



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:00 PM BST

PDB ID : 4A7H
EMDB ID: : EMD-1987
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 2)
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;
Raunser, S.
Deposited on : 2011-11-14
Resolution : 7.80 Å(reported)
Based on PDB ID : 3MFP;1LKX

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 : 1.7.1 (RC1), CSD as537be (2016)
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

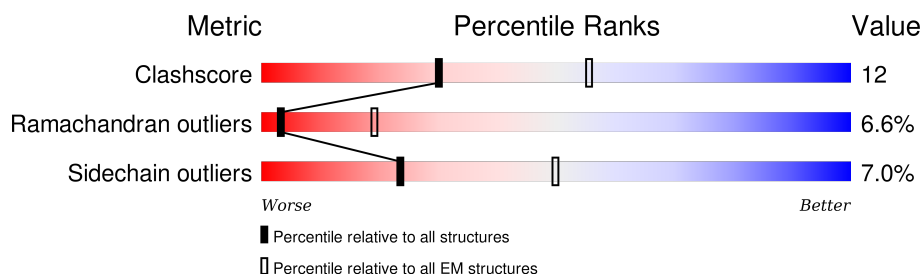
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	375	65% 25% 7% .
1	D	375	64% 26% 6% .
1	E	375	65% 26% 6% .
1	F	375	66% 25% 6% .
1	G	375	66% 25% 6% .
2	B	136	96% .
2	H	136	99% .
3	C	697	78% 16% . .
3	I	697	78% 17% . .

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Mol	Chain	Length	Quality of chain
3	J	697	<div><div></div><div>77%</div><div>18%</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	G	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1-ALPHA CHAIN.

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	I	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	CONFLICT	UNP Q03479
C	334	GLU	SER	ENGINEERED MUTATION	UNP Q03479
I	77	MET	ILE	CONFLICT	UNP Q03479
I	215	ASP	ASN	CONFLICT	UNP Q03479
I	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

- # ADP
-

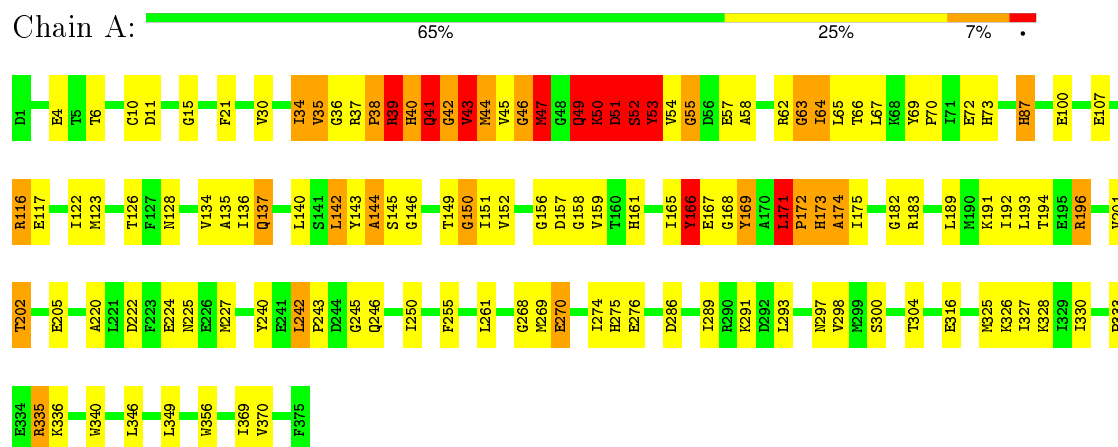
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	G	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

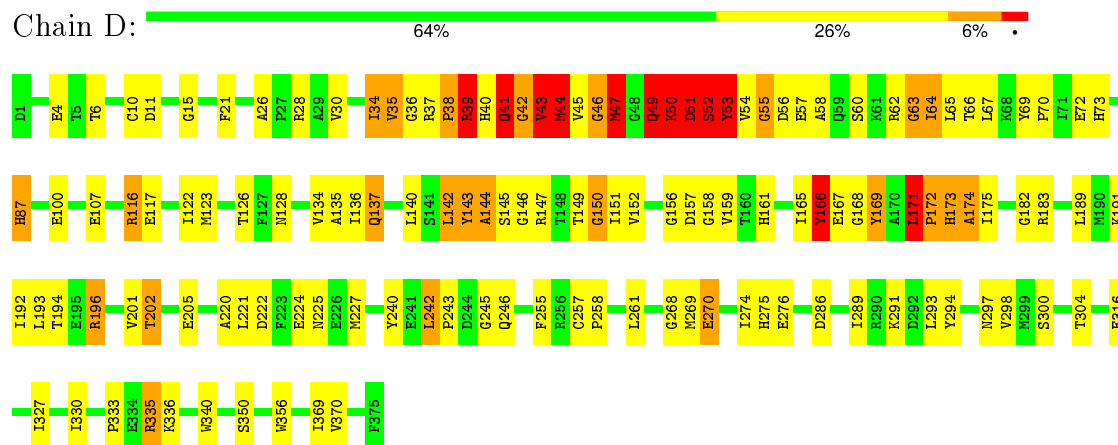
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

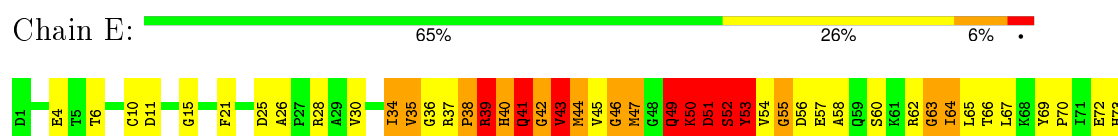
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



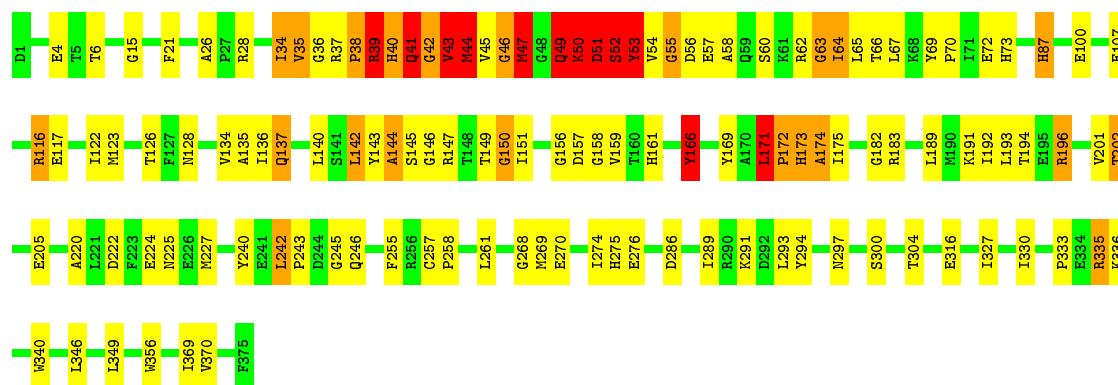
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





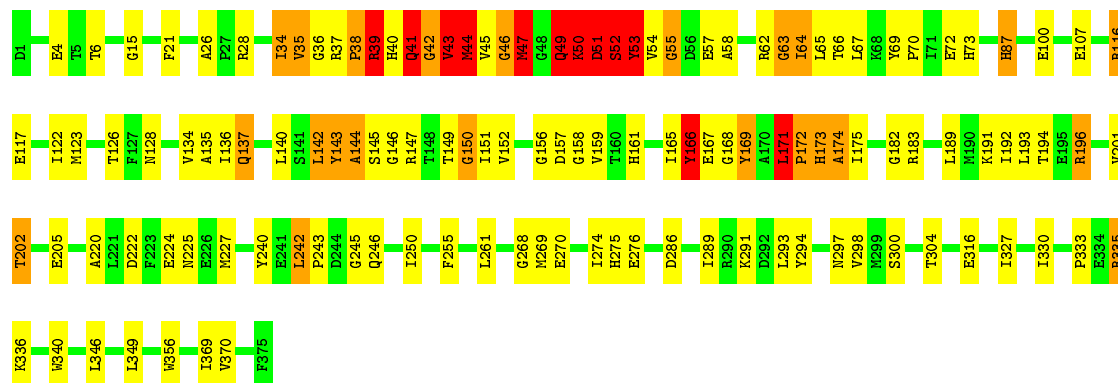
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain F: 66% 25% 6% .



- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain G: 66% 25% 6% .



- Molecule 2: TROPOMYOSIN 1-ALPHA CHAIN

Chain B: 96% .



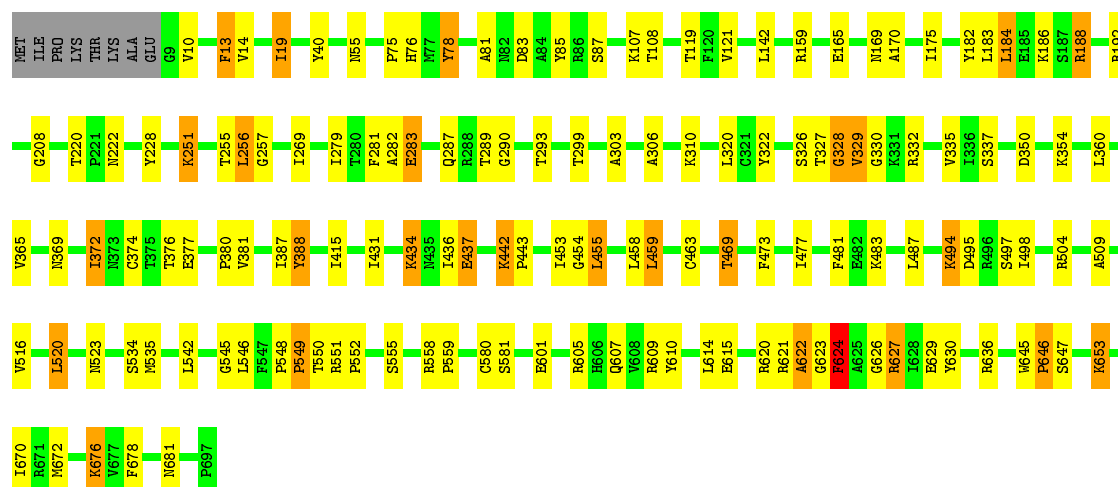
- Molecule 2: TROPOMYOSIN 1-ALPHA CHAIN

Chain H: 99% .



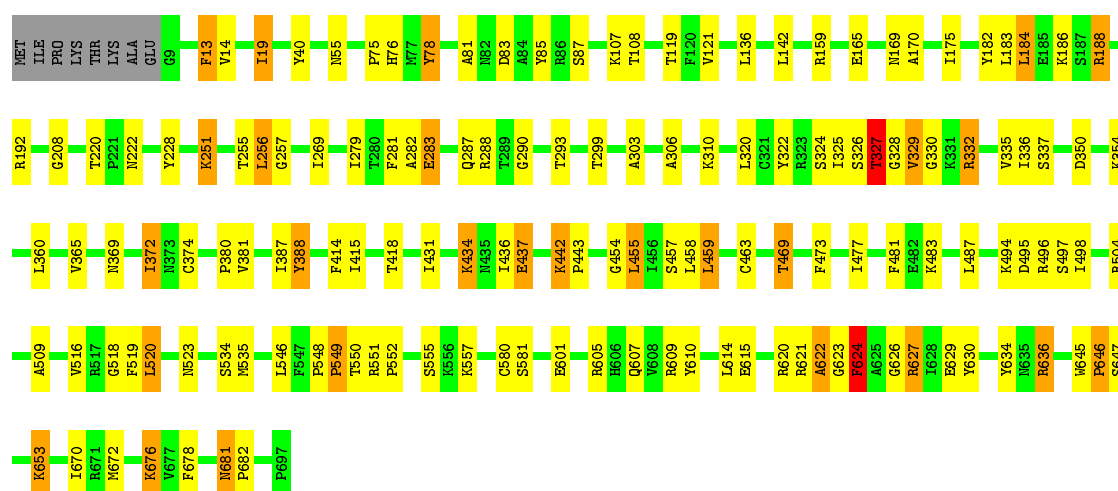
• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain C: 78% 16%



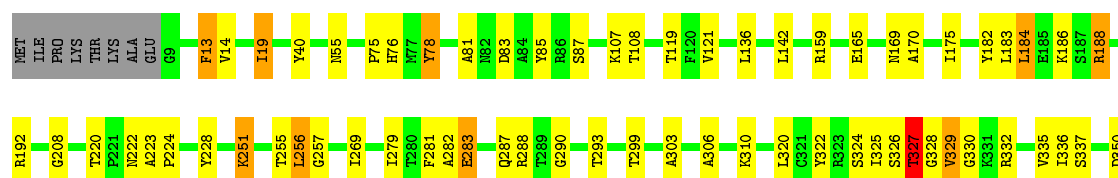
• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain I: 78% 17%



• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J: 77% 18%





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	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	80000	Depositor
Image detector	TEMCAM-F816	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	0.93	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	D	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	E	0.92	13/2984 (0.4%)	0.67	10/4040 (0.2%)
1	F	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	G	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
2	B	0.20	0/1107	0.31	0/1471
2	H	0.24	0/1107	0.38	0/1471
3	C	0.26	0/5590	0.38	0/7527
3	I	0.22	0/5590	0.37	0/7527
3	J	0.22	0/5590	0.37	0/7527
All	All	0.63	65/33904 (0.2%)	0.53	54/45723 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	166	TYR	CD2-CE2	19.25	1.68	1.39
1	D	166	TYR	CD2-CE2	19.25	1.68	1.39
1	A	166	TYR	CD2-CE2	19.24	1.68	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	TYR	CD2-CE2	19.24	1.68	1.39
1	E	166	TYR	CD2-CE2	19.18	1.68	1.39
1	G	166	TYR	CD1-CE1	18.68	1.67	1.39
1	F	166	TYR	CD1-CE1	18.67	1.67	1.39
1	D	166	TYR	CD1-CE1	18.67	1.67	1.39
1	E	166	TYR	CD1-CE1	18.67	1.67	1.39
1	A	166	TYR	CD1-CE1	18.66	1.67	1.39
1	F	166	TYR	CE2-CZ	18.48	1.62	1.38
1	D	166	TYR	CE2-CZ	18.47	1.62	1.38
1	A	166	TYR	CE2-CZ	18.45	1.62	1.38
1	E	166	TYR	CE2-CZ	18.45	1.62	1.38
1	G	166	TYR	CE2-CZ	18.44	1.62	1.38
1	E	166	TYR	CE1-CZ	15.37	1.58	1.38
1	F	166	TYR	CE1-CZ	15.35	1.58	1.38
1	A	166	TYR	CE1-CZ	15.34	1.58	1.38
1	G	166	TYR	CE1-CZ	15.34	1.58	1.38
1	D	166	TYR	CE1-CZ	15.33	1.58	1.38
1	F	166	TYR	CG-CD1	12.05	1.54	1.39
1	G	166	TYR	CG-CD1	12.05	1.54	1.39
1	D	166	TYR	CG-CD1	12.04	1.54	1.39
1	E	166	TYR	CG-CD1	12.03	1.54	1.39
1	A	166	TYR	CG-CD1	12.03	1.54	1.39
1	E	166	TYR	CG-CD2	11.29	1.53	1.39
1	A	166	TYR	CG-CD2	11.28	1.53	1.39
1	G	166	TYR	CG-CD2	11.26	1.53	1.39
1	F	166	TYR	CG-CD2	11.23	1.53	1.39
1	D	166	TYR	CG-CD2	11.22	1.53	1.39
1	G	150	GLY	N-CA	9.97	1.61	1.46
1	F	150	GLY	N-CA	9.97	1.61	1.46
1	A	150	GLY	N-CA	9.95	1.60	1.46
1	E	150	GLY	N-CA	9.93	1.60	1.46
1	D	150	GLY	N-CA	9.91	1.60	1.46
1	D	43	VAL	CA-CB	8.42	1.72	1.54
1	E	43	VAL	CA-CB	8.39	1.72	1.54
1	A	43	VAL	CA-CB	8.38	1.72	1.54
1	G	43	VAL	CA-CB	8.37	1.72	1.54
1	F	43	VAL	CA-CB	8.35	1.72	1.54
1	E	149	THR	C-N	6.75	1.45	1.33
1	D	149	THR	C-N	6.74	1.45	1.33
1	F	149	THR	C-N	6.72	1.45	1.33
1	A	149	THR	C-N	6.71	1.45	1.33
1	G	149	THR	C-N	6.69	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	GLN	N-CA	6.05	1.58	1.46
1	F	41	GLN	N-CA	6.05	1.58	1.46
1	A	41	GLN	N-CA	6.04	1.58	1.46
1	E	41	GLN	N-CA	6.04	1.58	1.46
1	G	41	GLN	N-CA	6.02	1.58	1.46
1	G	49	GLN	CG-CD	5.83	1.64	1.51
1	F	49	GLN	CG-CD	5.82	1.64	1.51
1	A	49	GLN	CG-CD	5.81	1.64	1.51
1	E	49	GLN	CG-CD	5.81	1.64	1.51
1	D	49	GLN	CG-CD	5.77	1.64	1.51
1	G	53	TYR	CE1-CZ	-5.38	1.31	1.38
1	A	53	TYR	CE1-CZ	-5.36	1.31	1.38
1	D	53	TYR	CE1-CZ	-5.35	1.31	1.38
1	F	53	TYR	CE1-CZ	-5.33	1.31	1.38
1	E	53	TYR	CE1-CZ	-5.32	1.31	1.38
1	G	43	VAL	CA-C	5.11	1.66	1.52
1	F	43	VAL	CA-C	5.11	1.66	1.52
1	E	43	VAL	CA-C	5.10	1.66	1.52
1	A	43	VAL	CA-C	5.10	1.66	1.52
1	D	43	VAL	CA-C	5.09	1.66	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	THR	C-N-CA	9.74	142.76	122.30
1	G	149	THR	C-N-CA	9.73	142.74	122.30
1	A	149	THR	C-N-CA	9.73	142.73	122.30
1	E	149	THR	C-N-CA	9.73	142.73	122.30
1	D	149	THR	C-N-CA	9.72	142.72	122.30
1	D	53	TYR	CB-CA-C	9.25	128.90	110.40
1	F	53	TYR	CB-CA-C	9.24	128.89	110.40
1	A	53	TYR	CB-CA-C	9.24	128.88	110.40
1	G	53	TYR	CB-CA-C	9.23	128.86	110.40
1	E	53	TYR	CB-CA-C	9.23	128.85	110.40
1	F	43	VAL	CG1-CB-CG2	-7.15	99.46	110.90
1	G	43	VAL	CG1-CB-CG2	-7.14	99.47	110.90
1	E	43	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	A	43	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	D	43	VAL	CG1-CB-CG2	-7.11	99.53	110.90
1	G	43	VAL	CA-CB-CG2	6.64	120.86	110.90
1	E	43	VAL	CA-CB-CG2	6.63	120.84	110.90
1	A	43	VAL	CA-CB-CG2	6.62	120.84	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	VAL	CA-CB-CG2	6.61	120.81	110.90
1	F	43	VAL	CA-CB-CG2	6.60	120.81	110.90
1	F	47	MET	CB-CA-C	6.04	122.48	110.40
1	G	47	MET	CB-CA-C	6.02	122.44	110.40
1	A	47	MET	CB-CA-C	6.01	122.43	110.40
1	D	47	MET	CB-CA-C	6.01	122.41	110.40
1	D	39	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	39	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	39	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	39	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	39	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	F	46	GLY	C-N-CA	5.84	136.31	121.70
1	D	46	GLY	C-N-CA	5.84	136.30	121.70
1	A	46	GLY	C-N-CA	5.83	136.28	121.70
1	G	46	GLY	C-N-CA	5.83	136.28	121.70
1	E	46	GLY	C-N-CA	5.83	136.26	121.70
1	D	44	MET	CA-CB-CG	5.38	122.45	113.30
1	G	44	MET	CA-CB-CG	5.38	122.45	113.30
1	F	44	MET	CA-CB-CG	5.37	122.43	113.30
1	A	44	MET	CA-CB-CG	5.35	122.40	113.30
1	E	44	MET	CA-CB-CG	5.34	122.39	113.30
1	F	52	SER	C-N-CA	5.34	135.04	121.70
1	D	52	SER	C-N-CA	5.33	135.04	121.70
1	G	52	SER	C-N-CA	5.33	135.03	121.70
1	A	52	SER	C-N-CA	5.33	135.03	121.70
1	E	52	SER	C-N-CA	5.33	135.03	121.70
1	E	46	GLY	CA-C-N	-5.32	105.50	117.20
1	A	46	GLY	CA-C-N	-5.31	105.51	117.20
1	G	46	GLY	CA-C-N	-5.31	105.52	117.20
1	F	46	GLY	CA-C-N	-5.31	105.52	117.20
1	D	46	GLY	CA-C-N	-5.30	105.53	117.20
1	G	52	SER	N-CA-CB	-5.29	102.56	110.50
1	E	52	SER	N-CA-CB	-5.28	102.58	110.50
1	F	52	SER	N-CA-CB	-5.27	102.59	110.50
1	D	52	SER	N-CA-CB	-5.27	102.59	110.50
1	A	52	SER	N-CA-CB	-5.26	102.60	110.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	D	43	VAL	Mainchain
1	E	43	VAL	Mainchain
1	F	43	VAL	Mainchain
1	G	43	VAL	Mainchain

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	140	0
1	D	2934	0	2895	125	0
1	E	2934	0	2895	124	0
1	F	2934	0	2895	121	0
1	G	2934	0	2894	122	0
2	B	1104	0	1104	3	0
2	H	1104	0	1104	1	0
3	C	5494	0	5488	77	0
3	I	5494	0	5488	82	0
3	J	5494	0	5488	86	0
4	A	27	0	12	3	0
4	D	27	0	12	3	0
4	E	27	0	12	3	0
4	F	27	0	12	3	0
4	G	27	0	12	3	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	G	1	0	0	0	0
All	All	33500	0	33206	795	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 12.

All (795) 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:F:43:VAL:O	1:G:169:TYR:OH	1.53	1.21
1:A:169:TYR:OH	1:E:43:VAL:O	1.62	1.14
1:D:157:ASP:N	4:D:376:ADP:O3B	1.82	1.13
1:E:157:ASP:N	4:E:376:ADP:O3B	1.82	1.13
1:A:157:ASP:N	4:A:376:ADP:O3B	1.82	1.12
1:A:43:VAL:O	1:D:169:TYR:OH	1.63	1.12
1:F:157:ASP:N	4:F:376:ADP:O3B	1.82	1.11
1:G:157:ASP:N	4:G:376:ADP:O3B	1.82	1.11
1:D:30:VAL:HG22	3:I:327:THR:CG2	1.84	1.08
1:G:36:GLY:O	1:G:52:SER:CA	2.03	1.07
1:A:42:GLY:C	1:D:167:GLU:O	1.92	1.07
1:F:36:GLY:O	1:F:52:SER:CA	2.03	1.06
1:A:36:GLY:O	1:A:52:SER:CA	2.03	1.06
1:D:36:GLY:O	1:D:52:SER:CA	2.03	1.05
1:E:36:GLY:O	1:E:52:SER:CA	2.03	1.05
1:E:30:VAL:HG22	3:J:327:THR:CG2	1.85	1.05
1:A:36:GLY:O	1:A:52:SER:HA	1.59	1.02
1:A:42:GLY:O	1:D:167:GLU:O	1.77	1.02
1:A:41:GLN:NE2	1:D:169:TYR:HD1	1.56	1.02
1:D:36:GLY:O	1:D:52:SER:HA	1.59	1.02
1:F:42:GLY:O	1:G:167:GLU:O	1.78	1.01
1:E:36:GLY:O	1:E:52:SER:HA	1.59	1.01
1:A:167:GLU:O	1:E:42:GLY:C	2.00	1.00
1:F:36:GLY:O	1:F:52:SER:HA	1.59	0.99
1:G:36:GLY:O	1:G:52:SER:HA	1.59	0.99
1:F:42:GLY:C	1:G:167:GLU:O	2.03	0.97
1:A:169:TYR:HD1	1:E:41:GLN:NE2	1.60	0.97
1:A:53:TYR:OH	1:D:167:GLU:OE2	1.82	0.95
1:A:167:GLU:O	1:E:42:GLY:O	1.83	0.95
1:F:53:TYR:OH	1:G:167:GLU:OE2	1.85	0.94
1:A:41:GLN:NE2	1:D:169:TYR:CD1	2.36	0.93
1:E:38:PRO:HG3	1:E:49:GLN:HG2	1.52	0.92
1:D:30:VAL:HG22	3:I:327:THR:HG21	1.50	0.92
1:A:167:GLU:OE2	1:E:53:TYR:OH	1.85	0.92
1:A:38:PRO:HG3	1:A:49:GLN:HG2	1.52	0.92
1:E:54:VAL:HG22	1:E:55:GLY:H	1.35	0.92
1:D:38:PRO:HG3	1:D:49:GLN:HG2	1.52	0.91
1:E:350:SER:HG	3:J:457:SER:HG	1.00	0.91
1:E:30:VAL:HG22	3:J:327:THR:HG21	1.48	0.91
1:F:54:VAL:HG22	1:F:55:GLY:H	1.35	0.91
1:A:54:VAL:HG22	1:A:55:GLY:H	1.34	0.90
1:D:350:SER:HG	3:I:457:SER:HG	1.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:CD1	1:E:41:GLN:NE2	2.39	0.90
1:G:54:VAL:HG22	1:G:55:GLY:H	1.35	0.89
1:G:38:PRO:HG3	1:G:49:GLN:HG2	1.52	0.89
1:D:54:VAL:HG22	1:D:55:GLY:H	1.35	0.89
1:F:38:PRO:HG3	1:F:49:GLN:HG2	1.52	0.89
1:A:38:PRO:HG3	1:A:49:GLN:CG	2.05	0.87
1:D:38:PRO:HG3	1:D:49:GLN:CG	2.05	0.87
1:E:38:PRO:HG3	1:E:49:GLN:CG	2.05	0.86
1:E:30:VAL:CG2	3:J:327:THR:HG22	2.06	0.86
1:F:38:PRO:HG3	1:F:49:GLN:CG	2.05	0.86
1:G:38:PRO:HG3	1:G:49:GLN:CG	2.05	0.86
1:F:41:GLN:NE2	1:G:169:TYR:HD1	1.73	0.85
1:A:51:ASP:O	1:A:53:TYR:N	2.10	0.85
1:D:30:VAL:CG2	3:I:327:THR:HG22	2.06	0.85
1:F:36:GLY:O	1:F:52:SER:CB	2.26	0.84
1:F:51:ASP:O	1:F:53:TYR:N	2.10	0.84
1:G:36:GLY:O	1:G:52:SER:CB	2.26	0.84
1:G:51:ASP:C	1:G:53:TYR:H	1.80	0.84
1:G:51:ASP:O	1:G:53:TYR:N	2.10	0.84
1:D:51:ASP:O	1:D:53:TYR:N	2.10	0.84
1:E:51:ASP:O	1:E:53:TYR:N	2.10	0.83
1:A:35:VAL:HG13	1:A:52:SER:CB	2.08	0.83
1:D:35:VAL:HG13	1:D:52:SER:CB	2.08	0.83
1:F:35:VAL:HG13	1:F:52:SER:CB	2.08	0.83
1:E:35:VAL:HG13	1:E:52:SER:CB	2.08	0.83
1:G:35:VAL:HG13	1:G:52:SER:CB	2.08	0.83
1:E:36:GLY:O	1:E:52:SER:CB	2.26	0.83
1:D:36:GLY:O	1:D:52:SER:CB	2.26	0.83
1:F:51:ASP:C	1:F:53:TYR:H	1.80	0.83
1:A:36:GLY:O	1:A:52:SER:CB	2.26	0.82
1:D:30:VAL:CG2	3:I:327:THR:CG2	2.59	0.81
3:C:188:ARG:O	3:C:192:ARG:NH1	2.14	0.81
3:I:188:ARG:O	3:I:192:ARG:NH1	2.14	0.81
3:J:188:ARG:O	3:J:192:ARG:NH1	2.14	0.81
1:G:36:GLY:O	1:G:52:SER:HB3	1.82	0.80
1:D:51:ASP:C	1:D:53:TYR:H	1.80	0.80
1:A:36:GLY:O	1:A:52:SER:HB3	1.82	0.80
1:F:42:GLY:O	1:F:43:VAL:HG22	1.82	0.80
1:D:36:GLY:O	1:D:52:SER:HB3	1.82	0.80
1:G:42:GLY:O	1:G:43:VAL:HG22	1.82	0.79
1:E:30:VAL:CG2	3:J:327:THR:CG2	2.59	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLY:O	1:E:52:SER:HB3	1.82	0.79
1:A:42:GLY:O	1:A:43:VAL:HG22	1.82	0.79
1:E:49:GLN:HG3	1:E:50:LYS:N	1.98	0.79
1:A:51:ASP:C	1:A:53:TYR:H	1.80	0.79
1:D:42:GLY:O	1:D:43:VAL:HG22	1.82	0.79
1:F:36:GLY:O	1:F:52:SER:HB3	1.82	0.78
1:A:49:GLN:HG3	1:A:50:LYS:N	1.98	0.78
3:J:630:TYR:OH	3:J:672:MET:SD	2.40	0.78
3:I:630:TYR:OH	3:I:672:MET:SD	2.40	0.78
1:E:42:GLY:O	1:E:43:VAL:HG22	1.82	0.78
3:C:630:TYR:OH	3:C:672:MET:SD	2.40	0.78
1:G:49:GLN:HG3	1:G:50:LYS:N	1.98	0.78
1:F:49:GLN:HG3	1:F:50:LYS:N	1.98	0.77
1:E:51:ASP:C	1:E:53:TYR:H	1.80	0.77
1:D:49:GLN:HG3	1:D:50:LYS:N	1.98	0.77
1:F:41:GLN:NE2	1:G:169:TYR:CD1	2.53	0.75
1:A:54:VAL:HG22	1:A:55:GLY:N	2.02	0.75
1:F:54:VAL:HG22	1:F:55:GLY:N	2.02	0.75
1:E:54:VAL:HG22	1:E:55:GLY:N	2.02	0.74
1:D:54:VAL:HG22	1:D:55:GLY:N	2.02	0.73
1:G:54:VAL:HG22	1:G:55:GLY:N	2.02	0.73
1:A:168:GLY:C	1:E:40:HIS:CE1	2.62	0.73
1:D:142:LEU:O	1:D:144:ALA:N	2.22	0.73
1:F:142:LEU:O	1:F:144:ALA:N	2.22	0.73
1:E:142:LEU:O	1:E:144:ALA:N	2.22	0.72
1:G:142:LEU:O	1:G:144:ALA:N	2.22	0.72
1:A:142:LEU:O	1:A:144:ALA:N	2.22	0.72
1:A:173:HIS:O	1:A:175:ILE:N	2.23	0.72
1:D:173:HIS:O	1:D:175:ILE:N	2.23	0.72
1:E:30:VAL:HG22	3:J:327:THR:HG22	1.65	0.71
1:F:173:HIS:O	1:F:175:ILE:N	2.23	0.71
1:D:196:ARG:O	1:D:196:ARG:NE	2.23	0.71
1:G:173:HIS:O	1:G:175:ILE:N	2.23	0.71
1:E:173:HIS:O	1:E:175:ILE:N	2.23	0.71
1:E:196:ARG:NE	1:E:196:ARG:O	2.23	0.70
1:G:196:ARG:O	1:G:196:ARG:NE	2.23	0.70
1:A:196:ARG:NE	1:A:196:ARG:O	2.23	0.70
1:D:172:PRO:O	1:G:191:LYS:NZ	2.22	0.70
1:F:196:ARG:NE	1:F:196:ARG:O	2.23	0.70
1:E:171:LEU:HB2	1:E:172:PRO:HD3	1.74	0.70
1:D:171:LEU:HB2	1:D:172:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:OE1	1:D:169:TYR:O	2.10	0.69
1:G:171:LEU:HB2	1:G:172:PRO:HD3	1.74	0.69
1:F:43:VAL:O	1:G:169:TYR:CZ	2.46	0.68
1:A:171:LEU:HB2	1:A:172:PRO:HD3	1.74	0.68
1:D:35:VAL:HG13	1:D:52:SER:OG	1.94	0.68
1:F:171:LEU:HB2	1:F:172:PRO:HD3	1.74	0.68
1:A:35:VAL:HG13	1:A:52:SER:OG	1.94	0.68
1:G:35:VAL:HG13	1:G:52:SER:OG	1.94	0.68
1:A:40:HIS:CE1	1:D:168:GLY:C	2.67	0.68
1:F:35:VAL:HG13	1:F:52:SER:OG	1.94	0.67
1:F:35:VAL:HG13	1:F:52:SER:HB2	1.75	0.67
1:E:35:VAL:HG13	1:E:52:SER:HB2	1.75	0.67
1:E:35:VAL:HG13	1:E:52:SER:OG	1.94	0.67
1:F:336:LYS:HE3	4:F:376:ADP:PA	2.35	0.67
1:G:35:VAL:HG13	1:G:52:SER:HB2	1.75	0.67
1:E:336:LYS:HE3	4:E:376:ADP:PA	2.35	0.67
1:G:336:LYS:HE3	4:G:376:ADP:PA	2.35	0.67
1:G:53:TYR:C	1:G:58:ALA:HB2	2.15	0.67
1:A:336:LYS:HE3	4:A:376:ADP:PA	2.35	0.67
3:C:494:LYS:HG3	3:C:494:LYS:O	1.94	0.67
1:E:53:TYR:C	1:E:58:ALA:HB2	2.16	0.66
1:A:53:TYR:C	1:A:58:ALA:HB2	2.16	0.66
1:F:53:TYR:C	1:F:58:ALA:HB2	2.15	0.66
1:A:35:VAL:HG13	1:A:52:SER:HB2	1.75	0.66
1:D:53:TYR:C	1:D:58:ALA:HB2	2.16	0.66
1:D:336:LYS:HE3	4:D:376:ADP:PA	2.35	0.66
1:D:35:VAL:HG13	1:D:52:SER:HB2	1.75	0.66
3:C:269:ILE:HD12	3:C:546:LEU:HD11	1.78	0.64
3:C:558:ARG:HB2	3:C:559:PRO:HD3	1.80	0.64
3:I:269:ILE:HD12	3:I:546:LEU:HD11	1.79	0.64
3:J:19:ILE:O	3:J:19:ILE:HG23	1.97	0.64
3:J:269:ILE:HD12	3:J:546:LEU:HD11	1.79	0.64
1:G:117:GLU:N	1:G:117:GLU:OE1	2.31	0.64
1:F:117:GLU:N	1:F:117:GLU:OE1	2.31	0.63
3:J:365:VAL:O	3:J:369:ASN:ND2	2.31	0.63
1:A:169:TYR:O	1:E:41:GLN:OE1	2.16	0.63
1:D:37:ARG:HB3	1:D:38:PRO:CD	2.29	0.63
1:D:117:GLU:OE1	1:D:117:GLU:N	2.31	0.63
1:F:40:HIS:CE1	1:G:168:GLY:C	2.72	0.63
1:A:37:ARG:HB3	1:A:38:PRO:CD	2.29	0.63
1:G:333:PRO:O	1:G:335:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ARG:HB3	1:F:38:PRO:CD	2.29	0.63
3:C:365:VAL:O	3:C:369:ASN:ND2	2.31	0.63
1:D:122:ILE:O	1:D:126:THR:OG1	2.17	0.63
3:I:365:VAL:O	3:I:369:ASN:ND2	2.31	0.63
1:E:117:GLU:N	1:E:117:GLU:OE1	2.31	0.63
1:E:37:ARG:HB3	1:E:38:PRO:CD	2.29	0.63
1:E:122:ILE:O	1:E:126:THR:OG1	2.17	0.63
3:I:19:ILE:O	3:I:19:ILE:HG23	1.97	0.63
1:G:122:ILE:O	1:G:126:THR:OG1	2.17	0.63
1:G:37:ARG:HB3	1:G:38:PRO:CD	2.29	0.62
3:C:19:ILE:O	3:C:19:ILE:HG23	1.97	0.62
1:F:333:PRO:O	1:F:335:ARG:NH2	2.32	0.62
1:A:333:PRO:O	1:A:335:ARG:NH2	2.32	0.62
1:E:191:LYS:NZ	1:F:172:PRO:O	2.28	0.62
1:A:117:GLU:OE1	1:A:117:GLU:N	2.31	0.62
1:E:333:PRO:O	1:E:335:ARG:NH2	2.32	0.62
1:A:168:GLY:O	1:E:40:HIS:CE1	2.52	0.62
1:F:122:ILE:O	1:F:126:THR:OG1	2.17	0.62
1:D:269:MET:N	1:G:39:ARG:HH21	1.98	0.62
1:A:122:ILE:O	1:A:126:THR:OG1	2.17	0.61
1:D:333:PRO:O	1:D:335:ARG:NH2	2.32	0.61
1:A:172:PRO:O	1:F:191:LYS:NZ	2.22	0.61
1:A:43:VAL:O	1:D:169:TYR:CZ	2.52	0.61
3:I:495:ASP:OD2	3:I:497:SER:OG	2.19	0.60
3:J:495:ASP:OD2	3:J:497:SER:OG	2.19	0.60
1:G:54:VAL:CG2	1:G:55:GLY:H	2.13	0.60
3:C:495:ASP:OD2	3:C:497:SER:OG	2.19	0.60
1:D:43:VAL:HG23	1:D:46:GLY:HA3	1.83	0.60
3:C:494:LYS:O	3:C:494:LYS:CG	2.49	0.60
1:A:43:VAL:HG23	1:A:46:GLY:HA3	1.83	0.60
1:E:43:VAL:HG23	1:E:46:GLY:HA3	1.82	0.60
1:D:38:PRO:HG3	1:D:49:GLN:CD	2.22	0.60
1:A:40:HIS:CE1	1:D:168:GLY:O	2.55	0.59
1:F:43:VAL:HG23	1:F:46:GLY:HA3	1.83	0.59
1:E:38:PRO:HG3	1:E:49:GLN:CD	2.22	0.59
1:G:43:VAL:HG23	1:G:46:GLY:HA3	1.83	0.59
3:C:463:CYS:SG	3:C:523:ASN:ND2	2.76	0.59
3:I:463:CYS:SG	3:I:523:ASN:ND2	2.76	0.59
1:F:43:VAL:HG12	1:G:165:ILE:HD11	1.85	0.59
1:D:26:ALA:O	1:D:28:ARG:NH1	2.36	0.59
1:E:54:VAL:CG2	1:E:55:GLY:H	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:CG	1:A:49:GLN:HG2	2.31	0.58
1:G:26:ALA:O	1:G:28:ARG:NH1	2.36	0.58
3:J:376:THR:OG1	3:J:377:GLU:OE1	2.11	0.58
1:A:38:PRO:HG3	1:A:49:GLN:CD	2.23	0.58
1:D:45:VAL:C	1:D:47:MET:H	2.06	0.58
1:E:45:VAL:C	1:E:47:MET:H	2.06	0.58
3:J:107:LYS:O	3:J:108:THR:N	2.36	0.58
3:J:463:CYS:SG	3:J:523:ASN:ND2	2.76	0.58
1:A:54:VAL:CG2	1:A:55:GLY:H	2.13	0.58
1:F:38:PRO:HG3	1:F:49:GLN:CD	2.23	0.58
1:E:42:GLY:O	1:E:43:VAL:CG2	2.52	0.58
1:E:26:ALA:O	1:E:28:ARG:NH1	2.36	0.58
1:A:45:VAL:C	1:A:47:MET:H	2.06	0.58
1:F:26:ALA:O	1:F:28:ARG:NH1	2.36	0.58
1:D:38:PRO:CG	1:D:49:GLN:HG2	2.31	0.57
3:I:107:LYS:O	3:I:108:THR:N	2.36	0.57
1:F:45:VAL:C	1:F:47:MET:H	2.06	0.57
1:A:43:VAL:N	1:D:168:GLY:HA2	2.19	0.57
1:G:38:PRO:HG3	1:G:49:GLN:CD	2.23	0.57
3:C:107:LYS:O	3:C:108:THR:N	2.36	0.57
1:F:171:LEU:N	1:F:171:LEU:HD12	2.19	0.57
1:G:42:GLY:O	1:G:43:VAL:CG2	2.52	0.57
1:A:42:GLY:O	1:A:43:VAL:CG2	2.52	0.57
1:D:242:LEU:HD23	1:D:243:PRO:HD2	1.86	0.57
1:G:202:THR:N	1:G:205:GLU:OE2	2.38	0.57
1:G:171:LEU:HD12	1:G:171:LEU:N	2.19	0.57
1:D:54:VAL:CG2	1:D:55:GLY:H	2.13	0.57
1:F:38:PRO:CG	1:F:49:GLN:HG2	2.31	0.57
1:D:171:LEU:HD12	1:D:171:LEU:N	2.19	0.57
1:G:45:VAL:C	1:G:47:MET:H	2.06	0.57
1:E:171:LEU:HD12	1:E:171:LEU:N	2.19	0.57
1:E:242:LEU:HD23	1:E:243:PRO:HD2	1.86	0.57
1:A:202:THR:N	1:A:205:GLU:OE2	2.38	0.57
1:A:169:TYR:CZ	1:E:43:VAL:O	2.55	0.56
1:A:242:LEU:HD23	1:A:243:PRO:HD2	1.86	0.56
1:G:242:LEU:HD23	1:G:243:PRO:HD2	1.86	0.56
1:F:242:LEU:HD23	1:F:243:PRO:HD2	1.85	0.56
1:F:150:GLY:O	1:F:166:TYR:CG	2.59	0.56
1:E:202:THR:N	1:E:205:GLU:OE2	2.38	0.56
1:E:150:GLY:O	1:E:166:TYR:CG	2.59	0.56
1:D:202:THR:N	1:D:205:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD12	1:A:171:LEU:N	2.19	0.56
1:A:150:GLY:O	1:A:166:TYR:CG	2.59	0.56
1:A:269:MET:N	1:F:39:ARG:HH21	2.04	0.56
3:C:376:THR:OG1	3:C:377:GLU:OE1	2.11	0.56
1:G:150:GLY:O	1:G:166:TYR:CG	2.59	0.56
1:A:275:HIS:ND1	1:A:316:GLU:OE1	2.39	0.56
1:D:150:GLY:O	1:D:166:TYR:CG	2.59	0.55
1:G:275:HIS:ND1	1:G:316:GLU:OE1	2.39	0.55
1:G:304:THR:O	1:G:335:ARG:NH1	2.40	0.55
1:F:304:THR:O	1:F:335:ARG:NH1	2.40	0.55
1:F:43:VAL:N	1:G:168:GLY:HA2	2.20	0.55
1:F:49:GLN:CG	1:F:50:LYS:N	2.69	0.55
1:D:42:GLY:O	1:D:43:VAL:CG2	2.52	0.55
1:F:202:THR:N	1:F:205:GLU:OE2	2.38	0.55
1:E:275:HIS:ND1	1:E:316:GLU:OE1	2.40	0.55
1:F:191:LYS:O	1:F:194:THR:OG1	2.24	0.55
1:G:38:PRO:CG	1:G:49:GLN:HG2	2.31	0.55
3:J:326:SER:O	3:J:327:THR:HB	2.05	0.55
1:E:304:THR:O	1:E:335:ARG:NH1	2.40	0.55
1:F:38:PRO:HD3	1:F:49:GLN:OE1	2.07	0.55
1:D:38:PRO:HD3	1:D:49:GLN:OE1	2.07	0.55
1:A:304:THR:O	1:A:335:ARG:NH1	2.40	0.55
3:I:622:ALA:HB3	3:I:678:PHE:CE2	2.41	0.55
1:F:42:GLY:O	1:F:43:VAL:CG2	2.52	0.55
1:E:38:PRO:HD3	1:E:49:GLN:OE1	2.07	0.55
1:G:191:LYS:O	1:G:194:THR:OG1	2.24	0.55
3:C:322:TYR:HB3	3:C:337:SER:HA	1.89	0.55
1:D:304:THR:O	1:D:335:ARG:NH1	2.40	0.55
3:C:622:ALA:HB3	3:C:678:PHE:CE2	2.41	0.55
1:A:38:PRO:HD3	1:A:49:GLN:OE1	2.07	0.55
1:D:49:GLN:CG	1:D:50:LYS:N	2.69	0.55
3:I:326:SER:O	3:I:327:THR:HB	2.06	0.54
1:D:275:HIS:ND1	1:D:316:GLU:OE1	2.39	0.54
1:F:275:HIS:ND1	1:F:316:GLU:OE1	2.39	0.54
3:J:622:ALA:HB3	3:J:678:PHE:CE2	2.41	0.54
1:G:38:PRO:HD3	1:G:49:GLN:OE1	2.07	0.54
3:I:580:CYS:SG	3:I:581:SER:N	2.81	0.54
1:G:171:LEU:HD13	1:G:172:PRO:HD3	1.90	0.54
1:F:41:GLN:OE1	1:G:169:TYR:O	2.26	0.54
1:F:171:LEU:HD13	1:F:172:PRO:HD3	1.90	0.54
3:J:580:CYS:SG	3:J:581:SER:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:509:ALA:HB1	3:I:610:TYR:HB2	1.90	0.54
3:C:282:ALA:O	3:C:283:GLU:C	2.47	0.54
3:C:509:ALA:HB1	3:C:610:TYR:HB2	1.90	0.54
3:I:142:LEU:HG	3:I:256:LEU:HD12	1.90	0.54
1:E:49:GLN:CG	1:E:50:LYS:N	2.69	0.53
3:C:142:LEU:HG	3:C:256:LEU:HD12	1.90	0.53
1:A:30:VAL:O	1:A:30:VAL:HG23	2.08	0.53
1:E:336:LYS:HE3	4:E:376:ADP:O2A	2.09	0.53
1:G:336:LYS:HE3	4:G:376:ADP:O2A	2.09	0.53
3:J:322:TYR:HB3	3:J:337:SER:HA	1.91	0.53
3:J:142:LEU:HG	3:J:256:LEU:HD12	1.90	0.53
3:J:509:ALA:HB1	3:J:610:TYR:HB2	1.90	0.53
1:A:336:LYS:HE3	4:A:376:ADP:O2A	2.09	0.53
1:A:34:ILE:O	1:A:35:VAL:HG23	2.09	0.53
3:I:322:TYR:HB3	3:I:337:SER:HA	1.91	0.53
1:A:39:ARG:HH21	1:G:269:MET:N	2.06	0.53
1:A:72:GLU:O	1:A:73:HIC:C	2.57	0.53
1:E:171:LEU:HD13	1:E:172:PRO:HD3	1.90	0.53
1:E:191:LYS:O	1:E:194:THR:OG1	2.24	0.53
1:A:49:GLN:CG	1:A:50:LYS:N	2.69	0.53
3:J:282:ALA:O	3:J:283:GLU:C	2.46	0.53
1:E:37:ARG:HB3	1:E:38:PRO:HD2	1.91	0.53
1:A:37:ARG:HB3	1:A:38:PRO:HD2	1.91	0.53
1:A:171:LEU:HD13	1:A:172:PRO:HD3	1.90	0.53
1:D:336:LYS:HE3	4:D:376:ADP:O2A	2.09	0.53
1:D:171:LEU:HD13	1:D:172:PRO:HD3	1.90	0.53
1:G:72:GLU:O	1:G:73:HIC:C	2.57	0.53
1:A:43:VAL:HG12	1:D:165:ILE:HD11	1.92	0.53
1:F:336:LYS:HE3	4:F:376:ADP:O2A	2.09	0.53
1:D:72:GLU:O	1:D:73:HIC:C	2.57	0.53
1:E:34:ILE:O	1:E:35:VAL:HG23	2.09	0.52
1:D:191:LYS:O	1:D:194:THR:OG1	2.24	0.52
3:I:282:ALA:O	3:I:283:GLU:C	2.46	0.52
3:C:580:CYS:SG	3:C:581:SER:N	2.81	0.52
1:G:49:GLN:CG	1:G:50:LYS:N	2.69	0.52
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.92	0.52
1:F:54:VAL:CG2	1:F:55:GLY:H	2.13	0.52
1:F:40:HIS:CD2	1:G:171:LEU:HD21	2.44	0.52
1:F:72:GLU:O	1:F:73:HIC:C	2.57	0.52
1:D:34:ILE:O	1:D:35:VAL:HG23	2.09	0.52
1:D:37:ARG:HB3	1:D:38:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLU:O	1:E:73:HIC:C	2.57	0.52
1:G:107:GLU:HB2	1:G:134:VAL:HG22	1.92	0.52
1:F:34:ILE:O	1:F:35:VAL:HG23	2.09	0.52
1:G:107:GLU:N	1:G:135:ALA:O	2.43	0.52
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.92	0.52
1:A:191:LYS:O	1:A:194:THR:OG1	2.24	0.52
1:F:304:THR:HB	1:F:335:ARG:HD2	1.92	0.52
3:J:455:LEU:O	3:J:459:LEU:N	2.43	0.52
1:F:107:GLU:N	1:F:135:ALA:O	2.43	0.51
1:G:34:ILE:O	1:G:35:VAL:HG23	2.09	0.51
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.92	0.51
1:G:34:ILE:HD13	1:G:34:ILE:H	1.76	0.51
3:C:455:LEU:O	3:C:459:LEU:N	2.43	0.51
1:A:107:GLU:N	1:A:135:ALA:O	2.43	0.51
1:A:168:GLY:HA2	1:E:43:VAL:N	2.26	0.51
1:A:34:ILE:H	1:A:34:ILE:HD13	1.76	0.51
3:J:473:PHE:CZ	3:J:477:ILE:HD11	2.45	0.51
1:E:34:ILE:H	1:E:34:ILE:HD13	1.76	0.51
1:G:304:THR:HB	1:G:335:ARG:HD2	1.92	0.51
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.92	0.51
1:F:37:ARG:HB3	1:F:38:PRO:HD2	1.91	0.51
1:G:37:ARG:HB3	1:G:38:PRO:HD2	1.91	0.51
1:D:41:GLN:O	1:D:43:VAL:N	2.44	0.51
1:E:304:THR:HB	1:E:335:ARG:HD2	1.92	0.51
1:D:107:GLU:N	1:D:135:ALA:O	2.43	0.51
3:C:454:GLY:O	3:C:458:LEU:N	2.44	0.51
1:F:34:ILE:H	1:F:34:ILE:HD13	1.76	0.51
1:A:304:THR:HB	1:A:335:ARG:HD2	1.92	0.51
3:I:455:LEU:O	3:I:459:LEU:N	2.43	0.51
1:E:107:GLU:N	1:E:135:ALA:O	2.43	0.51
3:I:81:ALA:O	3:I:85:TYR:N	2.44	0.51
3:J:454:GLY:O	3:J:458:LEU:N	2.44	0.51
3:I:473:PHE:CZ	3:I:477:ILE:HD11	2.45	0.51
3:J:621:ARG:HB3	3:J:678:PHE:HZ	1.76	0.51
3:I:454:GLY:O	3:I:458:LEU:N	2.44	0.51
1:E:39:ARG:HH21	1:F:269:MET:N	2.08	0.51
1:E:38:PRO:CG	1:E:49:GLN:HG2	2.31	0.51
1:F:300:SER:HA	1:F:335:ARG:HB2	1.93	0.51
3:C:473:PHE:CZ	3:C:477:ILE:HD11	2.45	0.51
1:E:300:SER:HA	1:E:335:ARG:HB2	1.93	0.50
1:D:304:THR:HB	1:D:335:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:HD13	1:D:34:ILE:H	1.76	0.50
1:A:300:SER:HA	1:A:335:ARG:HB2	1.93	0.50
3:I:621:ARG:HB3	3:I:678:PHE:HZ	1.76	0.50
1:G:300:SER:HA	1:G:335:ARG:HB2	1.93	0.50
3:C:621:ARG:HB3	3:C:678:PHE:HZ	1.76	0.50
1:E:41:GLN:O	1:E:43:VAL:N	2.44	0.50
3:C:81:ALA:O	3:C:85:TYR:N	2.44	0.50
1:F:41:GLN:O	1:F:43:VAL:N	2.44	0.50
1:D:300:SER:HA	1:D:335:ARG:HB2	1.93	0.50
1:D:222:ASP:OD2	1:D:225:ASN:ND2	2.45	0.50
1:E:222:ASP:OD2	1:E:225:ASN:ND2	2.45	0.50
1:G:222:ASP:OD2	1:G:225:ASN:ND2	2.45	0.50
1:F:222:ASP:OD2	1:F:225:ASN:ND2	2.45	0.50
3:I:550:THR:HG22	3:I:551:ARG:HG3	1.94	0.50
3:C:550:THR:HG22	3:C:551:ARG:HG3	1.94	0.50
1:A:165:ILE:HD11	1:E:43:VAL:HG12	1.94	0.49
1:A:43:VAL:HB	1:D:143:TYR:OH	2.11	0.49
3:I:436:ILE:O	3:I:437:GLU:C	2.50	0.49
1:E:224:GLU:OE1	1:E:224:GLU:N	2.45	0.49
3:C:320:LEU:HD21	3:C:534:SER:HB2	1.94	0.49
1:F:40:HIS:CE1	1:G:168:GLY:O	2.65	0.49
3:I:320:LEU:HD21	3:I:534:SER:HB2	1.94	0.49
3:C:436:ILE:O	3:C:437:GLU:C	2.50	0.49
3:J:436:ILE:O	3:J:437:GLU:C	2.50	0.49
1:F:224:GLU:OE1	1:F:224:GLU:N	2.45	0.49
3:J:306:ALA:O	3:J:310:LYS:N	2.45	0.49
1:A:224:GLU:N	1:A:224:GLU:OE1	2.45	0.49
3:C:306:ALA:O	3:C:310:LYS:N	2.45	0.49
3:J:81:ALA:O	3:J:85:TYR:N	2.44	0.49
3:J:320:LEU:HD21	3:J:534:SER:HB2	1.94	0.49
3:J:550:THR:HG22	3:J:551:ARG:HG3	1.94	0.49
1:E:51:ASP:C	1:E:53:TYR:N	2.60	0.49
3:I:306:ALA:O	3:I:310:LYS:N	2.45	0.49
1:E:349:LEU:HA	3:J:461:GLU:HB2	1.95	0.49
3:I:326:SER:O	3:I:327:THR:CB	2.60	0.49
3:C:645:TRP:O	3:C:647:SER:N	2.46	0.49
3:J:326:SER:O	3:J:327:THR:CB	2.60	0.49
1:A:222:ASP:OD2	1:A:225:ASN:ND2	2.45	0.49
3:C:299:THR:O	3:C:303:ALA:N	2.42	0.49
1:A:43:VAL:HG23	1:A:46:GLY:CA	2.43	0.49
3:C:119:THR:O	3:C:121:VAL:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:CA	1:D:167:GLU:O	2.59	0.48
1:D:43:VAL:HG23	1:D:46:GLY:CA	2.43	0.48
1:E:43:VAL:HG23	1:E:46:GLY:CA	2.43	0.48
1:D:224:GLU:OE1	1:D:224:GLU:N	2.45	0.48
1:F:43:VAL:HB	1:G:143:TYR:OH	2.14	0.48
1:A:41:GLN:O	1:A:43:VAL:N	2.44	0.48
1:G:41:GLN:O	1:G:43:VAL:N	2.44	0.48
3:I:119:THR:O	3:I:121:VAL:N	2.44	0.48
3:I:645:TRP:O	3:I:647:SER:N	2.46	0.48
3:C:607:GLN:HA	3:C:610:TYR:CE2	2.49	0.48
3:J:607:GLN:HA	3:J:610:TYR:CE2	2.49	0.48
3:C:55:ASN:ND2	3:C:55:ASN:O	2.47	0.48
3:J:645:TRP:O	3:J:647:SER:N	2.46	0.48
3:I:607:GLN:HA	3:I:610:TYR:CE2	2.49	0.48
1:A:191:LYS:NZ	1:G:172:PRO:O	2.33	0.48
1:F:107:GLU:OE2	1:F:116:ARG:NH1	2.47	0.48
1:E:107:GLU:OE2	1:E:116:ARG:NH1	2.47	0.48
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.47	0.48
3:J:119:THR:O	3:J:121:VAL:N	2.44	0.48
3:J:442:LYS:N	3:J:443:PRO:HD3	2.29	0.48
1:G:224:GLU:OE1	1:G:224:GLU:N	2.45	0.48
3:J:55:ASN:ND2	3:J:55:ASN:O	2.47	0.48
1:G:107:GLU:OE2	1:G:116:ARG:NH1	2.47	0.48
3:C:350:ASP:HB3	3:C:354:LYS:HE3	1.96	0.48
3:I:324:SER:HA	3:I:336:ILE:HG22	1.95	0.48
3:J:324:SER:HA	3:J:336:ILE:HG22	1.95	0.48
3:I:621:ARG:HG2	3:I:676:LYS:HG3	1.96	0.47
3:J:621:ARG:HG2	3:J:676:LYS:HG3	1.96	0.47
3:I:350:ASP:HB3	3:I:354:LYS:HE3	1.96	0.47
1:F:43:VAL:HG23	1:F:46:GLY:CA	2.43	0.47
3:C:453:ILE:O	3:C:453:ILE:HG22	2.14	0.47
1:F:286:ASP:O	1:F:289:ILE:HG22	2.15	0.47
1:G:43:VAL:HG23	1:G:46:GLY:CA	2.43	0.47
1:F:56:ASP:O	1:F:60:SER:OG	2.22	0.47
1:G:286:ASP:O	1:G:289:ILE:HG22	2.15	0.47
3:J:624:PHE:O	3:J:627:ARG:NH1	2.47	0.47
3:J:350:ASP:HB3	3:J:354:LYS:HE3	1.96	0.47
3:C:621:ARG:HG2	3:C:676:LYS:HG3	1.96	0.47
1:F:73:HIC:O	1:F:73:HIC:CG	2.63	0.47
3:I:624:PHE:O	3:I:627:ARG:NH1	2.47	0.47
1:E:73:HIC:CG	1:E:73:HIC:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:GLU:OE2	1:D:116:ARG:NH1	2.47	0.47
1:A:286:ASP:O	1:A:289:ILE:HG22	2.15	0.47
3:I:442:LYS:N	3:I:443:PRO:HD3	2.29	0.47
3:I:55:ASN:O	3:I:55:ASN:ND2	2.47	0.47
1:A:43:VAL:H	1:D:168:GLY:HA2	1.80	0.47
3:J:299:THR:O	3:J:303:ALA:N	2.42	0.47
1:D:73:HIC:O	1:D:73:HIC:CG	2.63	0.46
1:G:220:ALA:HB2	1:G:255:PHE:HB2	1.97	0.46
1:D:286:ASP:O	1:D:289:ILE:HG22	2.15	0.46
1:D:171:LEU:CB	1:D:172:PRO:HD3	2.44	0.46
3:C:459:LEU:HD22	3:C:523:ASN:ND2	2.31	0.46
3:J:459:LEU:HD22	3:J:523:ASN:ND2	2.31	0.46
3:C:431:ILE:HG23	3:C:653:LYS:HB3	1.98	0.46
3:J:431:ILE:HG23	3:J:653:LYS:HB3	1.97	0.46
1:E:286:ASP:O	1:E:289:ILE:HG22	2.15	0.46
3:I:431:ILE:HG23	3:I:653:LYS:HB3	1.97	0.46
3:J:287:GLN:HG3	3:J:293:THR:HG23	1.97	0.46
3:I:459:LEU:HD22	3:I:523:ASN:ND2	2.31	0.46
3:C:442:LYS:N	3:C:443:PRO:HD3	2.29	0.46
1:A:171:LEU:CB	1:A:172:PRO:HD3	2.44	0.46
3:C:182:TYR:O	3:C:184:LEU:N	2.48	0.46
3:I:615:GLU:N	3:I:615:GLU:OE1	2.49	0.46
1:F:220:ALA:HB2	1:F:255:PHE:HB2	1.97	0.46
3:C:287:GLN:HG3	3:C:293:THR:HG23	1.97	0.46
3:C:186:LYS:HD2	3:C:354:LYS:HD3	1.98	0.46
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.97	0.46
3:J:645:TRP:HB3	3:J:646:PRO:HD2	1.97	0.46
3:J:186:LYS:HD2	3:J:354:LYS:HD3	1.98	0.46
3:C:326:SER:O	3:C:327:THR:HB	2.15	0.46
3:C:601:GLU:OE2	3:C:605:ARG:NH2	2.49	0.46
3:I:299:THR:O	3:I:303:ALA:N	2.42	0.46
1:F:54:VAL:N	1:F:58:ALA:HB2	2.31	0.46
1:E:54:VAL:N	1:E:58:ALA:HB2	2.31	0.46
1:A:39:ARG:HH21	1:G:268:GLY:C	2.19	0.46
3:J:469:THR:HA	3:J:520:LEU:HD11	1.98	0.46
3:I:469:THR:HA	3:I:520:LEU:HD11	1.98	0.46
3:J:388:TYR:N	3:J:388:TYR:CD1	2.84	0.46
1:A:73:HIC:O	1:A:73:HIC:CG	2.63	0.46
1:G:49:GLN:HG3	1:G:50:LYS:H	1.79	0.45
1:E:171:LEU:CB	1:E:172:PRO:HD3	2.44	0.45
1:F:274:ILE:HD12	1:F:275:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:551:ARG:HB3	3:C:555:SER:OG	2.17	0.45
3:I:186:LYS:HD2	3:I:354:LYS:HD3	1.98	0.45
3:I:83:ASP:O	3:I:87:SER:N	2.49	0.45
1:E:62:ARG:O	1:E:63:GLY:C	2.55	0.45
1:G:62:ARG:O	1:G:63:GLY:C	2.55	0.45
1:A:64:ILE:C	1:A:65:LEU:HD12	2.37	0.45
3:C:615:GLU:OE1	3:C:615:GLU:N	2.49	0.45
3:J:615:GLU:OE1	3:J:615:GLU:N	2.49	0.45
1:E:25:ASP:HB3	3:J:528:PHE:CE1	2.51	0.45
3:I:287:GLN:HG3	3:I:293:THR:HG23	1.97	0.45
1:G:54:VAL:N	1:G:58:ALA:HB2	2.31	0.45
1:F:171:LEU:CB	1:F:172:PRO:HD3	2.44	0.45
1:E:135:ALA:HB1	1:E:140:LEU:HD11	1.99	0.45
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.99	0.45
3:C:83:ASP:O	3:C:87:SER:N	2.49	0.45
1:D:268:GLY:C	1:G:39:ARG:NH2	2.69	0.45
1:E:274:ILE:HD12	1:E:275:HIS:N	2.31	0.45
1:D:274:ILE:HD12	1:D:275:HIS:N	2.31	0.45
3:J:551:ARG:HB3	3:J:555:SER:OG	2.17	0.45
3:C:645:TRP:HB3	3:C:646:PRO:HD2	1.97	0.45
1:G:289:ILE:O	1:G:293:LEU:HG	2.17	0.45
1:A:43:VAL:CG1	1:D:166:TYR:O	2.64	0.45
1:A:40:HIS:CD2	1:D:171:LEU:HD21	2.50	0.45
1:A:270:GLU:HG2	1:F:202:THR:HG22	1.97	0.45
1:G:73:HIC:O	1:G:73:HIC:CG	2.63	0.45
1:D:136:ILE:N	1:D:136:ILE:HD12	2.31	0.45
1:D:62:ARG:O	1:D:63:GLY:C	2.55	0.45
3:J:83:ASP:O	3:J:87:SER:N	2.49	0.45
3:C:624:PHE:O	3:C:627:ARG:NH1	2.47	0.45
1:D:270:GLU:HG2	1:G:202:THR:HG22	1.97	0.45
1:F:135:ALA:HB1	1:F:140:LEU:HD11	1.98	0.45
1:G:135:ALA:HB1	1:G:140:LEU:HD11	1.99	0.45
3:I:78:TYR:CZ	3:I:81:ALA:HB2	2.52	0.45
1:E:64:ILE:C	1:E:65:LEU:HD12	2.37	0.45
3:I:601:GLU:OE2	3:I:605:ARG:NH2	2.49	0.45
1:F:62:ARG:O	1:F:63:GLY:C	2.55	0.45
1:G:51:ASP:C	1:G:53:TYR:N	2.60	0.45
1:G:43:VAL:CG2	1:G:46:GLY:HA3	2.47	0.45
1:F:289:ILE:O	1:F:293:LEU:HG	2.17	0.45
1:F:49:GLN:HG3	1:F:50:LYS:H	1.79	0.45
1:G:274:ILE:HD12	1:G:275:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ALA:HB1	1:D:140:LEU:HD11	1.99	0.45
1:E:136:ILE:N	1:E:136:ILE:HD12	2.31	0.45
2:B:139:GLU:OE2	1:D:221:LEU:HD22	2.17	0.45
1:F:43:VAL:CG2	1:F:46:GLY:HA3	2.47	0.45
1:G:171:LEU:CB	1:G:172:PRO:HD3	2.44	0.45
1:A:173:HIS:O	1:A:174:ALA:C	2.55	0.45
1:F:173:HIS:O	1:F:174:ALA:C	2.55	0.45
1:G:136:ILE:HD12	1:G:136:ILE:N	2.31	0.45
3:I:645:TRP:HB3	3:I:646:PRO:HD2	1.97	0.45
1:A:297:ASN:O	1:A:330:ILE:N	2.50	0.45
1:E:220:ALA:HB2	1:E:255:PHE:HB2	1.97	0.45
1:A:328:LYS:HG3	3:C:289:THR:HB	1.99	0.45
1:A:54:VAL:N	1:A:58:ALA:HB2	2.31	0.45
3:C:360:LEU:HD13	3:C:546:LEU:HD22	1.99	0.45
1:D:268:GLY:C	1:G:39:ARG:HH21	2.19	0.45
3:J:601:GLU:OE2	3:J:605:ARG:NH2	2.49	0.45
1:F:51:ASP:C	1:F:53:TYR:N	2.60	0.45
1:D:54:VAL:N	1:D:58:ALA:HB2	2.31	0.45
1:D:173:HIS:O	1:D:174:ALA:C	2.55	0.45
1:A:274:ILE:HD12	1:A:275:HIS:N	2.31	0.45
1:A:289:ILE:O	1:A:293:LEU:HG	2.17	0.45
1:G:64:ILE:C	1:G:65:LEU:HD12	2.37	0.45
1:D:220:ALA:HB2	1:D:255:PHE:HB2	1.97	0.45
1:F:297:ASN:O	1:F:330:ILE:N	2.50	0.45
3:I:360:LEU:HD13	3:I:546:LEU:HD22	2.00	0.44
3:J:629:GLU:HA	3:J:676:LYS:HA	2.00	0.44
1:F:136:ILE:HD12	1:F:136:ILE:N	2.31	0.44
1:A:136:ILE:N	1:A:136:ILE:HD12	2.31	0.44
3:J:78:TYR:CZ	3:J:81:ALA:HB2	2.52	0.44
1:D:64:ILE:C	1:D:65:LEU:HD12	2.37	0.44
1:D:43:VAL:CG2	1:D:46:GLY:HA3	2.47	0.44
3:J:360:LEU:HD13	3:J:546:LEU:HD22	2.00	0.44
3:I:629:GLU:HA	3:I:676:LYS:HA	2.00	0.44
3:I:551:ARG:HB3	3:I:555:SER:OG	2.17	0.44
1:D:289:ILE:O	1:D:293:LEU:HG	2.17	0.44
1:F:64:ILE:C	1:F:65:LEU:HD12	2.37	0.44
1:D:297:ASN:O	1:D:330:ILE:N	2.50	0.44
1:A:169:TYR:N	1:E:40:HIS:CE1	2.85	0.44
1:D:49:GLN:HG3	1:D:50:LYS:H	1.80	0.44
3:C:78:TYR:CZ	3:C:81:ALA:HB2	2.52	0.44
1:E:297:ASN:O	1:E:330:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:HIS:O	1:E:174:ALA:C	2.55	0.44
3:C:629:GLU:HA	3:C:676:LYS:HA	2.00	0.44
1:E:289:ILE:O	1:E:293:LEU:HG	2.17	0.44
1:G:171:LEU:HD13	1:G:172:PRO:CD	2.48	0.44
1:A:171:LEU:HB2	1:A:172:PRO:CD	2.46	0.44
1:G:173:HIS:O	1:G:174:ALA:C	2.55	0.44
3:I:388:TYR:N	3:I:388:TYR:CD1	2.84	0.44
3:J:182:TYR:O	3:J:184:LEU:N	2.49	0.44
1:A:62:ARG:O	1:A:63:GLY:C	2.55	0.44
1:E:87:HIS:O	1:E:87:HIS:ND1	2.51	0.44
1:G:297:ASN:O	1:G:330:ILE:N	2.50	0.44
3:I:19:ILE:O	3:I:19:ILE:CG2	2.66	0.44
1:D:171:LEU:HD13	1:D:172:PRO:CD	2.48	0.44
1:E:171:LEU:HD13	1:E:172:PRO:CD	2.48	0.44
1:F:171:LEU:HD13	1:F:172:PRO:CD	2.48	0.44
3:J:19:ILE:O	3:J:19:ILE:CG2	2.66	0.44
3:J:251:LYS:O	3:J:255:THR:OG1	2.30	0.44
1:A:87:HIS:ND1	1:A:87:HIS:O	2.51	0.44
3:C:388:TYR:N	3:C:388:TYR:CD1	2.84	0.44
3:C:469:THR:HA	3:C:520:LEU:HD11	1.99	0.44
1:F:87:HIS:O	1:F:87:HIS:ND1	2.51	0.44
1:G:34:ILE:HB	1:G:67:LEU:HD22	2.00	0.43
1:E:275:HIS:NE2	1:E:276:GLU:OE2	2.51	0.43
1:D:56:ASP:O	1:D:60:SER:OG	2.22	0.43
2:B:199:THR:O	2:B:203:ASN:ND2	2.48	0.43
1:D:35:VAL:O	1:D:35:VAL:HG12	2.18	0.43
1:A:275:HIS:NE2	1:A:276:GLU:OE2	2.52	0.43
1:G:275:HIS:NE2	1:G:276:GLU:OE2	2.51	0.43
1:D:87:HIS:ND1	1:D:87:HIS:O	2.51	0.43
1:F:34:ILE:HB	1:F:67:LEU:HD22	2.00	0.43
1:A:43:VAL:CG2	1:A:46:GLY:HA3	2.47	0.43
1:F:275:HIS:NE2	1:F:276:GLU:OE2	2.52	0.43
3:J:624:PHE:CZ	3:J:626:GLY:O	2.71	0.43
3:C:328:GLY:O	3:C:329:VAL:HB	2.19	0.43
3:I:182:TYR:O	3:I:184:LEU:N	2.48	0.43
1:G:87:HIS:O	1:G:87:HIS:ND1	2.51	0.43
1:A:169:TYR:HA	1:E:40:HIS:HE1	1.83	0.43
1:D:275:HIS:NE2	1:D:276:GLU:OE2	2.52	0.43
1:E:136:ILE:O	1:E:140:LEU:HD13	2.19	0.43
1:F:35:VAL:O	1:F:35:VAL:HG12	2.19	0.43
1:G:171:LEU:HB2	1:G:172:PRO:CD	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:HB	1:D:67:LEU:HD22	2.00	0.43
1:A:171:LEU:HD13	1:A:172:PRO:CD	2.48	0.43
1:E:34:ILE:HB	1:E:67:LEU:HD22	2.00	0.43
1:A:50:LYS:O	1:A:52:SER:N	2.48	0.43
3:J:19:ILE:HD13	3:J:19:ILE:C	2.39	0.43
1:A:136:ILE:O	1:A:140:LEU:HD13	2.19	0.43
3:J:220:THR:O	3:J:222:ASN:N	2.51	0.43
1:E:35:VAL:HG12	1:E:35:VAL:O	2.18	0.43
1:A:34:ILE:HB	1:A:67:LEU:HD22	1.99	0.43
1:D:171:LEU:HB2	1:D:172:PRO:CD	2.46	0.43
1:D:136:ILE:O	1:D:140:LEU:HD13	2.19	0.43
3:C:624:PHE:CZ	3:C:626:GLY:O	2.71	0.43
3:I:481:PHE:HB3	3:I:487:LEU:HD23	2.01	0.43
3:I:19:ILE:C	3:I:19:ILE:HD13	2.39	0.43
3:C:19:ILE:C	3:C:19:ILE:HD13	2.39	0.43
3:J:548:PRO:O	3:J:549:PRO:C	2.57	0.43
1:A:325:MET:SD	1:A:327:ILE:HD11	2.59	0.43
1:F:55:GLY:C	1:F:57:GLU:N	2.73	0.43
1:G:39:ARG:HG2	1:G:66:THR:OG1	2.19	0.43
1:F:39:ARG:HG2	1:F:66:THR:OG1	2.19	0.43
1:E:50:LYS:O	1:E:52:SER:N	2.48	0.43
1:F:136:ILE:O	1:F:140:LEU:HD13	2.19	0.43
1:G:136:ILE:O	1:G:140:LEU:HD13	2.19	0.43
3:I:220:THR:O	3:I:222:ASN:N	2.51	0.43
3:C:175:ILE:HB	3:C:374:CYS:HB3	2.01	0.43
3:I:634:TYR:O	3:I:636:ARG:N	2.50	0.43
3:C:481:PHE:HB3	3:C:487:LEU:HD23	2.01	0.43
1:A:167:GLU:O	1:E:42:GLY:CA	2.65	0.42
1:G:50:LYS:O	1:G:52:SER:N	2.48	0.42
1:G:55:GLY:C	1:G:57:GLU:N	2.73	0.42
3:J:481:PHE:HB3	3:J:487:LEU:HD23	2.01	0.42
3:I:175:ILE:HB	3:I:374:CYS:HB3	2.01	0.42
1:D:50:LYS:O	1:D:52:SER:N	2.48	0.42
3:I:624:PHE:CZ	3:I:626:GLY:O	2.71	0.42
3:C:220:THR:O	3:C:222:ASN:N	2.51	0.42
3:J:175:ILE:HB	3:J:374:CYS:HB3	2.01	0.42
1:E:55:GLY:C	1:E:57:GLU:N	2.73	0.42
1:A:35:VAL:O	1:A:35:VAL:HG12	2.18	0.42
1:A:49:GLN:HG3	1:A:50:LYS:H	1.79	0.42
1:G:35:VAL:HG12	1:G:35:VAL:O	2.19	0.42
1:E:276:GLU:OE1	1:E:276:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:169:ASN:OD1	3:J:170:ALA:N	2.52	0.42
3:I:548:PRO:O	3:I:549:PRO:C	2.57	0.42
3:I:498:ILE:HD11	3:I:504:ARG:HE	1.84	0.42
1:E:43:VAL:CG2	1:E:46:GLY:HA3	2.46	0.42
1:A:276:GLU:OE1	1:A:276:GLU:N	2.53	0.42
1:F:202:THR:OG1	1:F:205:GLU:OE2	2.38	0.42
3:I:623:GLY:O	3:I:624:PHE:HB3	2.20	0.42
3:I:431:ILE:HG12	3:I:653:LYS:HD2	2.01	0.42
3:I:251:LYS:O	3:I:255:THR:OG1	2.30	0.42
3:C:169:ASN:OD1	3:C:170:ALA:N	2.53	0.42
3:C:548:PRO:O	3:C:549:PRO:C	2.57	0.42
1:G:276:GLU:OE1	1:G:276:GLU:N	2.53	0.42
1:D:276:GLU:N	1:D:276:GLU:OE1	2.53	0.42
1:F:276:GLU:N	1:F:276:GLU:OE1	2.53	0.42
3:C:183:LEU:O	3:C:184:LEU:HB3	2.19	0.42
3:C:623:GLY:O	3:C:624:PHE:HB3	2.20	0.42
3:C:498:ILE:HD11	3:C:504:ARG:HE	1.84	0.42
1:G:42:GLY:C	1:G:44:MET:H	2.21	0.42
1:E:39:ARG:HH21	1:F:268:GLY:C	2.21	0.42
3:I:183:LEU:O	3:I:184:LEU:HB3	2.19	0.42
3:J:498:ILE:HD11	3:J:504:ARG:HE	1.84	0.42
3:C:251:LYS:O	3:C:255:THR:OG1	2.30	0.42
1:G:202:THR:OG1	1:G:205:GLU:OE2	2.38	0.42
3:J:622:ALA:HB3	3:J:678:PHE:CZ	2.55	0.42
1:A:55:GLY:C	1:A:57:GLU:N	2.73	0.42
3:J:623:GLY:O	3:J:624:PHE:HB3	2.20	0.42
3:C:431:ILE:HG12	3:C:653:LYS:HD2	2.01	0.42
1:E:56:ASP:O	1:E:60:SER:OG	2.22	0.42
3:I:434:LYS:N	3:I:434:LYS:HD3	2.35	0.42
1:D:53:TYR:N	1:D:53:TYR:CD1	2.88	0.42
1:D:42:GLY:C	1:D:44:MET:H	2.22	0.42
3:I:622:ALA:HB3	3:I:678:PHE:CZ	2.54	0.42
1:E:53:TYR:CD1	1:E:53:TYR:N	2.88	0.42
1:A:53:TYR:N	1:A:53:TYR:CD1	2.88	0.42
3:I:369:ASN:HA	3:I:372:ILE:HB	2.02	0.42
3:C:19:ILE:CG2	3:C:19:ILE:O	2.66	0.42
1:D:269:MET:CA	1:G:39:ARG:HH21	2.33	0.42
1:E:202:THR:OG1	1:E:205:GLU:OE2	2.38	0.42
3:C:622:ALA:HB3	3:C:678:PHE:CZ	2.54	0.42
3:I:169:ASN:OD1	3:I:170:ALA:N	2.53	0.42
3:J:434:LYS:HD3	3:J:434:LYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:165:GLU:HB3	3:J:381:VAL:HG13	2.02	0.42
1:A:39:ARG:HG2	1:A:66:THR:OG1	2.19	0.41
1:G:53:TYR:N	1:G:53:TYR:CD1	2.88	0.41
3:C:369:ASN:HA	3:C:372:ILE:HB	2.02	0.41
1:A:39:ARG:NH2	1:G:268:GLY:C	2.73	0.41
3:J:183:LEU:O	3:J:184:LEU:HB3	2.19	0.41
1:D:189:LEU:HG	1:D:193:LEU:HD13	2.02	0.41
1:E:49:GLN:HG3	1:E:50:LYS:H	1.79	0.41
1:A:43:VAL:HG13	1:D:166:TYR:O	2.19	0.41
1:G:47:MET:O	1:G:49:GLN:N	2.51	0.41
3:J:369:ASN:HA	3:J:372:ILE:HB	2.02	0.41
1:E:39:ARG:HG2	1:E:66:THR:OG1	2.19	0.41
3:C:165:GLU:HB3	3:C:381:VAL:HG13	2.02	0.41
3:C:434:LYS:N	3:C:434:LYS:HD3	2.35	0.41
3:I:165:GLU:HB3	3:I:381:VAL:HG13	2.02	0.41
1:F:171:LEU:HB2	1:F:172:PRO:CD	2.46	0.41
1:A:202:THR:OG1	1:A:205:GLU:OE2	2.38	0.41
1:A:326:LYS:HD3	1:A:328:LYS:HE3	2.00	0.41
1:F:42:GLY:C	1:F:44:MET:H	2.22	0.41
1:D:202:THR:OG1	1:D:205:GLU:OE2	2.38	0.41
3:I:415:ILE:HD12	3:I:442:LYS:HD2	2.03	0.41
3:C:415:ILE:HD12	3:C:442:LYS:HD2	2.03	0.41
1:A:62:ARG:O	1:A:65:LEU:N	2.53	0.41
1:A:159:VAL:HG23	1:A:161:HIS:CE1	2.56	0.41
1:F:257:CYS:HB3	1:F:258:PRO:HD3	2.02	0.41
3:I:621:ARG:O	3:I:622:ALA:HB2	2.21	0.41
3:I:681:ASN:HA	3:I:682:PRO:HD3	1.97	0.41
1:G:346:LEU:HD23	1:G:349:LEU:HD12	2.03	0.41
1:D:39:ARG:HG2	1:D:66:THR:OG1	2.19	0.41
1:G:189:LEU:HG	1:G:193:LEU:HD13	2.02	0.41
1:D:257:CYS:HB3	1:D:258:PRO:HD3	2.02	0.41
1:F:40:HIS:CE1	1:G:169:TYR:N	2.89	0.41
1:D:55:GLY:C	1:D:57:GLU:N	2.73	0.41
3:I:142:LEU:HD13	3:I:142:LEU:C	2.41	0.41
3:J:415:ILE:HD12	3:J:442:LYS:HD2	2.03	0.41
1:E:62:ARG:O	1:E:65:LEU:N	2.53	0.41
1:G:62:ARG:O	1:G:65:LEU:N	2.53	0.41
1:D:152:VAL:HA	1:D:298:VAL:HB	2.02	0.41
1:F:53:TYR:CD1	1:F:53:TYR:N	2.88	0.41
1:E:34:ILE:HD13	1:E:34:ILE:N	2.36	0.41
1:A:171:LEU:HD21	1:E:40:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ASP:O	1:G:53:TYR:CA	2.69	0.41
3:J:136:LEU:HD21	3:J:372:ILE:HG23	2.03	0.41
1:A:268:GLY:C	1:F:39:ARG:HH21	2.23	0.41
3:C:621:ARG:O	3:C:622:ALA:HB2	2.21	0.41
3:J:142:LEU:C	3:J:142:LEU:HD13	2.41	0.41
3:J:431:ILE:HG12	3:J:653:LYS:HD2	2.01	0.41
3:C:40:TYR:CZ	3:C:75:PRO:HA	2.56	0.41
1:E:294:TYR:HB3	1:E:327:ILE:HD13	2.03	0.41
1:D:294:TYR:HB3	1:D:327:ILE:HD13	2.03	0.41
3:J:634:TYR:O	3:J:636:ARG:N	2.50	0.41
3:J:40:TYR:CZ	3:J:75:PRO:HA	2.56	0.41
1:E:189:LEU:HG	1:E:193:LEU:HD13	2.02	0.41
1:F:294:TYR:HB3	1:F:327:ILE:HD13	2.03	0.41
3:J:414:PHE:O	3:J:418:THR:N	2.51	0.41
1:G:250:ILE:O	1:G:250:ILE:HG13	2.21	0.41
1:G:294:TYR:HB3	1:G:327:ILE:HD13	2.03	0.41
1:F:346:LEU:HD23	1:F:349:LEU:HD12	2.03	0.41
1:F:47:MET:O	1:F:49:GLN:N	2.51	0.41
3:I:136:LEU:HD21	3:I:372:ILE:HG23	2.03	0.41
3:I:40:TYR:CZ	3:I:75:PRO:HA	2.56	0.41
1:F:189:LEU:HG	1:F:193:LEU:HD13	2.02	0.41
1:A:189:LEU:HG	1:A:193:LEU:HD13	2.02	0.41
1:F:34:ILE:N	1:F:34:ILE:HD13	2.36	0.40
1:E:47:MET:O	1:E:49:GLN:N	2.51	0.40
1:G:152:VAL:HA	1:G:298:VAL:HB	2.02	0.40
1:A:346:LEU:HD23	1:A:349:LEU:HD12	2.03	0.40
1:A:152:VAL:HA	1:A:298:VAL:HB	2.02	0.40
1:D:159:VAL:HG23	1:D:161:HIS:CE1	2.56	0.40
1:F:159:VAL:HG23	1:F:161:HIS:CE1	2.56	0.40
1:A:169:TYR:CA	1:E:40:HIS:CE1	3.04	0.40
1:D:52:SER:C	1:D:53:TYR:HD1	2.24	0.40
1:D:62:ARG:O	1:D:65:LEU:N	2.53	0.40
1:F:62:ARG:O	1:F:65:LEU:N	2.53	0.40
1:E:345:ILE:HG12	3:J:464:LEU:HB3	2.03	0.40
1:F:40:HIS:HE1	1:G:169:TYR:HA	1.87	0.40
1:E:52:SER:C	1:E:53:TYR:HD1	2.24	0.40
1:A:268:GLY:C	1:F:39:ARG:NH2	2.75	0.40
1:G:159:VAL:HG23	1:G:161:HIS:CE1	2.56	0.40
1:A:10:CYS:SG	1:A:11:ASP:N	2.95	0.40
3:J:223:ALA:N	3:J:224:PRO:CD	2.85	0.40
2:B:169:LEU:HD22	2:H:165:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:CYS:SG	1:D:11:ASP:N	2.95	0.40
3:C:10:VAL:O	3:C:10:VAL:HG12	2.21	0.40
1:E:10:CYS:SG	1:E:11:ASP:N	2.95	0.40
1:F:50:LYS:O	1:F:52:SER:N	2.48	0.40
3:I:326:SER:H	3:I:332:ARG:HB2	1.86	0.40
3:J:621:ARG:O	3:J:622:ALA:HB2	2.21	0.40
3:I:414:PHE:O	3:I:418:THR:N	2.51	0.40
3:I:518:GLY:O	3:I:519:PHE:C	2.60	0.40
1:E:152:VAL:HA	1:E:298:VAL:HB	2.03	0.40
1:A:250:ILE:HG13	1:A:250:ILE:O	2.21	0.40
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.02	0.40
1:F:52:SER:C	1:F:53:TYR:HD1	2.24	0.40
1:A:52:SER:C	1:A:53:TYR:HD1	2.24	0.40
3:C:542:LEU:O	3:C:545:GLY:N	2.55	0.40
3:J:387:ILE:HD13	3:J:387:ILE:H	1.87	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	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	1	14
1	D	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	1	14
1	E	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	1	14
1	F	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	1	14
1	G	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	1	14
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	680/697 (98%)	551 (81%)	99 (15%)	30 (4%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	680/697 (98%)	551 (81%)	98 (14%)	31 (5%)	3	33
3	J	680/697 (98%)	551 (81%)	98 (14%)	31 (5%)	3	33
All	All	4168/4238 (98%)	3341 (80%)	550 (13%)	277 (7%)	3	24

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	42	GLY
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	51	ASP
1	A	52	SER
1	A	63	GLY
1	A	143	TYR
1	A	172	PRO
1	A	174	ALA
3	C	78	TYR
3	C	469	THR
1	D	41	GLN
1	D	42	GLY
1	D	43	VAL
1	D	47	MET
1	D	49	GLN
1	D	51	ASP
1	D	52	SER
1	D	63	GLY
1	D	143	TYR
1	D	172	PRO
1	D	174	ALA
1	E	41	GLN
1	E	42	GLY
1	E	43	VAL
1	E	47	MET
1	E	49	GLN
1	E	51	ASP
1	E	52	SER
1	E	63	GLY
1	E	143	TYR
1	E	172	PRO

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Mol	Chain	Res	Type
1	E	174	ALA
1	F	41	GLN
1	F	42	GLY
1	F	43	VAL
1	F	47	MET
1	F	49	GLN
1	F	51	ASP
1	F	52	SER
1	F	63	GLY
1	F	143	TYR
1	F	172	PRO
1	F	174	ALA
1	G	41	GLN
1	G	42	GLY
1	G	43	VAL
1	G	47	MET
1	G	49	GLN
1	G	51	ASP
1	G	52	SER
1	G	63	GLY
1	G	143	TYR
1	G	172	PRO
1	G	174	ALA
3	I	78	TYR
3	I	469	THR
3	J	78	TYR
3	J	469	THR
1	A	50	LYS
1	A	245	GLY
3	C	76	HIS
3	C	283	GLU
3	C	290	GLY
3	C	335	VAL
3	C	437	GLU
3	C	622	ALA
1	D	15	GLY
1	D	50	LYS
1	D	245	GLY
1	E	50	LYS
1	E	245	GLY
1	F	50	LYS
1	F	245	GLY

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Mol	Chain	Res	Type
1	G	50	LYS
1	G	245	GLY
3	I	76	HIS
3	I	283	GLU
3	I	290	GLY
3	I	335	VAL
3	I	437	GLU
3	I	622	ALA
3	J	76	HIS
3	J	283	GLU
3	J	290	GLY
3	J	335	VAL
3	J	437	GLU
3	J	622	ALA
1	A	15	GLY
1	A	21	PHE
1	A	38	PRO
1	A	44	MET
1	A	53	TYR
1	A	100	GLU
1	A	128	ASN
1	A	137	GLN
1	A	144	ALA
1	A	145	SER
1	A	158	GLY
1	A	171	LEU
1	A	182	GLY
1	A	370	VAL
3	C	184	LEU
3	C	257	GLY
3	C	624	PHE
3	C	636	ARG
1	D	6	THR
1	D	21	PHE
1	D	38	PRO
1	D	44	MET
1	D	53	TYR
1	D	100	GLU
1	D	128	ASN
1	D	137	GLN
1	D	144	ALA
1	D	145	SER

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Mol	Chain	Res	Type
1	D	158	GLY
1	D	171	LEU
1	D	182	GLY
1	D	370	VAL
1	E	15	GLY
1	E	21	PHE
1	E	38	PRO
1	E	44	MET
1	E	53	TYR
1	E	100	GLU
1	E	128	ASN
1	E	137	GLN
1	E	144	ALA
1	E	145	SER
1	E	158	GLY
1	E	171	LEU
1	E	182	GLY
1	E	370	VAL
1	F	6	THR
1	F	15	GLY
1	F	21	PHE
1	F	38	PRO
1	F	44	MET
1	F	53	TYR
1	F	100	GLU
1	F	128	ASN
1	F	137	GLN
1	F	144	ALA
1	F	145	SER
1	F	158	GLY
1	F	171	LEU
1	F	182	GLY
1	F	370	VAL
1	G	15	GLY
1	G	21	PHE
1	G	38	PRO
1	G	44	MET
1	G	53	TYR
1	G	100	GLU
1	G	128	ASN
1	G	137	GLN
1	G	144	ALA

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Mol	Chain	Res	Type
1	G	145	SER
1	G	158	GLY
1	G	171	LEU
1	G	182	GLY
1	G	370	VAL
3	I	184	LEU
3	I	257	GLY
3	I	624	PHE
3	I	636	ARG
3	J	184	LEU
3	J	257	GLY
3	J	624	PHE
3	J	636	ARG
1	A	4	GLU
1	A	6	THR
3	C	328	GLY
3	C	455	LEU
3	C	494	LYS
3	C	520	LEU
3	C	676	LYS
1	D	4	GLU
1	E	4	GLU
1	E	6	THR
1	F	4	GLU
1	G	4	GLU
1	G	6	THR
3	I	328	GLY
3	I	455	LEU
3	I	494	LYS
3	I	520	LEU
3	I	676	LYS
3	J	327	THR
3	J	328	GLY
3	J	455	LEU
3	J	494	LYS
3	J	520	LEU
3	J	676	LYS
1	A	146	GLY
3	C	13	PHE
3	C	330	GLY
3	C	380	PRO
3	C	483	LYS

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Mol	Chain	Res	Type
3	C	549	PRO
1	D	142	LEU
1	D	146	GLY
1	E	146	GLY
1	F	146	GLY
1	G	146	GLY
3	I	13	PHE
3	I	327	THR
3	I	330	GLY
3	I	380	PRO
3	I	483	LYS
3	I	549	PRO
3	J	13	PHE
3	J	330	GLY
3	J	380	PRO
3	J	483	LYS
3	J	549	PRO
1	A	142	LEU
3	C	279	ILE
3	C	552	PRO
3	C	646	PRO
1	E	142	LEU
1	F	142	LEU
1	G	142	LEU
3	I	279	ILE
3	I	552	PRO
3	I	646	PRO
3	J	279	ILE
3	J	552	PRO
3	J	646	PRO
1	A	369	ILE
3	C	329	VAL
1	D	369	ILE
1	E	369	ILE
1	F	369	ILE
1	G	369	ILE
3	I	329	VAL
3	J	329	VAL
1	A	35	VAL
1	A	156	GLY
3	C	14	VAL
3	C	208	GLY

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Mol	Chain	Res	Type
1	D	35	VAL
1	D	70	PRO
1	D	156	GLY
1	E	35	VAL
1	E	156	GLY
1	F	35	VAL
1	F	70	PRO
1	F	156	GLY
1	G	35	VAL
1	G	156	GLY
3	I	14	VAL
3	I	208	GLY
3	J	14	VAL
3	J	208	GLY
1	A	55	GLY
1	A	70	PRO
3	C	372	ILE
3	C	681	ASN
1	D	55	GLY
1	E	55	GLY
1	E	70	PRO
1	F	55	GLY
1	G	55	GLY
1	G	70	PRO
3	I	372	ILE
3	I	681	ASN
3	J	372	ILE
3	J	681	ASN
1	A	201	VAL
1	D	201	VAL
1	E	201	VAL
1	F	201	VAL
1	G	201	VAL

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%)	283 (89%)	34 (11%)	8	36
1	D	317/317 (100%)	282 (89%)	35 (11%)	8	34
1	E	317/317 (100%)	283 (89%)	34 (11%)	8	36
1	F	317/317 (100%)	282 (89%)	35 (11%)	8	34
1	G	317/317 (100%)	282 (89%)	35 (11%)	8	34
2	B	118/118 (100%)	117 (99%)	1 (1%)	86	94
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	586 (96%)	23 (4%)	40	73
3	I	609/616 (99%)	580 (95%)	29 (5%)	31	67
3	J	609/616 (99%)	580 (95%)	29 (5%)	31	67
All	All	3648/3669 (99%)	3393 (93%)	255 (7%)	23	56

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	39	ARG
1	A	40	HIS
1	A	47	MET
1	A	49	GLN
1	A	50	LYS
1	A	51	ASP
1	A	52	SER
1	A	53	TYR
1	A	64	ILE
1	A	69	TYR
1	A	87	HIS
1	A	116	ARG
1	A	123	MET
1	A	137	GLN
1	A	151	ILE
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	202	THR

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Mol	Chain	Res	Type
1	A	227	MET
1	A	240	TYR
1	A	242	LEU
1	A	246	GLN
1	A	261	LEU
1	A	270	GLU
1	A	291	LYS
1	A	335	ARG
1	A	340	TRP
1	A	356	TRP
2	B	154	ILE
3	C	13	PHE
3	C	19	ILE
3	C	159	ARG
3	C	188	ARG
3	C	228	TYR
3	C	251	LYS
3	C	256	LEU
3	C	281	PHE
3	C	332	ARG
3	C	387	ILE
3	C	388	TYR
3	C	434	LYS
3	C	442	LYS
3	C	459	LEU
3	C	516	VAL
3	C	535	MET
3	C	609	ARG
3	C	614	LEU
3	C	620	ARG
3	C	624	PHE
3	C	627	ARG
3	C	653	LYS
3	C	670	ILE
1	D	34	ILE
1	D	39	ARG
1	D	40	HIS
1	D	47	MET
1	D	49	GLN
1	D	50	LYS
1	D	51	ASP
1	D	52	SER

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Mol	Chain	Res	Type
1	D	53	TYR
1	D	64	ILE
1	D	69	TYR
1	D	87	HIS
1	D	116	ARG
1	D	123	MET
1	D	137	GLN
1	D	147	ARG
1	D	151	ILE
1	D	166	TYR
1	D	169	TYR
1	D	171	LEU
1	D	173	HIS
1	D	183	ARG
1	D	192	ILE
1	D	196	ARG
1	D	202	THR
1	D	227	MET
1	D	240	TYR
1	D	242	LEU
1	D	246	GLN
1	D	261	LEU
1	D	270	GLU
1	D	291	LYS
1	D	335	ARG
1	D	340	TRP
1	D	356	TRP
1	E	34	ILE
1	E	39	ARG
1	E	40	HIS
1	E	49	GLN
1	E	50	LYS
1	E	51	ASP
1	E	52	SER
1	E	53	TYR
1	E	64	ILE
1	E	69	TYR
1	E	87	HIS
1	E	116	ARG
1	E	123	MET
1	E	137	GLN
1	E	147	ARG

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Mol	Chain	Res	Type
1	E	151	ILE
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	202	THR
1	E	227	MET
1	E	240	TYR
1	E	242	LEU
1	E	246	GLN
1	E	261	LEU
1	E	270	GLU
1	E	291	LYS
1	E	335	ARG
1	E	340	TRP
1	E	356	TRP
1	F	34	ILE
1	F	39	ARG
1	F	40	HIS
1	F	47	MET
1	F	49	GLN
1	F	50	LYS
1	F	51	ASP
1	F	52	SER
1	F	53	TYR
1	F	64	ILE
1	F	69	TYR
1	F	87	HIS
1	F	116	ARG
1	F	123	MET
1	F	137	GLN
1	F	147	ARG
1	F	151	ILE
1	F	166	TYR
1	F	169	TYR
1	F	171	LEU
1	F	173	HIS
1	F	183	ARG
1	F	192	ILE

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Mol	Chain	Res	Type
1	F	196	ARG
1	F	202	THR
1	F	227	MET
1	F	240	TYR
1	F	242	LEU
1	F	246	GLN
1	F	261	LEU
1	F	270	GLU
1	F	291	LYS
1	F	335	ARG
1	F	340	TRP
1	F	356	TRP
1	G	34	ILE
1	G	39	ARG
1	G	40	HIS
1	G	47	MET
1	G	49	GLN
1	G	50	LYS
1	G	51	ASP
1	G	52	SER
1	G	53	TYR
1	G	64	ILE
1	G	69	TYR
1	G	87	HIS
1	G	116	ARG
1	G	123	MET
1	G	137	GLN
1	G	147	ARG
1	G	151	ILE
1	G	166	TYR
1	G	169	TYR
1	G	171	LEU
1	G	173	HIS
1	G	183	ARG
1	G	192	ILE
1	G	196	ARG
1	G	202	THR
1	G	227	MET
1	G	240	TYR
1	G	242	LEU
1	G	246	GLN
1	G	261	LEU

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Mol	Chain	Res	Type
1	G	270	GLU
1	G	291	LYS
1	G	335	ARG
1	G	340	TRP
1	G	356	TRP
3	I	13	PHE
3	I	19	ILE
3	I	159	ARG
3	I	188	ARG
3	I	228	TYR
3	I	251	LYS
3	I	256	LEU
3	I	281	PHE
3	I	288	ARG
3	I	325	ILE
3	I	327	THR
3	I	329	VAL
3	I	332	ARG
3	I	387	ILE
3	I	388	TYR
3	I	434	LYS
3	I	442	LYS
3	I	459	LEU
3	I	496	ARG
3	I	516	VAL
3	I	535	MET
3	I	557	LYS
3	I	609	ARG
3	I	614	LEU
3	I	620	ARG
3	I	624	PHE
3	I	627	ARG
3	I	653	LYS
3	I	670	ILE
3	J	13	PHE
3	J	19	ILE
3	J	159	ARG
3	J	188	ARG
3	J	228	TYR
3	J	251	LYS
3	J	256	LEU
3	J	281	PHE

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Mol	Chain	Res	Type
3	J	288	ARG
3	J	325	ILE
3	J	327	THR
3	J	329	VAL
3	J	332	ARG
3	J	387	ILE
3	J	388	TYR
3	J	434	LYS
3	J	442	LYS
3	J	459	LEU
3	J	496	ARG
3	J	516	VAL
3	J	535	MET
3	J	557	LYS
3	J	609	ARG
3	J	614	LEU
3	J	620	ARG
3	J	624	PHE
3	J	627	ARG
3	J	653	LYS
3	J	670	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	88	HIS
1	A	137	GLN
1	A	161	HIS
1	A	252	ASN
2	B	216	GLN
3	C	95	GLN
3	C	125	GLN
3	C	154	ASN
3	C	167	GLN
3	C	313	GLN
3	C	402	ASN
3	C	523	ASN
3	C	536	GLN
1	D	88	HIS
1	D	137	GLN
1	D	161	HIS

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Mol	Chain	Res	Type
1	D	252	ASN
1	E	40	HIS
1	E	88	HIS
1	E	92	ASN
1	E	137	GLN
1	E	161	HIS
1	E	252	ASN
1	F	40	HIS
1	F	137	GLN
1	F	161	HIS
1	F	252	ASN
1	G	88	HIS
1	G	137	GLN
1	G	161	HIS
1	G	252	ASN
3	I	95	GLN
3	I	125	GLN
3	I	154	ASN
3	I	167	GLN
3	I	313	GLN
3	I	402	ASN
3	I	523	ASN
3	I	536	GLN
3	J	95	GLN
3	J	125	GLN
3	J	154	ASN
3	J	167	GLN
3	J	313	GLN
3	J	402	ASN
3	J	523	ASN
3	J	536	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	6,11,12	1.25	1 (16%)	6,14,16	1.41	2 (33%)
1	HIC	D	73	1	6,11,12	1.26	1 (16%)	6,14,16	1.41	2 (33%)
1	HIC	E	73	1	6,11,12	1.26	1 (16%)	6,14,16	1.41	2 (33%)
1	HIC	F	73	1	6,11,12	1.25	1 (16%)	6,14,16	1.41	2 (33%)
1	HIC	G	73	1	6,11,12	1.25	1 (16%)	6,14,16	1.42	2 (33%)

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	G	73	1	-	0/4/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	HIC	CB-CA	2.11	1.58	1.53
1	D	73	HIC	CB-CA	2.12	1.58	1.53
1	A	73	HIC	CB-CA	2.12	1.58	1.53
1	F	73	HIC	CB-CA	2.13	1.58	1.53
1	E	73	HIC	CB-CA	2.15	1.58	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	HIC	O-C-CA	-2.70	118.49	125.72
1	A	73	HIC	O-C-CA	-2.69	118.51	125.72
1	G	73	HIC	O-C-CA	-2.69	118.51	125.72
1	D	73	HIC	O-C-CA	-2.69	118.52	125.72
1	E	73	HIC	O-C-CA	-2.68	118.54	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	73	HIC	CG-CD2-NE2	-2.10	105.21	107.63
1	A	73	HIC	CG-CD2-NE2	-2.10	105.21	107.63
1	D	73	HIC	CG-CD2-NE2	-2.09	105.22	107.63
1	F	73	HIC	CG-CD2-NE2	-2.09	105.22	107.63
1	E	73	HIC	CG-CD2-NE2	-2.09	105.23	107.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0
1	D	73	HIC	2	0
1	E	73	HIC	2	0
1	F	73	HIC	2	0
1	G	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	24,29,29	1.17	1 (4%)	23,45,45	1.50	3 (13%)
4	ADP	D	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)
4	ADP	E	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)
4	ADP	F	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	G	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.50	3 (13%)

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	G	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	G	376	ADP	C2-N1	2.86	1.39	1.33
4	F	376	ADP	C2-N1	2.87	1.39	1.33
4	D	376	ADP	C2-N1	2.89	1.39	1.33
4	E	376	ADP	C2-N1	2.91	1.39	1.33
4	A	376	ADP	C2-N1	2.91	1.39	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	376	ADP	N3-C2-N1	-4.64	125.22	128.87
4	D	376	ADP	N3-C2-N1	-4.63	125.23	128.87
4	F	376	ADP	N3-C2-N1	-4.61	125.25	128.87
4	A	376	ADP	N3-C2-N1	-4.59	125.26	128.87
4	G	376	ADP	N3-C2-N1	-4.56	125.29	128.87
4	A	376	ADP	C2-N1-C6	2.07	122.45	118.77
4	G	376	ADP	C2-N1-C6	2.07	122.46	118.77
4	E	376	ADP	C2-N1-C6	2.08	122.49	118.77
4	D	376	ADP	C2-N1-C6	2.09	122.49	118.77
4	F	376	ADP	C2-N1-C6	2.10	122.51	118.77
4	D	376	ADP	O3B-PB-O2B	2.23	115.62	107.44
4	E	376	ADP	O3B-PB-O2B	2.23	115.62	107.44
4	F	376	ADP	O3B-PB-O2B	2.24	115.66	107.44
4	G	376	ADP	O3B-PB-O2B	2.24	115.67	107.44
4	A	376	ADP	O3B-PB-O2B	2.24	115.67	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	376	ADP	3	0
4	D	376	ADP	3	0
4	E	376	ADP	3	0
4	F	376	ADP	3	0
4	G	376	ADP	3	0

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.