THR	N	3.75
1	J	107:LYS	C	108:THR	N	3.75
1	C	90:GLN	C	91:SER	N	3.23
1	G	90:GLN	C	91:SER	N	3.23
1	J	90:GLN	C	91:SER	N	3.22