



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 10:02 PM UTC

PDB ID : 5JLH / pdb_00005jlh
EMDB ID : EMD-8164
Title : Cryo-EM structure of a human cytoplasmic actomyosin complex at near-atomic resolution
Authors : von der Ecken, J.; Heissler, S.M.; Pathan-Chhatbar, S.; Manstein, D.J.; Raunser, S.
Deposited on : 2016-04-27
Resolution : 3.90 Å (reported)
Based on initial models : 4PD3, 3J8A, 4A7F

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

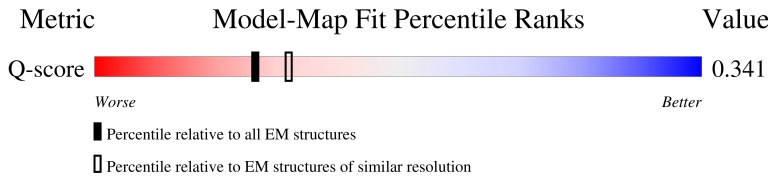
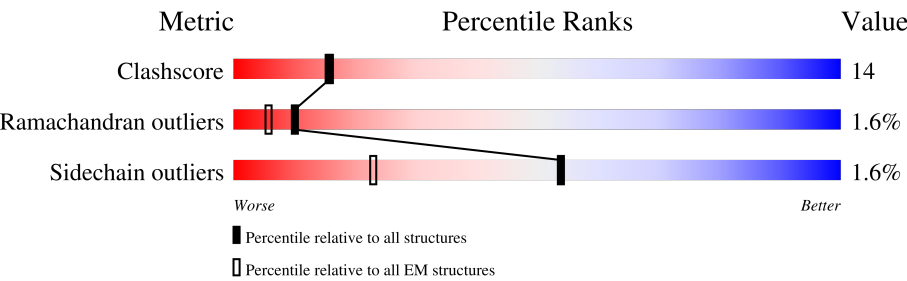
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.



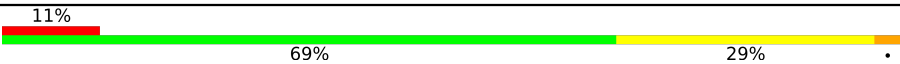
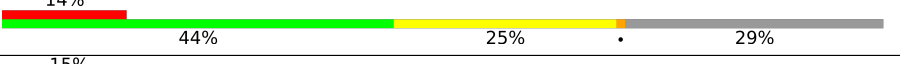
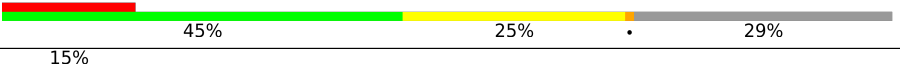
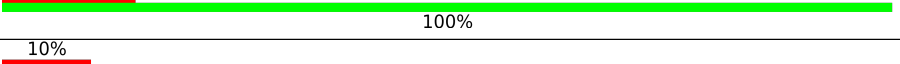
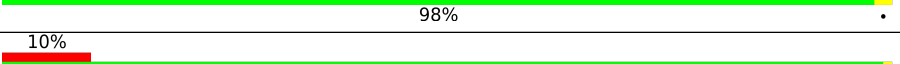
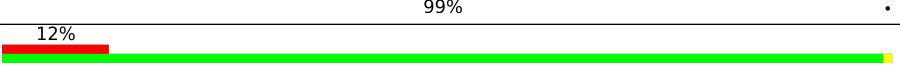
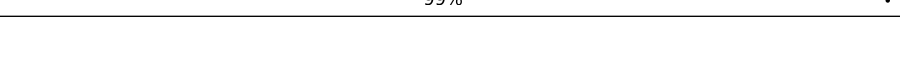
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	9% 68% 29% .
1	B	374	41% 72% 25% .
1	C	374	30% 70% 28% .

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Mol	Chain	Length	Quality of chain
1	D	374	
1	E	374	
2	F	1039	
2	G	1039	
3	H	135	
3	I	135	
3	J	135	
3	K	135	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 29177 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, cytoplasmic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	B	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	C	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	D	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	E	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		

- Molecule 2 is a protein called Myosin-14,Alpha-actinin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	737	Total	C	N	O	S	0	0
			5866	3711	1045	1083	27		
2	G	737	Total	C	N	O	S	0	0
			5866	3711	1045	1083	27		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	800	ALA	-	linker	UNP Q7Z406
F	801	SER	-	linker	UNP Q7Z406
G	800	ALA	-	linker	UNP Q7Z406
G	801	SER	-	linker	UNP Q7Z406

- Molecule 3 is a protein called Tropomyosin alpha-3 chain.

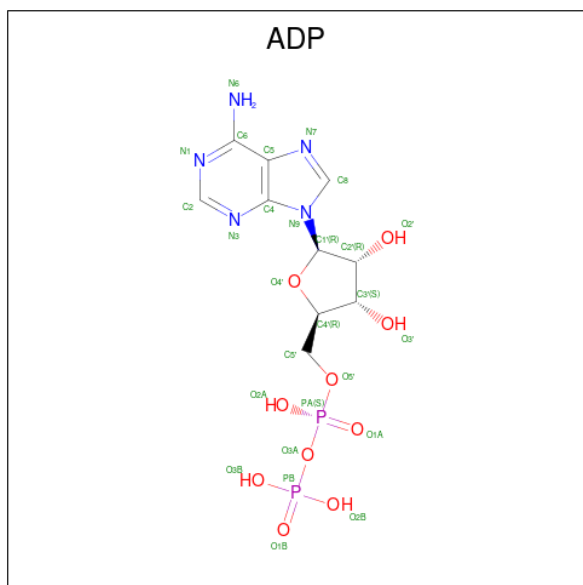
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	135	Total	C	N	O	0	0
			675	405	135	135		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	135	Total	C	N	O	0	0
			675	405	135	135		
3	J	135	Total	C	N	O	0	0
			675	405	135	135		
3	K	135	Total	C	N	O	0	0
			675	405	135	135		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	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	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

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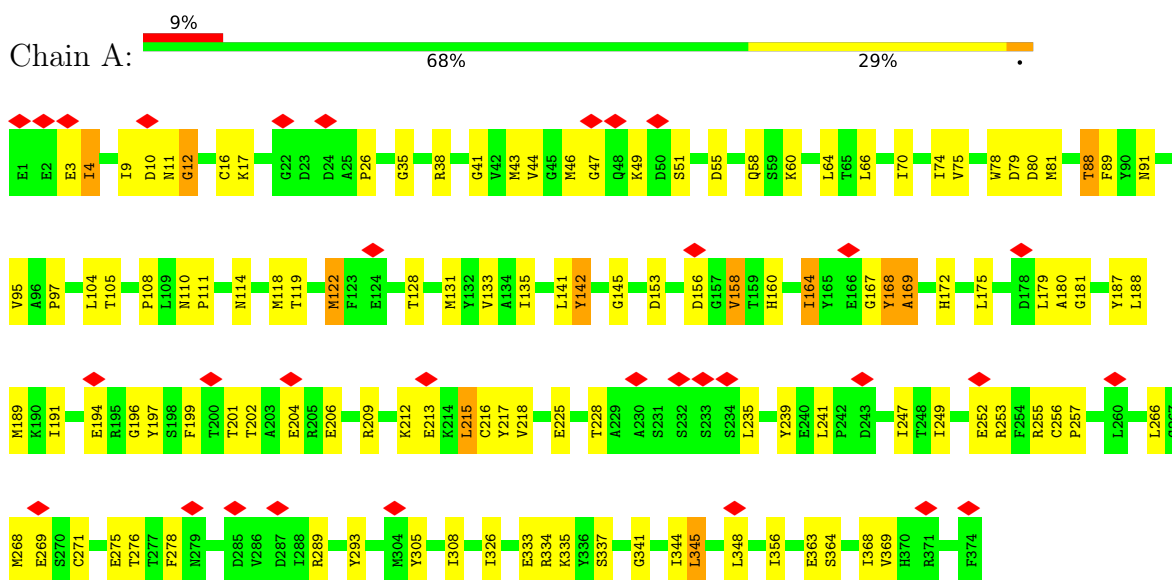
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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total 1	Mg 1	0
5	C	1	Total 1	Mg 1	0
5	D	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0

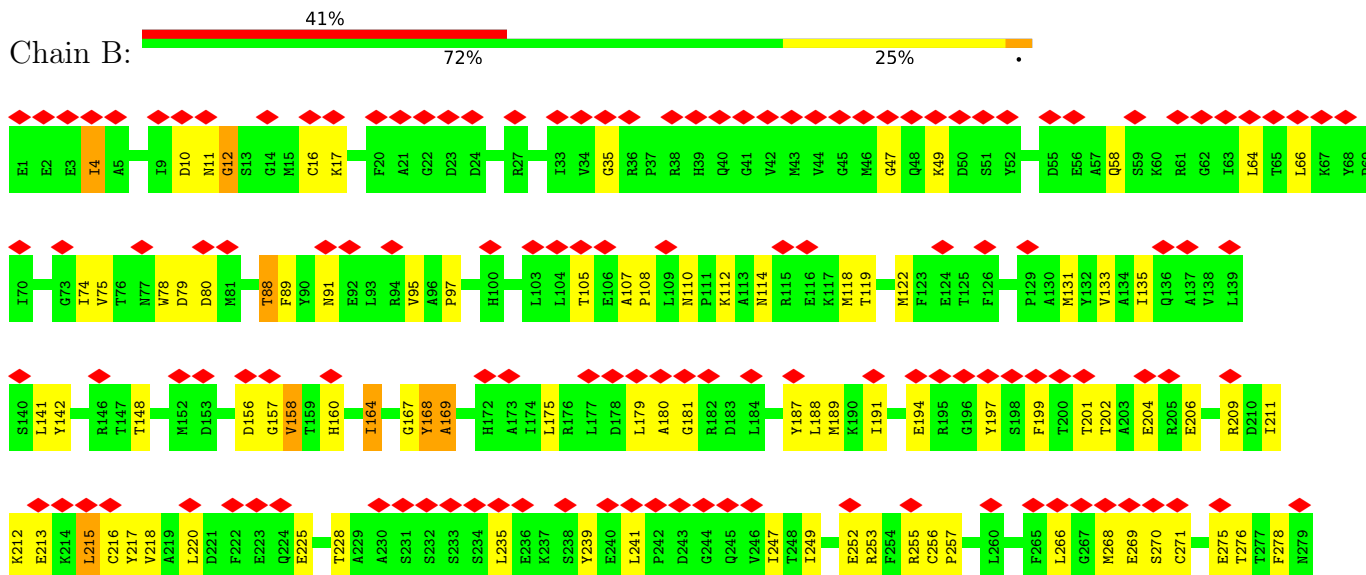
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

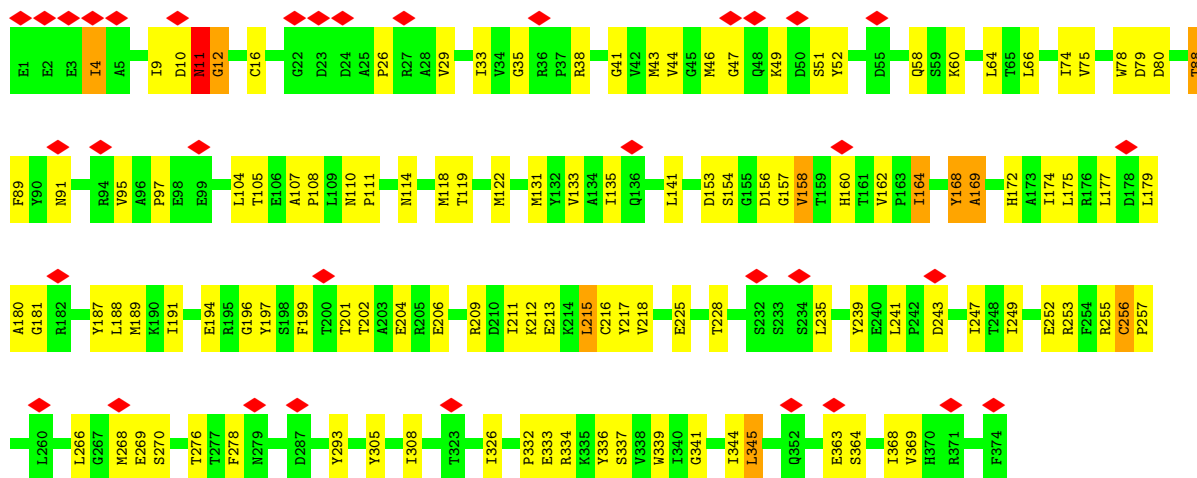
- Molecule 1: Actin, cytoplasmic 2



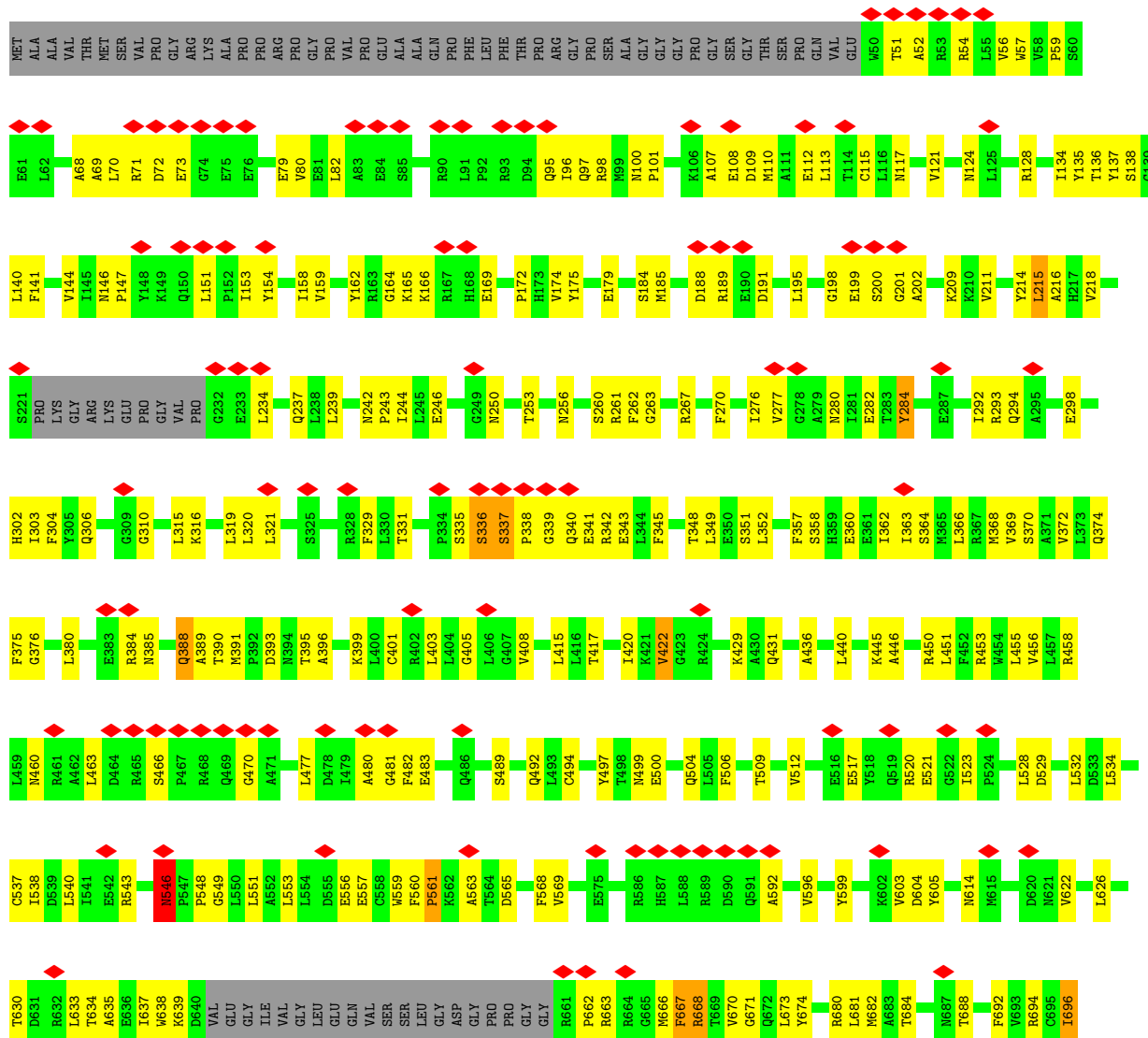
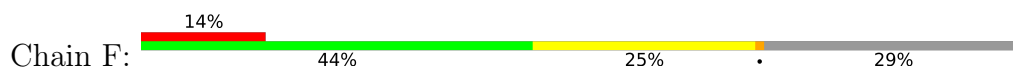
- Molecule 1: Actin, cytoplasmic 2

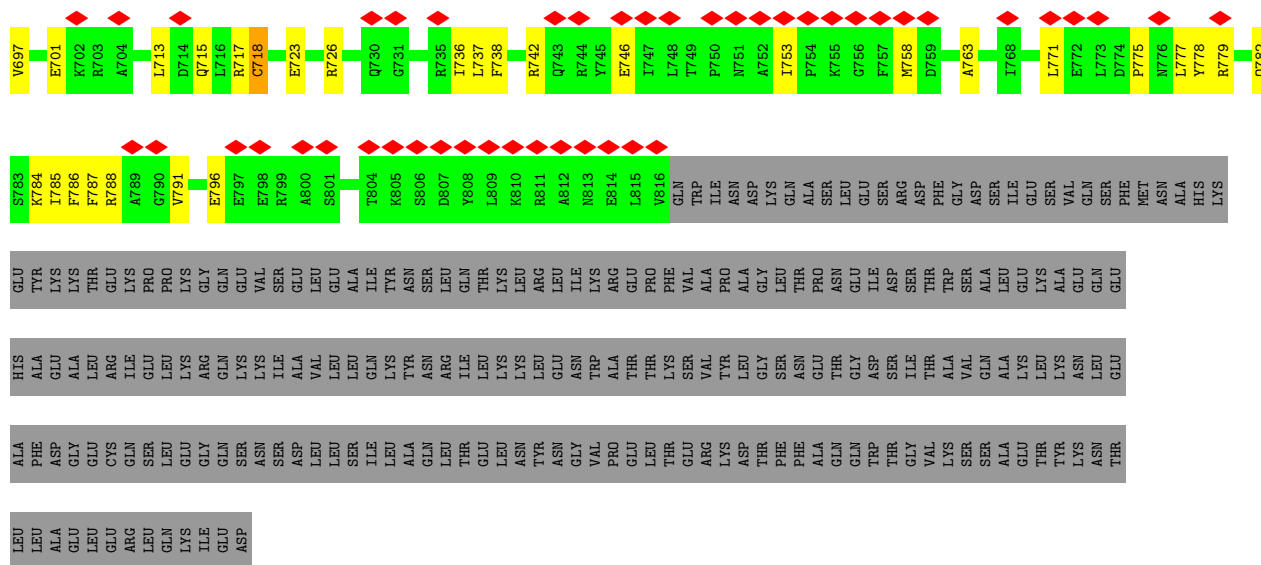




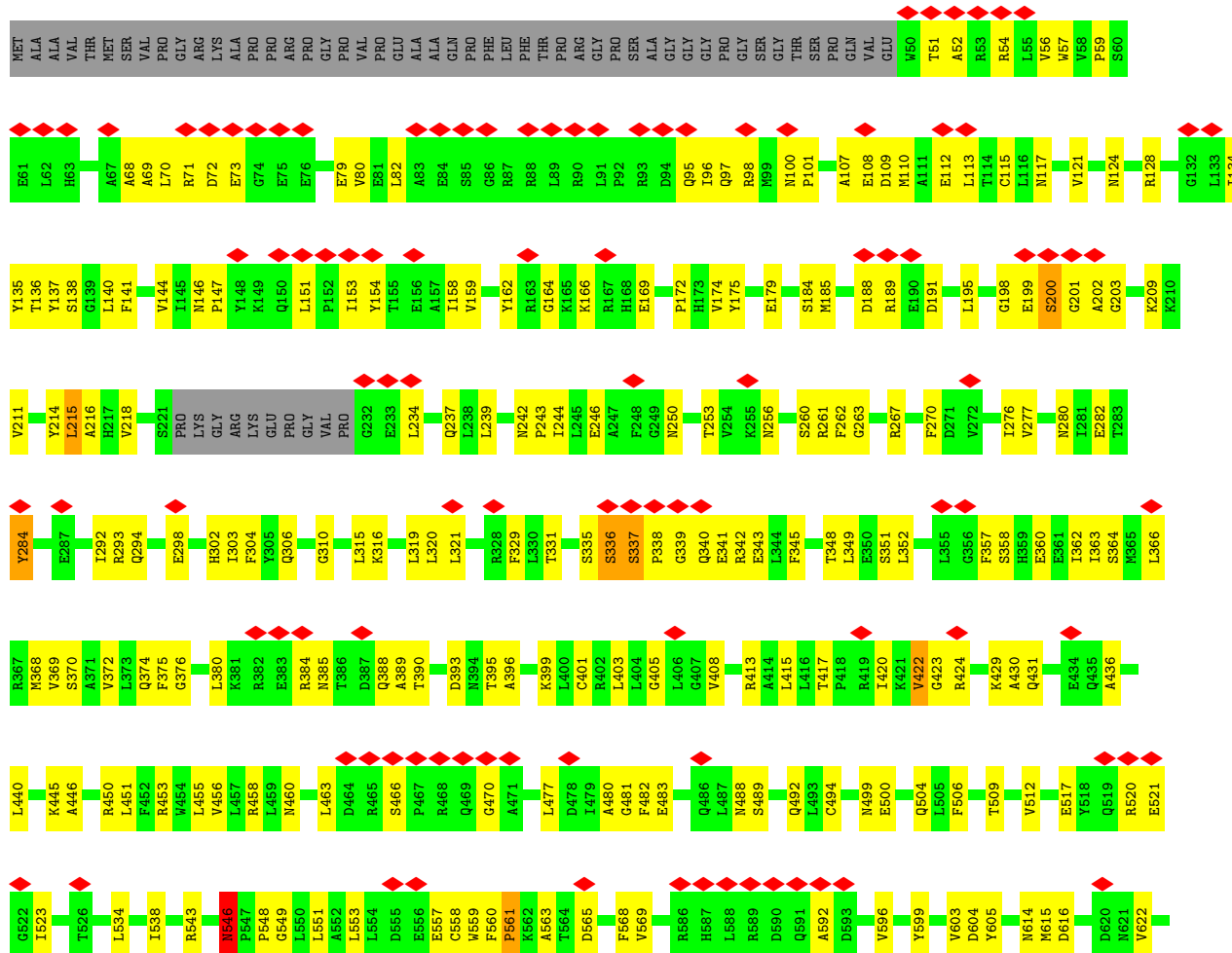


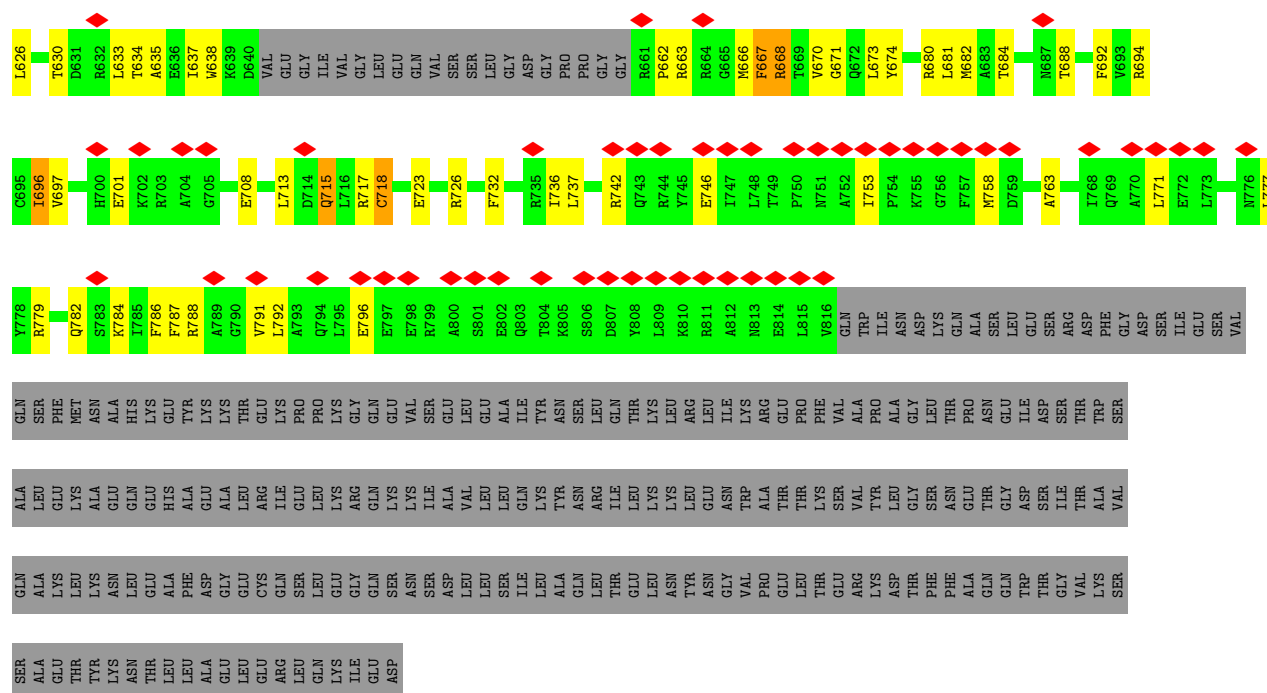
• Molecule 2: Myosin-14,Alpha-actinin A



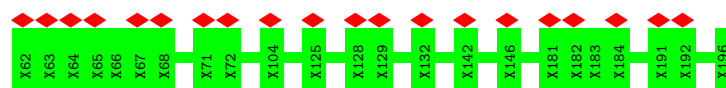


• Molecule 2: Myosin-14,Alpha-actinin A

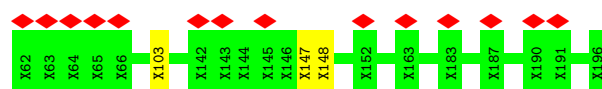




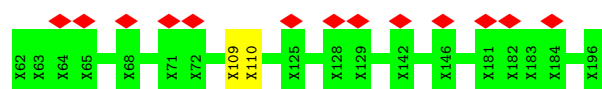
- Molecule 3: Tropomyosin alpha-3 chain



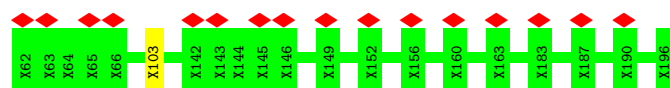
- Molecule 3: Tropomyosin alpha-3 chain



- Molecule 3: Tropomyosin alpha-3 chain



- Molecule 3: Tropomyosin alpha-3 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=166.9°, rise=27.50 Å, axial sym=C1	Depositor
Number of particles used	118000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	16	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.049	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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 > 5$	RMSZ	# $ Z > 5$
1	A	1.13	2/2984 (0.1%)	1.27	8/4039 (0.2%)
1	B	1.05	1/2984 (0.0%)	1.24	8/4039 (0.2%)
1	C	1.07	2/2984 (0.1%)	1.24	6/4039 (0.1%)
1	D	1.10	0/2984	1.27	10/4039 (0.2%)
1	E	1.12	6/2984 (0.2%)	1.27	8/4039 (0.2%)
2	F	1.02	2/5980 (0.0%)	1.21	7/8074 (0.1%)
2	G	1.03	3/5980 (0.1%)	1.22	12/8074 (0.1%)
All	All	1.06	16/26880 (0.1%)	1.24	59/36343 (0.2%)

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	D	0	1
1	E	0	2
2	F	0	2
2	G	0	1
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	MET	C-O	-6.04	1.17	1.24
1	C	122	MET	C-O	-5.63	1.17	1.24
1	C	278	PHE	C-O	-5.56	1.17	1.24
1	E	154	SER	CA-C	-5.49	1.46	1.52
1	A	345	LEU	CA-C	-5.37	1.45	1.52
1	E	345	LEU	CA-C	-5.37	1.45	1.52
2	G	682	MET	CA-C	-5.29	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	682	MET	CA-C	-5.27	1.46	1.52
2	G	622	VAL	C-O	-5.25	1.18	1.24
1	E	122	MET	C-O	-5.16	1.18	1.24
2	G	200	SER	CA-C	5.14	1.59	1.52
1	E	215	LEU	C-O	-5.12	1.18	1.24
1	E	256	CYS	C-O	-5.10	1.19	1.24
1	A	122	MET	C-O	-5.07	1.18	1.24
2	F	622	VAL	C-O	-5.04	1.18	1.24
1	E	12	GLY	N-CA	5.04	1.51	1.45

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	GLY	N-CA-C	-8.96	100.45	112.82
1	B	12	GLY	N-CA-C	-8.89	100.56	112.82
1	D	12	GLY	N-CA-C	-8.85	100.61	112.82
1	A	12	GLY	N-CA-C	-8.84	100.63	112.82
1	D	88	THR	CB-CA-C	-8.33	97.81	110.88
1	E	88	THR	CB-CA-C	-8.06	98.22	110.88
2	F	276	ILE	CB-CA-C	-7.92	101.81	111.08
2	G	276	ILE	CB-CA-C	-7.83	101.91	111.08
1	A	88	THR	CB-CA-C	-7.68	98.83	110.88
1	E	12	GLY	N-CA-C	-7.42	103.05	112.54
1	B	88	THR	CB-CA-C	-7.04	99.83	110.88
1	C	88	THR	CB-CA-C	-6.92	100.01	110.88
1	E	308	ILE	CB-CA-C	-6.88	103.16	111.97
1	A	215	LEU	N-CA-C	6.88	118.78	111.28
1	A	308	ILE	CB-CA-C	-6.56	103.57	111.97
2	G	336	SER	CA-C-N	6.54	133.47	121.70
2	G	336	SER	C-N-CA	6.54	133.47	121.70
1	D	308	ILE	CB-CA-C	-6.49	103.66	111.97
2	F	336	SER	CA-C-N	6.49	133.38	121.70
2	F	336	SER	C-N-CA	6.49	133.38	121.70
1	C	308	ILE	CB-CA-C	-6.43	103.73	111.97
1	B	215	LEU	N-CA-C	6.43	118.28	111.28
1	D	215	LEU	N-CA-C	6.34	118.19	111.28
1	D	91	ASN	N-CA-C	6.26	118.18	111.36
2	G	708	GLU	CA-C-O	6.24	123.34	119.29
1	E	215	LEU	N-CA-C	6.21	118.85	111.33
1	B	308	ILE	CB-CA-C	-6.20	104.04	111.97
1	E	91	ASN	N-CA-C	6.16	118.08	111.36
1	A	91	ASN	N-CA-C	6.13	118.04	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASN	N-CA-C	6.12	118.03	111.36
1	C	91	ASN	N-CA-C	6.01	117.91	111.36
2	G	546	ASN	CA-C-N	-5.97	114.22	120.38
2	G	546	ASN	C-N-CA	-5.97	114.22	120.38
1	E	11	ASN	N-CA-C	5.96	116.95	108.54
1	D	110	ASN	N-CA-C	-5.82	102.27	110.29
1	C	215	LEU	N-CA-C	5.78	118.32	111.33
1	A	110	ASN	N-CA-C	-5.73	102.94	110.39
2	G	203	GLY	N-CA-C	-5.68	105.77	115.08
2	F	546	ASN	CA-C-N	-5.62	114.59	120.38
2	F	546	ASN	C-N-CA	-5.62	114.59	120.38
1	D	364	SER	N-CA-C	5.40	119.87	113.28
1	A	88	THR	N-CA-CB	5.38	117.82	110.01
2	G	701	GLU	CB-CA-C	-5.37	100.70	110.63
1	B	211	ILE	CB-CA-C	-5.36	105.12	111.97
1	E	110	ASN	N-CA-C	-5.28	103.00	110.29
1	E	211	ILE	CB-CA-C	-5.28	105.22	111.97
1	D	88	THR	N-CA-CB	5.22	117.58	110.01
1	D	211	ILE	CB-CA-C	-5.19	105.33	111.97
1	B	110	ASN	N-CA-C	-5.17	103.15	110.29
2	G	413	ARG	CB-CA-C	-5.14	102.27	110.79
2	F	701	GLU	CB-CA-C	-5.12	101.16	110.63
2	G	715	GLN	CB-CA-C	5.12	119.55	110.85
1	A	142	TYR	CB-CA-C	-5.11	102.86	110.88
1	C	211	ILE	CB-CA-C	-5.08	105.47	111.97
1	D	289	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	F	388	GLN	N-CA-C	5.07	118.23	111.75
1	B	364	SER	N-CA-C	5.05	119.44	113.28
2	G	732	PHE	CA-C-N	5.04	124.65	119.05
2	G	732	PHE	C-N-CA	5.04	124.65	119.05

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	336	TYR	Mainchain
1	E	11	ASN	Peptide
1	E	336	TYR	Mainchain
2	F	546	ASN	Peptide
2	F	639	LYS	Peptide
2	G	546	ASN	Peptide

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	2921	0	2890	96	0
1	B	2921	0	2890	75	0
1	C	2921	0	2890	81	0
1	D	2921	0	2890	88	0
1	E	2921	0	2890	85	0
2	F	5866	0	5777	216	0
2	G	5866	0	5775	208	0
3	H	675	0	137	0	0
3	I	675	0	137	9	0
3	J	675	0	137	8	0
3	K	675	0	137	1	0
4	A	27	0	12	3	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	29177	0	26610	807	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 14.

All (807) 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)
2:G:384:ARG:HH12	3:J:110:UNK:CA	1.05	1.57
2:G:384:ARG:NH1	3:J:110:UNK:HA	1.29	1.39
2:G:384:ARG:HD2	3:J:109:UNK:CB	1.73	1.16
2:G:384:ARG:NH1	3:J:110:UNK:CA	1.89	1.13
2:G:384:ARG:CD	3:J:109:UNK:CB	2.32	1.05
2:F:352:LEU:HD13	2:F:362:ILE:HD12	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:352:LEU:HD13	2:G:362:ILE:HD12	1.45	0.96
2:G:384:ARG:NH1	3:J:110:UNK:N	1.95	0.84
2:G:384:ARG:HH12	3:J:110:UNK:HA	0.67	0.83
2:G:294:GLN:HB2	2:G:331:THR:HG21	1.59	0.82
2:F:294:GLN:HB2	2:F:331:THR:HG21	1.59	0.82
2:F:384:ARG:HH12	3:I:148:UNK:HA	1.47	0.80
2:G:250:ASN:ND2	2:G:260:SER:HA	1.97	0.79
2:F:384:ARG:HH22	3:I:148:UNK:HA	1.47	0.78
2:F:341:GLU:O	2:F:343:GLU:N	2.16	0.77
1:D:141:LEU:HD22	1:D:164:ILE:HG21	1.67	0.77
1:C:141:LEU:HD22	1:C:164:ILE:HG21	1.66	0.77
1:A:141:LEU:HD22	1:A:164:ILE:HG21	1.66	0.76
1:B:141:LEU:HD22	1:B:164:ILE:HG21	1.66	0.76
2:F:250:ASN:ND2	2:F:260:SER:HA	1.99	0.76
2:G:200:SER:HA	2:G:256:ASN:HD22	1.49	0.76
2:G:341:GLU:O	2:G:343:GLU:N	2.15	0.76
1:A:215:LEU:O	1:A:253:ARG:HD3	1.86	0.75
2:F:200:SER:HA	2:F:256:ASN:HD22	1.49	0.75
1:B:215:LEU:O	1:B:253:ARG:HD3	1.85	0.75
2:F:453:ARG:O	2:F:456:VAL:HG12	1.86	0.75
2:G:483:GLU:HB2	2:G:492:GLN:HE22	1.52	0.75
2:G:453:ARG:O	2:G:456:VAL:HG12	1.87	0.75
1:E:141:LEU:HD22	1:E:164:ILE:HG21	1.69	0.74
1:E:215:LEU:O	1:E:253:ARG:HD3	1.87	0.74
2:F:483:GLU:HB2	2:F:492:GLN:HE22	1.52	0.74
2:F:216:ALA:HB2	2:F:234:LEU:HD21	1.69	0.73
1:D:215:LEU:O	1:D:253:ARG:HD3	1.88	0.73
1:A:168:TYR:HA	1:C:41:GLY:HA2	1.71	0.72
1:A:41:GLY:HA2	1:B:168:TYR:HA	1.69	0.72
1:A:44:VAL:N	1:B:142:TYR:OH	2.22	0.72
1:C:215:LEU:O	1:C:253:ARG:HD3	1.89	0.72
1:A:46:MET:SD	1:B:167:GLY:HA3	2.30	0.72
2:G:216:ALA:HB2	2:G:234:LEU:HD21	1.71	0.72
2:G:134:ILE:HG23	2:G:135:TYR:CD2	2.26	0.71
2:G:405:GLY:HA2	2:G:630:THR:HG22	1.73	0.71
1:E:119:THR:HG21	1:E:369:VAL:HG22	1.73	0.70
2:F:405:GLY:HA2	2:F:630:THR:HG22	1.73	0.70
2:F:134:ILE:HG23	2:F:135:TYR:CD2	2.25	0.70
2:G:56:VAL:HG12	2:G:96:ILE:HG22	1.73	0.70
1:D:119:THR:HG21	1:D:369:VAL:HG22	1.73	0.69
1:D:142:TYR:OH	1:E:44:VAL:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:VAL:HG12	2:F:96:ILE:HG22	1.72	0.69
1:B:119:THR:HG21	1:B:369:VAL:HG22	1.74	0.68
1:A:119:THR:HG21	1:A:369:VAL:HG22	1.74	0.68
2:F:200:SER:HB2	2:F:201:GLY:HA3	1.76	0.68
1:C:156:ASP:O	1:C:180:ALA:HB1	1.94	0.67
1:D:156:ASP:O	1:D:180:ALA:HB1	1.95	0.67
2:F:98:ARG:HB2	2:F:115:CYS:SG	2.34	0.67
1:D:108:PRO:HA	1:D:135:ILE:HD11	1.76	0.67
2:G:200:SER:HB2	2:G:201:GLY:HA3	1.76	0.67
2:G:668:ARG:HE	2:G:673:LEU:HD11	1.59	0.67
2:G:98:ARG:HB2	2:G:115:CYS:SG	2.34	0.67
1:D:168:TYR:HA	1:E:41:GLY:HA2	1.77	0.67
2:G:316:LYS:HG3	2:G:321:LEU:HB2	1.77	0.67
1:A:156:ASP:O	1:A:180:ALA:HB1	1.94	0.66
1:A:44:VAL:H	1:B:142:TYR:HH	1.41	0.66
2:G:101:PRO:HG2	2:G:796:GLU:HG2	1.78	0.66
1:A:142:TYR:OH	1:C:44:VAL:N	2.28	0.66
1:C:119:THR:HG21	1:C:369:VAL:HG22	1.76	0.66
2:F:101:PRO:HG2	2:F:796:GLU:HG2	1.78	0.66
1:A:256:CYS:HB3	1:A:257:PRO:HD3	1.77	0.66
1:B:108:PRO:HA	1:B:135:ILE:HD11	1.78	0.66
2:F:668:ARG:HE	2:F:673:LEU:HD11	1.60	0.66
1:E:156:ASP:O	1:E:180:ALA:HB1	1.95	0.66
2:G:614:ASN:HA	2:G:670:VAL:HG22	1.78	0.66
1:B:156:ASP:O	1:B:180:ALA:HB1	1.95	0.66
1:C:108:PRO:HA	1:C:135:ILE:HD11	1.77	0.65
2:F:310:GLY:HA2	2:F:342:ARG:HA	1.76	0.65
1:A:108:PRO:HA	1:A:135:ILE:HD11	1.78	0.65
1:E:58:GLN:NE2	1:E:206:GLU:OE1	2.30	0.65
1:D:293:TYR:HB3	1:D:326:ILE:HD12	1.79	0.65
1:E:293:TYR:HB3	1:E:326:ILE:HD12	1.79	0.65
1:E:108:PRO:HA	1:E:135:ILE:HD11	1.78	0.65
2:F:215:LEU:HD21	2:F:270:PHE:CE1	2.31	0.65
2:G:310:GLY:HA2	2:G:342:ARG:HA	1.77	0.64
2:F:543:ARG:NE	2:F:546:ASN:OD1	2.17	0.64
1:A:305:TYR:CD1	4:A:401:ADP:H2	2.15	0.64
2:F:384:ARG:NH2	3:I:148:UNK:HA	2.11	0.64
2:G:198:GLY:HA3	2:G:481:GLY:N	2.13	0.64
2:F:316:LYS:HG3	2:F:321:LEU:HB2	1.78	0.64
2:F:384:ARG:NH1	3:I:148:UNK:HA	2.11	0.64
2:F:384:ARG:HH22	3:I:148:UNK:CA	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:215:LEU:HD21	2:G:270:PHE:CE1	2.32	0.64
1:A:293:TYR:HB3	1:A:326:ILE:HD12	1.80	0.63
1:D:305:TYR:CD1	4:D:401:ADP:H2	2.16	0.63
1:B:191:ILE:O	1:B:194:GLU:HG2	1.98	0.63
1:C:191:ILE:O	1:C:194:GLU:HG2	1.99	0.63
2:F:110:MET:HE1	2:F:121:VAL:HG13	1.80	0.63
2:F:198:GLY:HA3	2:F:481:GLY:N	2.14	0.63
2:G:543:ARG:NE	2:G:546:ASN:OD1	2.17	0.63
1:B:187:TYR:HB2	1:B:266:LEU:HD21	1.81	0.63
1:D:191:ILE:O	1:D:194:GLU:HG2	1.99	0.63
1:A:191:ILE:O	1:A:194:GLU:HG2	1.99	0.62
1:C:293:TYR:HB3	1:C:326:ILE:HD12	1.81	0.62
2:F:97:GLN:HB3	2:F:117:ASN:ND2	2.15	0.62
1:C:141:LEU:CD2	1:C:164:ILE:HG21	2.29	0.62
1:D:256:CYS:HB3	1:D:257:PRO:HD3	1.82	0.62
1:A:187:TYR:HB2	1:A:266:LEU:HD21	1.81	0.62
2:G:110:MET:HE1	2:G:121:VAL:HG13	1.80	0.62
1:B:305:TYR:CD1	4:B:401:ADP:H2	2.17	0.62
2:G:282:GLU:OE1	2:G:284:TYR:OH	2.14	0.62
1:A:293:TYR:HB3	1:A:326:ILE:CD1	2.30	0.62
1:B:141:LEU:CD2	1:B:164:ILE:HG21	2.29	0.62
1:E:305:TYR:CD1	4:E:401:ADP:H2	2.18	0.62
1:A:141:LEU:CD2	1:A:164:ILE:HG21	2.30	0.61
1:B:256:CYS:HB3	1:B:257:PRO:HD3	1.83	0.61
1:C:305:TYR:CD1	4:C:401:ADP:H2	2.19	0.61
1:E:75:VAL:CG2	1:E:78:TRP:CZ2	2.83	0.61
1:A:191:ILE:HG23	1:A:252:GLU:HG3	1.82	0.61
1:B:293:TYR:HB3	1:B:326:ILE:HD12	1.82	0.61
1:C:293:TYR:HB3	1:C:326:ILE:CD1	2.31	0.61
2:G:97:GLN:HB3	2:G:117:ASN:ND2	2.15	0.61
1:D:293:TYR:HB3	1:D:326:ILE:CD1	2.31	0.61
1:E:35:GLY:O	1:E:51:SER:OG	2.15	0.61
1:D:75:VAL:CG2	1:D:78:TRP:CZ2	2.84	0.61
1:D:141:LEU:CD2	1:D:164:ILE:HG21	2.31	0.61
1:E:293:TYR:HB3	1:E:326:ILE:CD1	2.31	0.61
2:F:315:LEU:HD23	2:F:319:LEU:HD13	1.83	0.61
2:F:614:ASN:HA	2:F:670:VAL:HG22	1.82	0.60
2:F:134:ILE:HG12	2:F:144:VAL:HG23	1.82	0.60
1:E:141:LEU:CD2	1:E:164:ILE:HG21	2.31	0.60
1:E:191:ILE:HG23	1:E:252:GLU:HG3	1.84	0.60
2:G:315:LEU:HD23	2:G:319:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:548:PRO:CG	2:F:553:LEU:HD21	2.31	0.60
2:G:548:PRO:CG	2:G:553:LEU:HD21	2.32	0.60
1:B:293:TYR:HB3	1:B:326:ILE:CD1	2.32	0.60
1:C:187:TYR:HB2	1:C:266:LEU:HD21	1.83	0.60
1:A:58:GLN:NE2	1:A:206:GLU:OE1	2.34	0.60
1:C:256:CYS:HB3	1:C:257:PRO:HD3	1.84	0.60
1:D:333:GLU:OE1	2:G:429:LYS:HG3	2.01	0.60
1:E:187:TYR:HB2	1:E:266:LEU:HD21	1.85	0.59
2:G:134:ILE:HD12	2:G:147:PRO:HD3	1.84	0.59
2:G:134:ILE:HG12	2:G:144:VAL:HG23	1.83	0.59
2:G:200:SER:HA	2:G:256:ASN:ND2	2.17	0.59
2:G:667:PHE:O	2:G:668:ARG:C	2.45	0.59
1:D:167:GLY:HA3	1:E:46:MET:SD	2.42	0.59
2:F:504:GLN:HA	2:F:534:LEU:HD12	1.85	0.59
2:F:134:ILE:HD12	2:F:147:PRO:HD3	1.85	0.58
2:G:339:GLY:O	2:G:341:GLU:N	2.34	0.58
2:G:195:LEU:HD22	2:G:477:LEU:HD23	1.86	0.58
1:A:167:GLY:HA3	1:C:46:MET:SD	2.43	0.58
2:G:666:MET:O	2:G:667:PHE:C	2.46	0.58
1:C:75:VAL:CG2	1:C:78:TRP:CZ2	2.86	0.58
2:F:339:GLY:O	2:F:341:GLU:N	2.36	0.58
1:B:35:GLY:HA3	1:B:64:LEU:HD23	1.85	0.58
2:G:723:GLU:HA	2:G:726:ARG:HG2	1.85	0.58
1:C:191:ILE:HG23	1:C:252:GLU:HG3	1.85	0.58
1:D:35:GLY:HA3	1:D:64:LEU:HD23	1.86	0.58
1:D:187:TYR:HB2	1:D:266:LEU:HD21	1.86	0.58
1:E:191:ILE:O	1:E:194:GLU:HG2	2.04	0.58
2:G:787:PHE:HB3	2:G:791:VAL:HG21	1.85	0.58
2:F:200:SER:HA	2:F:256:ASN:ND2	2.17	0.57
1:C:35:GLY:HA3	1:C:64:LEU:HD23	1.84	0.57
2:F:302:HIS:O	2:F:306:GLN:HG2	2.04	0.57
1:A:35:GLY:HA3	1:A:64:LEU:HD23	1.85	0.57
1:E:35:GLY:HA3	1:E:64:LEU:HD23	1.86	0.57
2:G:302:HIS:O	2:G:306:GLN:HG2	2.04	0.57
1:D:58:GLN:NE2	1:D:206:GLU:OE1	2.36	0.57
2:F:195:LEU:HD22	2:F:477:LEU:HD23	1.86	0.57
1:B:191:ILE:HG23	1:B:252:GLU:HG3	1.87	0.57
1:B:75:VAL:CG2	1:B:78:TRP:CZ2	2.87	0.57
1:D:191:ILE:HG23	1:D:252:GLU:HG3	1.87	0.57
1:E:256:CYS:HB3	1:E:257:PRO:HD3	1.87	0.57
1:A:75:VAL:CG2	1:A:78:TRP:CZ2	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:VAL:HG22	1:E:257:PRO:HB2	1.87	0.56
1:A:333:GLU:OE1	2:F:429:LYS:HG3	2.05	0.56
1:E:75:VAL:HG21	1:E:78:TRP:CZ2	2.41	0.56
2:F:282:GLU:OE1	2:F:284:TYR:OH	2.14	0.56
1:A:218:VAL:HG22	1:A:257:PRO:HB2	1.87	0.56
2:G:200:SER:OG	2:G:202:ALA:N	2.39	0.56
2:F:560:PHE:CD1	2:F:561:PRO:HD2	2.40	0.56
2:F:667:PHE:O	2:F:668:ARG:C	2.49	0.56
1:D:75:VAL:HG21	1:D:78:TRP:CZ2	2.41	0.56
1:D:88:THR:OG1	1:D:89:PHE:N	2.39	0.56
1:B:269:GLU:HG2	1:D:38:ARG:HD3	1.87	0.56
2:F:666:MET:O	2:F:667:PHE:C	2.47	0.56
2:F:506:PHE:HD1	2:F:692:PHE:CD2	2.24	0.56
2:G:482:PHE:HB3	2:G:718:CYS:HB2	1.88	0.56
2:F:68:ALA:HB1	2:F:80:VAL:HG12	1.87	0.56
2:F:200:SER:OG	2:F:202:ALA:N	2.38	0.56
2:F:723:GLU:HA	2:F:726:ARG:HG2	1.86	0.56
2:F:787:PHE:HB3	2:F:791:VAL:HG21	1.86	0.56
1:B:58:GLN:NE2	1:B:206:GLU:OE1	2.40	0.55
1:B:194:GLU:OE2	1:B:255:ARG:NH2	2.39	0.55
2:G:787:PHE:HB3	2:G:791:VAL:CG2	2.37	0.55
2:F:374:GLN:HE22	2:F:399:LYS:HE2	1.71	0.55
2:F:787:PHE:HB3	2:F:791:VAL:CG2	2.37	0.55
1:E:194:GLU:OE2	1:E:255:ARG:NH2	2.39	0.55
1:A:194:GLU:OE2	1:A:255:ARG:NH2	2.39	0.55
2:G:506:PHE:HD1	2:G:692:PHE:CD2	2.25	0.55
1:D:194:GLU:OE2	1:D:255:ARG:NH2	2.40	0.55
2:G:244:ILE:HG22	2:G:455:LEU:HD21	1.89	0.55
2:G:124:ASN:O	2:G:128:ARG:HG2	2.07	0.55
2:G:560:PHE:CD1	2:G:561:PRO:HD2	2.42	0.55
1:C:194:GLU:OE2	1:C:255:ARG:NH2	2.40	0.55
2:F:294:GLN:HB2	2:F:331:THR:CG2	2.34	0.55
2:G:59:PRO:HG2	2:G:95:GLN:HB3	1.89	0.55
2:G:68:ALA:HB1	2:G:80:VAL:HG12	1.87	0.55
1:B:220:LEU:HD23	3:I:103:UNK:CB	2.37	0.54
2:F:124:ASN:O	2:F:128:ARG:HG2	2.07	0.54
2:G:191:ASP:HB2	2:G:688:THR:HG22	1.88	0.54
1:E:88:THR:OG1	1:E:89:PHE:N	2.39	0.54
1:C:75:VAL:HG21	1:C:78:TRP:CZ2	2.42	0.54
1:C:168:TYR:O	1:C:169:ALA:HB2	2.08	0.54
1:D:145:GLY:C	2:G:561:PRO:HB3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:VAL:HG12	1:E:160:HIS:CE1	2.42	0.54
2:F:244:ILE:HG22	2:F:455:LEU:HD21	1.90	0.54
1:B:168:TYR:O	1:B:169:ALA:HB2	2.08	0.54
2:F:200:SER:HB2	2:F:201:GLY:CA	2.38	0.54
2:G:200:SER:HB2	2:G:201:GLY:CA	2.38	0.54
1:A:75:VAL:HG21	1:A:78:TRP:CZ2	2.43	0.54
1:B:364:SER:HB2	1:B:368:ILE:HG21	1.90	0.54
1:C:364:SER:HB2	1:C:368:ILE:HG21	1.90	0.54
1:D:75:VAL:HG21	1:D:78:TRP:CH2	2.43	0.54
2:F:348:THR:O	2:F:351:SER:OG	2.22	0.54
2:G:504:GLN:HA	2:G:534:LEU:HD12	1.89	0.54
1:A:364:SER:HB2	1:A:368:ILE:HG21	1.90	0.54
2:F:191:ASP:HB2	2:F:688:THR:HG22	1.90	0.54
1:A:216:CYS:HA	1:A:253:ARG:HG2	1.90	0.54
1:D:158:VAL:HG12	1:D:160:HIS:CE1	2.43	0.54
2:F:59:PRO:HG2	2:F:95:GLN:HB3	1.88	0.53
2:F:107:ALA:O	2:F:128:ARG:NH1	2.41	0.53
2:G:521:GLU:O	2:G:782:GLN:HG2	2.08	0.53
1:E:75:VAL:HG21	1:E:78:TRP:CH2	2.43	0.53
1:E:364:SER:HB2	1:E:368:ILE:HG21	1.90	0.53
2:G:736:ILE:HG22	2:G:737:LEU:O	2.08	0.53
1:D:218:VAL:HG22	1:D:257:PRO:HB2	1.90	0.53
2:G:117:ASN:O	2:G:121:VAL:HG23	2.08	0.53
1:A:158:VAL:HG12	1:A:160:HIS:CE1	2.43	0.53
1:B:225:GLU:HA	1:B:228:THR:HG22	1.91	0.53
2:G:336:SER:CB	2:G:338:PRO:HD2	2.38	0.53
2:F:521:GLU:O	2:F:782:GLN:HG2	2.09	0.53
2:G:319:LEU:HD21	2:G:366:LEU:HB3	1.91	0.53
1:E:216:CYS:HA	1:E:253:ARG:HG2	1.91	0.53
2:F:117:ASN:O	2:F:121:VAL:HG23	2.07	0.53
2:F:153:ILE:HG22	2:F:154:TYR:H	1.74	0.53
2:G:153:ILE:HG22	2:G:154:TYR:N	2.23	0.53
1:B:75:VAL:HG21	1:B:78:TRP:CZ2	2.44	0.53
1:B:218:VAL:HG22	1:B:257:PRO:HB2	1.91	0.53
2:F:319:LEU:HD21	2:F:366:LEU:HB3	1.91	0.53
2:G:107:ALA:O	2:G:128:ARG:NH1	2.41	0.53
1:D:201:THR:HB	1:D:204:GLU:OE1	2.09	0.53
1:E:247:ILE:HG22	1:E:249:ILE:HG23	1.91	0.53
2:F:336:SER:CB	2:F:338:PRO:HD2	2.39	0.53
2:F:482:PHE:HB3	2:F:718:CYS:HB2	1.89	0.53
2:G:292:ILE:HD13	2:G:329:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:TYR:O	1:D:169:ALA:HB2	2.09	0.53
2:F:153:ILE:HG22	2:F:154:TYR:N	2.23	0.53
2:F:559:TRP:CE2	2:F:667:PHE:HD1	2.27	0.53
2:G:277:VAL:HG11	2:G:470:GLY:O	2.08	0.53
1:B:112:LYS:HG3	1:D:194:GLU:HB2	1.90	0.53
1:C:218:VAL:HG22	1:C:257:PRO:HB2	1.91	0.53
1:D:364:SER:HB2	1:D:368:ILE:HG21	1.91	0.53
1:E:58:GLN:HE22	1:E:206:GLU:CD	2.16	0.53
1:E:131:MET:HE2	1:E:133:VAL:HG13	1.90	0.53
1:E:168:TYR:O	1:E:169:ALA:HB2	2.09	0.53
2:F:237:GLN:HE21	2:F:463:LEU:HD23	1.74	0.53
2:F:736:ILE:HG22	2:F:737:LEU:O	2.08	0.53
2:G:70:LEU:HD21	2:G:73:GLU:HB3	1.91	0.53
2:G:237:GLN:HE21	2:G:463:LEU:HD23	1.73	0.53
2:G:713:LEU:O	2:G:717:ARG:HG3	2.08	0.53
1:C:58:GLN:NE2	1:C:206:GLU:OE1	2.38	0.52
1:C:225:GLU:HA	1:C:228:THR:HG22	1.90	0.52
2:F:292:ILE:HD13	2:F:329:PHE:CE2	2.44	0.52
2:G:68:ALA:HB2	2:G:82:LEU:HD23	1.90	0.52
2:G:348:THR:O	2:G:351:SER:OG	2.22	0.52
1:A:38:ARG:HD3	1:D:269:GLU:HG2	1.91	0.52
1:A:43:MET:HG3	1:B:167:GLY:HA2	1.90	0.52
1:C:75:VAL:HG21	1:C:78:TRP:CH2	2.44	0.52
2:F:360:GLU:O	2:F:363:ILE:HG22	2.09	0.52
1:B:75:VAL:HG21	1:B:78:TRP:CH2	2.45	0.52
2:F:68:ALA:HB2	2:F:82:LEU:HD23	1.90	0.52
2:F:384:ARG:HH12	3:I:148:UNK:CA	2.20	0.52
1:A:225:GLU:HA	1:A:228:THR:HG22	1.92	0.52
1:D:131:MET:HE2	1:D:133:VAL:HG13	1.90	0.52
1:E:119:THR:HG21	1:E:369:VAL:CG2	2.38	0.52
2:F:500:GLU:HG2	2:F:538:ILE:HG12	1.92	0.52
2:G:360:GLU:O	2:G:363:ILE:HG22	2.10	0.52
2:G:500:GLU:HG2	2:G:538:ILE:HG12	1.91	0.52
1:D:333:GLU:OE1	2:G:429:LYS:CG	2.58	0.52
2:F:369:VAL:O	2:F:372:VAL:HG12	2.09	0.52
2:G:153:ILE:HG22	2:G:154:TYR:H	1.74	0.52
1:A:168:TYR:O	1:A:169:ALA:HB2	2.10	0.52
1:D:225:GLU:HA	1:D:228:THR:HG22	1.92	0.52
2:F:357:PHE:CE1	2:F:458:ARG:HG3	2.45	0.52
1:D:217:TYR:CE2	1:D:253:ARG:HD2	2.45	0.52
1:E:225:GLU:HA	1:E:228:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:LEU:HD21	2:F:73:GLU:HB3	1.91	0.51
2:F:405:GLY:CA	2:F:630:THR:HG22	2.39	0.51
1:B:158:VAL:HG12	1:B:160:HIS:CE1	2.45	0.51
1:C:196:GLY:HA2	1:E:111:PRO:HG3	1.91	0.51
2:F:277:VAL:HG11	2:F:470:GLY:O	2.09	0.51
1:C:158:VAL:HG12	1:C:160:HIS:CE1	2.45	0.51
2:F:560:PHE:CG	2:F:561:PRO:HD2	2.46	0.51
2:G:244:ILE:HD12	2:G:352:LEU:HD23	1.92	0.51
1:A:119:THR:HG21	1:A:369:VAL:CG2	2.40	0.51
1:C:114:ASN:O	1:C:118:MET:HB2	2.10	0.51
2:G:294:GLN:HB2	2:G:331:THR:CG2	2.34	0.51
2:G:405:GLY:CA	2:G:630:THR:HG22	2.39	0.51
2:G:110:MET:CE	2:G:121:VAL:HA	2.40	0.51
2:G:292:ILE:HG21	2:G:445:LYS:HD2	1.90	0.51
1:C:79:ASP:OD1	1:C:80:ASP:N	2.44	0.51
2:G:680:ARG:O	2:G:684:THR:HG23	2.10	0.51
2:F:244:ILE:HD12	2:F:352:LEU:HD23	1.91	0.51
2:F:523:ILE:HD12	2:F:786:PHE:CE2	2.45	0.51
2:G:523:ILE:HD12	2:G:786:PHE:CE2	2.46	0.51
2:G:483:GLU:HB2	2:G:492:GLN:NE2	2.24	0.51
2:G:737:LEU:HD23	2:G:784:LYS:HG2	1.93	0.51
1:B:131:MET:HE2	1:B:133:VAL:HG13	1.91	0.51
1:E:119:THR:HG22	1:E:131:MET:SD	2.51	0.51
2:F:483:GLU:HB2	2:F:492:GLN:NE2	2.23	0.51
2:F:737:LEU:HD23	2:F:784:LYS:HG2	1.93	0.51
2:G:368:MET:HG3	2:G:451:LEU:HD22	1.93	0.51
2:G:69:ALA:O	2:G:80:VAL:HG13	2.11	0.50
2:G:415:LEU:CD2	2:G:440:LEU:HD21	2.41	0.50
1:C:131:MET:HE2	1:C:133:VAL:HG13	1.91	0.50
1:D:247:ILE:HG22	1:D:249:ILE:HG23	1.94	0.50
1:E:114:ASN:O	1:E:118:MET:HB2	2.11	0.50
2:F:450:ARG:HB3	2:F:637:ILE:CG2	2.41	0.50
1:B:216:CYS:HA	1:B:253:ARG:HG2	1.94	0.50
2:F:368:MET:HG3	2:F:451:LEU:HD22	1.94	0.50
2:F:69:ALA:O	2:F:80:VAL:HG13	2.10	0.50
2:F:215:LEU:HD21	2:F:270:PHE:CZ	2.46	0.50
2:F:680:ARG:O	2:F:684:THR:HG23	2.11	0.50
1:C:35:GLY:O	1:C:51:SER:OG	2.18	0.50
1:C:119:THR:HG22	1:C:131:MET:SD	2.52	0.50
1:A:201:THR:HB	1:A:204:GLU:OE1	2.10	0.50
1:D:35:GLY:O	1:D:51:SER:OG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:LEU:CD1	2:F:362:ILE:HD12	2.30	0.50
2:F:415:LEU:CD2	2:F:440:LEU:HD21	2.40	0.50
2:G:517:GLU:OE1	2:G:520:ARG:NH2	2.34	0.50
2:F:110:MET:CE	2:F:121:VAL:HA	2.41	0.50
1:A:75:VAL:HG21	1:A:78:TRP:CH2	2.47	0.49
1:C:217:TYR:CE2	1:C:253:ARG:HD2	2.47	0.49
2:F:174:VAL:HG11	2:F:211:VAL:HG22	1.94	0.49
1:E:201:THR:HB	1:E:204:GLU:OE1	2.12	0.49
1:E:217:TYR:CE2	1:E:253:ARG:HD2	2.47	0.49
2:F:713:LEU:O	2:F:717:ARG:HG3	2.11	0.49
2:G:209:LYS:CD	2:G:239:LEU:HD23	2.43	0.49
2:G:242:ASN:O	2:G:246:GLU:HB2	2.12	0.49
1:B:88:THR:OG1	1:B:89:PHE:N	2.46	0.49
1:B:217:TYR:CE2	1:B:253:ARG:HD2	2.47	0.49
1:B:119:THR:HG21	1:B:369:VAL:CG2	2.40	0.49
1:B:201:THR:HB	1:B:204:GLU:OE1	2.12	0.49
1:C:216:CYS:HA	1:C:253:ARG:HG2	1.95	0.49
1:D:216:CYS:HA	1:D:253:ARG:HG2	1.95	0.49
2:F:57:TRP:O	2:F:96:ILE:HG23	2.13	0.49
2:F:244:ILE:HD12	2:F:352:LEU:CD2	2.42	0.49
2:F:696:ILE:HG23	2:F:715:GLN:OE1	2.13	0.49
1:A:58:GLN:HE22	1:A:206:GLU:CD	2.21	0.49
1:A:88:THR:OG1	1:A:89:PHE:N	2.44	0.49
2:F:670:VAL:HG23	2:F:671:GLY:N	2.28	0.49
1:D:175:LEU:HD23	1:D:276:THR:HB	1.95	0.49
2:F:209:LYS:CD	2:F:239:LEU:HD23	2.42	0.49
2:G:100:ASN:ND2	2:G:113:LEU:HD23	2.28	0.49
2:G:374:GLN:HE22	2:G:399:LYS:HE2	1.78	0.49
1:A:114:ASN:O	1:A:118:MET:HB2	2.12	0.48
2:F:100:ASN:ND2	2:F:113:LEU:HD23	2.28	0.48
2:F:499:ASN:HB3	2:F:599:TYR:OH	2.12	0.48
2:G:174:VAL:HG11	2:G:211:VAL:HG22	1.95	0.48
2:F:292:ILE:HG23	2:F:293:ARG:HG2	1.94	0.48
2:G:450:ARG:HB3	2:G:637:ILE:CG2	2.43	0.48
2:G:548:PRO:HG2	2:G:553:LEU:HD21	1.95	0.48
2:G:670:VAL:HG23	2:G:671:GLY:N	2.28	0.48
2:G:697:VAL:HG22	2:G:715:GLN:HE22	1.78	0.48
2:G:215:LEU:HD21	2:G:270:PHE:CZ	2.48	0.48
2:G:506:PHE:HD1	2:G:692:PHE:CE2	2.31	0.48
2:F:395:THR:HG23	2:F:396:ALA:N	2.29	0.48
2:G:292:ILE:HG23	2:G:293:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:388:GLN:O	2:G:389:ALA:HB3	2.14	0.48
2:G:499:ASN:HB3	2:G:599:TYR:OH	2.14	0.48
1:A:241:LEU:HD13	1:A:247:ILE:HG12	1.96	0.48
1:C:247:ILE:HG22	1:C:249:ILE:HG23	1.95	0.48
1:D:58:GLN:HE22	1:D:206:GLU:CD	2.22	0.48
1:D:114:ASN:O	1:D:118:MET:HB2	2.13	0.48
1:B:114:ASN:O	1:B:118:MET:HB2	2.12	0.48
1:D:119:THR:HG21	1:D:369:VAL:CG2	2.41	0.48
2:F:506:PHE:HD1	2:F:692:PHE:CE2	2.32	0.48
1:C:108:PRO:CA	1:C:135:ILE:HD11	2.44	0.48
1:E:79:ASP:OD1	1:E:80:ASP:N	2.46	0.48
2:F:242:ASN:O	2:F:246:GLU:HB2	2.13	0.48
2:G:188:ASP:O	2:G:189:ARG:HG2	2.13	0.48
1:B:119:THR:HG22	1:B:131:MET:SD	2.54	0.48
2:F:388:GLN:HA	2:F:431:GLN:O	2.14	0.48
2:F:592:ALA:HB3	2:F:604:ASP:HB3	1.95	0.48
1:A:131:MET:HE2	1:A:133:VAL:HG13	1.94	0.48
1:A:247:ILE:HG22	1:A:249:ILE:HG23	1.95	0.48
2:F:372:VAL:HA	2:F:375:PHE:HD2	1.79	0.48
2:F:548:PRO:HG2	2:F:553:LEU:HD21	1.95	0.48
1:C:44:VAL:O	2:F:560:PHE:CE1	2.67	0.47
2:F:393:ASP:CG	2:F:393:ASP:O	2.56	0.47
2:G:696:ILE:HG23	2:G:715:GLN:OE1	2.12	0.47
2:F:56:VAL:CG1	2:F:96:ILE:HG22	2.44	0.47
2:G:57:TRP:O	2:G:96:ILE:HG23	2.14	0.47
1:B:175:LEU:HD23	1:B:276:THR:HB	1.96	0.47
1:D:241:LEU:HD13	1:D:247:ILE:HG12	1.96	0.47
2:F:384:ARG:CZ	3:I:148:UNK:HA	2.44	0.47
2:G:388:GLN:HA	2:G:431:GLN:O	2.13	0.47
1:A:108:PRO:CA	1:A:135:ILE:HD11	2.43	0.47
1:C:201:THR:HB	1:C:204:GLU:OE1	2.13	0.47
2:F:551:LEU:HD23	2:F:551:LEU:HA	1.82	0.47
2:G:110:MET:HE1	2:G:121:VAL:HA	1.95	0.47
2:G:244:ILE:HD12	2:G:352:LEU:CD2	2.45	0.47
1:D:74:ILE:HA	1:D:114:ASN:HD21	1.79	0.47
2:G:369:VAL:O	2:G:372:VAL:HG12	2.14	0.47
2:G:558:CYS:SG	2:G:615:MET:SD	3.10	0.47
1:A:11:ASN:CG	1:A:16:CYS:HG	2.20	0.47
1:A:79:ASP:OD1	1:A:80:ASP:N	2.47	0.47
1:B:247:ILE:HG22	1:B:249:ILE:HG23	1.95	0.47
2:F:292:ILE:HG21	2:F:445:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:374:GLN:NE2	2:F:399:LYS:HE2	2.30	0.47
2:F:401:CYS:SG	2:F:408:VAL:HA	2.54	0.47
2:F:517:GLU:OE1	2:F:520:ARG:NH2	2.34	0.47
1:B:241:LEU:HD13	1:B:247:ILE:HG12	1.97	0.47
1:D:119:THR:HG22	1:D:131:MET:SD	2.54	0.47
1:D:142:TYR:HH	1:E:44:VAL:N	2.12	0.47
2:F:110:MET:HE1	2:F:121:VAL:HA	1.96	0.47
2:F:188:ASP:O	2:F:189:ARG:HG2	2.14	0.47
2:F:697:VAL:HG22	2:F:715:GLN:HE22	1.79	0.47
1:A:3:GLU:OE1	2:F:663:ARG:NH1	2.48	0.47
2:G:384:ARG:HH11	3:J:110:UNK:HA	1.58	0.47
2:G:596:VAL:HG22	2:G:605:TYR:HE2	1.80	0.47
2:G:634:THR:HG23	2:G:635:ALA:N	2.29	0.47
1:A:217:TYR:CE2	1:A:253:ARG:HD2	2.49	0.47
1:C:266:LEU:O	1:E:172:HIS:HB3	2.15	0.47
2:F:634:THR:HG23	2:F:635:ALA:N	2.29	0.47
1:A:197:TYR:CE2	1:A:247:ILE:HG23	2.50	0.46
2:F:135:TYR:CE1	2:F:174:VAL:HG23	2.50	0.46
2:G:395:THR:HG23	2:G:396:ALA:N	2.30	0.46
2:G:509:THR:O	2:G:512:VAL:HG22	2.15	0.46
2:G:565:ASP:O	2:G:568:PHE:HB3	2.15	0.46
1:D:142:TYR:OH	1:E:43:MET:HB3	2.14	0.46
2:G:592:ALA:HB3	2:G:604:ASP:HB3	1.96	0.46
2:F:198:GLY:HA3	2:F:481:GLY:H	1.80	0.46
2:F:388:GLN:O	2:F:389:ALA:HB3	2.14	0.46
2:F:509:THR:O	2:F:512:VAL:HG22	2.15	0.46
2:G:401:CYS:SG	2:G:408:VAL:HA	2.54	0.46
1:A:70:ILE:HD11	1:A:81:MET:HE1	1.97	0.46
1:A:209:ARG:NH1	1:A:213:GLU:OE2	2.49	0.46
1:B:108:PRO:CA	1:B:135:ILE:HD11	2.44	0.46
1:D:188:LEU:HD13	1:D:256:CYS:HB2	1.96	0.46
1:E:188:LEU:HD13	1:E:256:CYS:HB2	1.97	0.46
1:E:241:LEU:HD13	1:E:247:ILE:HG12	1.97	0.46
2:F:159:VAL:HG23	2:F:214:TYR:CD1	2.50	0.46
2:F:380:LEU:HD13	2:F:436:ALA:HB3	1.97	0.46
2:G:198:GLY:HA3	2:G:481:GLY:H	1.79	0.46
2:G:372:VAL:HA	2:G:375:PHE:HD2	1.80	0.46
2:G:626:LEU:HD13	2:G:638:TRP:NE1	2.31	0.46
1:A:119:THR:HG22	1:A:131:MET:SD	2.55	0.46
1:C:241:LEU:HD13	1:C:247:ILE:HG12	1.98	0.46
2:F:262:PHE:HD1	2:F:263:GLY:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:OD1	1:B:80:ASP:N	2.49	0.46
1:C:88:THR:OG1	1:C:89:PHE:N	2.46	0.46
1:C:175:LEU:HD23	1:C:276:THR:HB	1.96	0.46
2:F:592:ALA:CB	2:F:604:ASP:HB3	2.46	0.46
2:F:746:GLU:HG3	2:F:753:ILE:HD13	1.98	0.46
2:G:357:PHE:CE1	2:G:458:ARG:HG3	2.51	0.46
1:B:74:ILE:HA	1:B:114:ASN:HD21	1.80	0.46
1:C:58:GLN:HE22	1:C:206:GLU:CD	2.24	0.46
1:D:79:ASP:OD1	1:D:80:ASP:N	2.49	0.46
2:F:460:ASN:HA	2:F:463:LEU:HD12	1.98	0.46
2:F:199:GLU:OE2	2:F:697:VAL:HG22	2.15	0.46
2:G:135:TYR:CE1	2:G:174:VAL:HG23	2.51	0.46
1:E:74:ILE:HA	1:E:114:ASN:HD21	1.81	0.46
2:F:364:SER:HB3	2:F:633:LEU:HD22	1.98	0.46
2:F:384:ARG:HH22	3:I:147:UNK:C	2.29	0.46
2:G:364:SER:HB3	2:G:633:LEU:HD22	1.97	0.46
2:G:460:ASN:HA	2:G:463:LEU:HD12	1.97	0.46
2:G:558:CYS:SG	2:G:559:TRP:CD1	3.09	0.46
2:G:742:ARG:NH1	2:G:763:ALA:HB2	2.30	0.46
1:E:215:LEU:HD11	1:E:239:TYR:HB2	1.98	0.46
2:G:166:LYS:HB2	2:G:169:GLU:HG3	1.98	0.46
2:G:185:MET:HE1	2:G:270:PHE:CD2	2.51	0.46
2:G:199:GLU:OE2	2:G:697:VAL:HG22	2.16	0.46
1:C:4:ILE:HG22	1:C:4:ILE:O	2.17	0.45
1:C:119:THR:HG21	1:C:369:VAL:CG2	2.42	0.45
2:G:184:SER:O	2:G:188:ASP:CB	2.65	0.45
1:A:334:ARG:HA	1:A:337:SER:OG	2.16	0.45
1:B:188:LEU:HD13	1:B:256:CYS:HB2	1.99	0.45
1:C:197:TYR:CE2	1:C:247:ILE:HG23	2.51	0.45
1:D:189:MET:HE3	1:D:199:PHE:O	2.16	0.45
1:D:212:LYS:HA	1:D:216:CYS:SG	2.56	0.45
1:E:197:TYR:CE2	1:E:247:ILE:HG23	2.51	0.45
2:F:166:LYS:HB2	2:F:169:GLU:HG3	1.98	0.45
2:G:336:SER:HB3	2:G:338:PRO:HD2	1.98	0.45
1:D:26:PRO:HG2	2:G:422:VAL:HG23	1.98	0.45
2:F:261:ARG:HD3	2:F:261:ARG:HA	1.34	0.45
2:G:110:MET:CE	2:G:121:VAL:HG13	2.46	0.45
1:A:44:VAL:N	1:B:142:TYR:HH	2.05	0.45
1:A:111:PRO:HG3	1:E:196:GLY:HA2	1.99	0.45
1:A:218:VAL:HG22	1:A:257:PRO:CB	2.46	0.45
1:E:218:VAL:HG22	1:E:257:PRO:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:596:VAL:HG22	2:F:605:TYR:HE2	1.81	0.45
2:G:242:ASN:N	2:G:243:PRO:HD2	2.31	0.45
1:A:142:TYR:HH	1:C:44:VAL:N	2.13	0.45
1:C:74:ILE:HA	1:C:114:ASN:HD21	1.81	0.45
1:C:209:ARG:NH1	1:C:213:GLU:OE2	2.50	0.45
1:C:228:THR:HG23	1:C:235:LEU:HD11	1.98	0.45
2:F:184:SER:O	2:F:188:ASP:CB	2.64	0.45
2:F:548:PRO:HG3	2:F:553:LEU:HD21	1.99	0.45
2:F:626:LEU:HD13	2:F:638:TRP:NE1	2.32	0.45
2:F:788:ARG:O	2:F:791:VAL:HG22	2.17	0.45
2:G:336:SER:HA	2:G:337:SER:HB2	1.99	0.45
1:A:60:LYS:O	1:A:64:LEU:HD13	2.16	0.45
1:E:108:PRO:CA	1:E:135:ILE:HD11	2.45	0.45
2:G:364:SER:CB	2:G:633:LEU:HD22	2.46	0.45
1:A:179:LEU:HD23	1:A:268:MET:HE1	1.98	0.45
1:A:188:LEU:HD13	1:A:256:CYS:HB2	1.99	0.45
1:B:10:ASP:HA	1:B:105:THR:HG22	1.99	0.45
1:C:10:ASP:HA	1:C:105:THR:HG22	1.99	0.45
1:E:209:ARG:NH1	1:E:213:GLU:OE2	2.50	0.45
1:E:341:GLY:O	1:E:344:ILE:HG22	2.17	0.45
2:F:260:SER:O	2:F:480:ALA:HB2	2.17	0.45
2:G:393:ASP:O	2:G:393:ASP:CG	2.59	0.45
1:A:10:ASP:HA	1:A:105:THR:HG22	1.99	0.45
1:B:58:GLN:HE22	1:B:206:GLU:CD	2.24	0.45
1:B:181:GLY:O	1:B:212:LYS:NZ	2.50	0.45
2:G:110:MET:HB2	2:G:138:SER:HA	1.98	0.45
1:C:212:LYS:HA	1:C:216:CYS:SG	2.56	0.45
1:D:249:ILE:HG13	1:D:249:ILE:O	2.17	0.45
2:F:185:MET:HE1	2:F:270:PHE:CD2	2.51	0.45
2:G:592:ALA:CB	2:G:604:ASP:HB3	2.46	0.45
1:B:212:LYS:HA	1:B:216:CYS:SG	2.57	0.45
1:E:181:GLY:O	1:E:212:LYS:NZ	2.50	0.45
2:F:165:LYS:N	2:F:179:GLU:OE2	2.48	0.45
2:F:364:SER:CB	2:F:633:LEU:HD22	2.47	0.45
2:F:565:ASP:O	2:F:568:PHE:HB3	2.17	0.45
1:C:249:ILE:O	1:C:249:ILE:HG13	2.18	0.44
1:D:167:GLY:HA2	1:E:43:MET:HG3	1.98	0.44
1:D:197:TYR:CE2	1:D:247:ILE:HG23	2.52	0.44
2:F:267:ARG:HE	2:F:282:GLU:CD	2.25	0.44
2:F:320:LEU:HB3	2:F:399:LYS:HE3	2.00	0.44
2:F:336:SER:HB3	2:F:338:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:742:ARG:NH1	2:F:763:ALA:HB2	2.32	0.44
2:G:494:CYS:HB3	2:G:674:TYR:CZ	2.53	0.44
2:G:788:ARG:O	2:G:791:VAL:HG22	2.16	0.44
1:A:4:ILE:HG22	1:A:4:ILE:O	2.18	0.44
1:A:181:GLY:O	1:A:212:LYS:NZ	2.50	0.44
1:D:10:ASP:HA	1:D:105:THR:HG22	1.99	0.44
2:G:54:ARG:O	2:G:56:VAL:HG23	2.17	0.44
2:G:548:PRO:HG3	2:G:553:LEU:HD21	1.98	0.44
2:G:746:GLU:HG3	2:G:753:ILE:HD13	1.99	0.44
1:C:181:GLY:O	1:C:212:LYS:NZ	2.50	0.44
1:E:179:LEU:HD23	1:E:268:MET:HE1	1.99	0.44
1:E:228:THR:HG23	1:E:235:LEU:HD11	1.99	0.44
2:G:134:ILE:HD12	2:G:147:PRO:CD	2.48	0.44
2:G:335:SER:O	2:G:337:SER:OG	2.33	0.44
1:A:212:LYS:HA	1:A:216:CYS:SG	2.57	0.44
1:A:333:GLU:OE1	2:F:429:LYS:CG	2.64	0.44
1:B:4:ILE:O	1:B:4:ILE:HG22	2.17	0.44
1:B:189:MET:HE3	1:B:199:PHE:O	2.17	0.44
1:C:188:LEU:HD13	1:C:256:CYS:HB2	2.00	0.44
1:E:4:ILE:O	1:E:4:ILE:HG22	2.16	0.44
2:F:110:MET:HB2	2:F:138:SER:HA	1.98	0.44
2:F:209:LYS:HD2	2:F:239:LEU:HD23	1.99	0.44
2:G:110:MET:HA	2:G:113:LEU:HD13	2.00	0.44
2:G:159:VAL:HG23	2:G:214:TYR:CD1	2.53	0.44
2:G:267:ARG:HE	2:G:282:GLU:CD	2.25	0.44
2:G:345:PHE:CZ	2:G:349:LEU:HD11	2.52	0.44
1:A:228:THR:HG23	1:A:235:LEU:HD11	2.00	0.44
2:F:242:ASN:N	2:F:243:PRO:HD2	2.31	0.44
2:F:335:SER:O	2:F:337:SER:OG	2.33	0.44
2:G:209:LYS:HD2	2:G:239:LEU:HD23	1.98	0.44
1:A:172:HIS:HB3	1:E:266:LEU:O	2.17	0.44
1:A:249:ILE:O	1:A:249:ILE:HG13	2.16	0.44
1:B:197:TYR:CE2	1:B:247:ILE:HG23	2.53	0.44
1:C:11:ASN:CG	1:C:16:CYS:HG	2.20	0.44
1:C:215:LEU:HD11	1:C:239:TYR:HB2	1.98	0.44
1:D:108:PRO:CA	1:D:135:ILE:HD11	2.44	0.44
1:D:228:THR:HG23	1:D:235:LEU:HD11	2.00	0.44
1:E:175:LEU:HD23	1:E:276:THR:HB	1.99	0.44
2:G:380:LEU:HD13	2:G:436:ALA:HB3	2.00	0.44
2:G:446:ALA:O	2:G:450:ARG:HG2	2.18	0.44
1:A:26:PRO:HG2	2:F:422:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:OH	1:C:43:MET:HB3	2.17	0.44
1:B:228:THR:HG23	1:B:235:LEU:HD11	2.00	0.44
1:D:220:LEU:HD23	3:K:103:UNK:CB	2.48	0.44
2:F:175:TYR:CD1	2:F:214:TYR:HB2	2.53	0.44
2:F:237:GLN:NE2	2:F:463:LEU:HD23	2.33	0.44
2:G:72:ASP:HB3	2:G:79:GLU:HB3	2.00	0.44
2:G:175:TYR:CD1	2:G:214:TYR:HB2	2.53	0.44
1:B:332:PRO:O	1:B:333:GLU:CB	2.66	0.44
2:F:446:ALA:O	2:F:450:ARG:HG2	2.18	0.44
2:F:494:CYS:HB3	2:F:674:TYR:CZ	2.53	0.44
1:A:175:LEU:HD23	1:A:276:THR:HB	1.99	0.44
1:E:249:ILE:HG13	1:E:249:ILE:O	2.18	0.44
2:G:237:GLN:NE2	2:G:463:LEU:HD23	2.33	0.44
2:G:777:LEU:HD23	2:G:791:VAL:HG12	2.00	0.44
1:A:35:GLY:O	1:A:51:SER:OG	2.22	0.43
1:A:269:GLU:HG2	1:E:38:ARG:HD3	2.00	0.43
1:B:148:THR:HG21	1:B:291:ASP:OD2	2.18	0.43
1:E:11:ASN:CG	1:E:16:CYS:HG	2.21	0.43
2:F:110:MET:CE	2:F:121:VAL:HG13	2.46	0.43
2:F:146:ASN:ND2	2:F:202:ALA:O	2.50	0.43
2:F:336:SER:HA	2:F:337:SER:HB2	1.99	0.43
2:G:262:PHE:HD1	2:G:263:GLY:O	2.01	0.43
2:G:415:LEU:HD22	2:G:440:LEU:HD21	2.00	0.43
1:B:209:ARG:NH1	1:B:213:GLU:OE2	2.50	0.43
2:F:415:LEU:HD22	2:F:440:LEU:HD21	2.00	0.43
2:F:603:VAL:HG12	2:F:604:ASP:N	2.32	0.43
2:G:603:VAL:HG12	2:G:604:ASP:N	2.33	0.43
1:B:142:TYR:CZ	1:B:345:LEU:HD11	2.54	0.43
1:D:4:ILE:HG22	1:D:4:ILE:O	2.17	0.43
1:D:215:LEU:HD11	1:D:239:TYR:HB2	1.99	0.43
1:E:75:VAL:CG2	1:E:78:TRP:CE2	3.01	0.43
1:E:212:LYS:HA	1:E:216:CYS:SG	2.58	0.43
2:F:134:ILE:HD12	2:F:147:PRO:CD	2.48	0.43
2:F:164:GLY:N	2:F:179:GLU:OE2	2.51	0.43
2:F:489:SER:O	2:F:492:GLN:HB3	2.18	0.43
2:F:543:ARG:O	2:F:549:GLY:N	2.51	0.43
2:F:777:LEU:HD23	2:F:791:VAL:HG12	2.00	0.43
2:G:56:VAL:CG1	2:G:96:ILE:HG22	2.44	0.43
2:F:267:ARG:HD2	2:F:280:ASN:OD1	2.18	0.43
2:F:339:GLY:C	2:F:341:GLU:H	2.24	0.43
2:G:253:THR:HA	2:G:298:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:370:SER:HB3	2:G:403:LEU:HD21	2.00	0.43
2:G:557:GLU:HG3	2:G:563:ALA:HB1	2.01	0.43
1:A:348:LEU:HG	2:F:556:GLU:HG3	2.01	0.43
1:D:344:ILE:O	1:D:348:LEU:HD13	2.17	0.43
2:F:110:MET:HA	2:F:113:LEU:HD13	1.99	0.43
2:F:345:PHE:CZ	2:F:349:LEU:HD11	2.54	0.43
2:G:261:ARG:HA	2:G:261:ARG:HD3	1.34	0.43
2:G:320:LEU:HB3	2:G:399:LYS:HE3	2.01	0.43
1:B:11:ASN:CG	1:B:16:CYS:HG	2.20	0.43
1:C:341:GLY:O	1:C:344:ILE:HG22	2.18	0.43
1:D:218:VAL:HG22	1:D:257:PRO:CB	2.48	0.43
2:F:147:PRO:HG3	2:F:151:LEU:HD11	2.01	0.43
2:G:108:GLU:HG3	2:G:172:PRO:HG3	2.01	0.43
2:G:405:GLY:HA3	2:G:630:THR:H	1.83	0.43
1:C:148:THR:HG21	1:C:291:ASP:OD2	2.19	0.43
1:C:218:VAL:HG22	1:C:257:PRO:CB	2.49	0.43
2:F:158:ILE:HG12	2:F:162:TYR:CE2	2.54	0.43
2:G:260:SER:O	2:G:480:ALA:HB2	2.19	0.43
1:C:189:MET:HE3	1:C:199:PHE:O	2.18	0.43
1:D:181:GLY:O	1:D:212:LYS:NZ	2.52	0.43
2:F:54:ARG:O	2:F:56:VAL:HG23	2.18	0.43
2:F:405:GLY:HA3	2:F:630:THR:H	1.83	0.43
2:G:164:GLY:N	2:G:179:GLU:OE2	2.52	0.43
1:A:167:GLY:HA2	1:C:43:MET:HG3	2.01	0.43
1:D:179:LEU:HD23	1:D:268:MET:HE1	2.01	0.43
1:D:209:ARG:NH1	1:D:213:GLU:OE2	2.51	0.43
2:F:329:PHE:CE1	2:F:376:GLY:HA2	2.54	0.43
2:F:557:GLU:HG3	2:F:563:ALA:HB1	2.00	0.43
2:G:242:ASN:HB2	2:G:243:PRO:HD3	2.01	0.43
2:G:267:ARG:HD2	2:G:280:ASN:OD1	2.18	0.43
2:G:420:ILE:HD13	2:G:429:LYS:HB2	2.01	0.43
1:A:10:ASP:OD1	1:A:10:ASP:C	2.62	0.42
1:B:215:LEU:HD11	1:B:239:TYR:HB2	1.99	0.42
2:G:146:ASN:ND2	2:G:202:ALA:O	2.50	0.42
2:G:336:SER:CA	2:G:338:PRO:HD2	2.48	0.42
1:E:177:LEU:HD22	1:E:276:THR:HG21	2.00	0.42
2:F:109:ASP:HB3	2:F:112:GLU:HG2	2.00	0.42
2:F:626:LEU:HD13	2:F:638:TRP:CE2	2.54	0.42
1:B:179:LEU:HD23	1:B:268:MET:HE1	2.01	0.42
1:B:271:CYS:HB3	1:B:275:GLU:HB2	2.01	0.42
1:E:189:MET:HE3	1:E:199:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:ASP:HB3	2:G:112:GLU:HG2	2.00	0.42
2:G:136:THR:HG22	2:G:137:TYR:N	2.34	0.42
1:A:196:GLY:HA2	1:D:111:PRO:HG3	2.01	0.42
1:D:11:ASN:CG	1:D:16:CYS:HG	2.21	0.42
2:F:136:THR:HG22	2:F:137:TYR:N	2.34	0.42
2:G:358:SER:O	2:G:362:ILE:HG12	2.19	0.42
2:G:560:PHE:CG	2:G:561:PRO:HD2	2.53	0.42
2:G:626:LEU:HD13	2:G:638:TRP:CE2	2.55	0.42
1:A:17:LYS:NZ	1:A:335:LYS:O	2.52	0.42
1:C:334:ARG:HA	1:C:337:SER:OG	2.19	0.42
1:D:164:ILE:O	1:D:164:ILE:CG2	2.67	0.42
1:D:332:PRO:O	1:D:333:GLU:CB	2.67	0.42
2:G:51:THR:HG22	2:G:52:ALA:N	2.35	0.42
1:A:189:MET:HE3	1:A:199:PHE:O	2.20	0.42
1:B:249:ILE:O	1:B:249:ILE:HG13	2.20	0.42
1:C:179:LEU:HD23	1:C:268:MET:HE1	2.01	0.42
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.86	0.42
1:D:95:VAL:O	1:D:97:PRO:HD3	2.20	0.42
2:F:51:THR:HG22	2:F:52:ALA:N	2.35	0.42
2:F:108:GLU:HG3	2:F:172:PRO:HG3	2.00	0.42
2:F:335:SER:O	2:F:337:SER:CB	2.68	0.42
2:G:158:ILE:HG12	2:G:162:TYR:CE2	2.54	0.42
2:G:336:SER:HA	2:G:338:PRO:HD2	2.01	0.42
2:G:670:VAL:CG2	2:G:671:GLY:N	2.82	0.42
1:A:74:ILE:HA	1:A:114:ASN:HD21	1.85	0.42
1:D:75:VAL:CG2	1:D:78:TRP:CE2	3.03	0.42
2:F:670:VAL:CG2	2:F:671:GLY:N	2.82	0.42
2:G:335:SER:O	2:G:337:SER:CB	2.68	0.42
2:G:339:GLY:C	2:G:341:GLU:H	2.24	0.42
1:A:344:ILE:O	1:A:348:LEU:HD13	2.20	0.42
1:B:17:LYS:NZ	1:B:335:LYS:O	2.51	0.42
1:B:107:ALA:HB1	1:B:160:HIS:NE2	2.34	0.42
1:B:218:VAL:HG22	1:B:257:PRO:CB	2.49	0.42
1:B:364:SER:CB	1:B:368:ILE:HG21	2.50	0.42
1:C:95:VAL:O	1:C:97:PRO:HD3	2.20	0.42
2:G:329:PHE:CE1	2:G:376:GLY:HA2	2.54	0.42
2:G:543:ARG:O	2:G:549:GLY:N	2.53	0.42
1:C:107:ALA:HB1	1:C:160:HIS:NE2	2.35	0.42
1:D:9:ILE:HB	1:D:104:LEU:HD23	2.01	0.42
1:E:95:VAL:O	1:E:97:PRO:HD3	2.20	0.42
2:F:370:SER:HB3	2:F:403:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:523:ILE:HD13	2:F:779:ARG:CB	2.50	0.42
2:F:537:CYS:O	2:F:540:LEU:HB3	2.19	0.42
2:G:175:TYR:CE1	2:G:214:TYR:HB2	2.55	0.42
2:G:214:TYR:CZ	2:G:218:VAL:HG21	2.55	0.42
1:A:95:VAL:O	1:A:97:PRO:HD3	2.20	0.42
1:D:29:VAL:O	1:D:29:VAL:HG23	2.20	0.42
1:D:356:ILE:CG2	1:D:368:ILE:HD11	2.50	0.42
2:F:336:SER:CA	2:F:338:PRO:HD2	2.49	0.42
2:G:147:PRO:HG3	2:G:151:LEU:HD11	2.01	0.42
2:G:303:ILE:HG23	2:G:304:PHE:N	2.35	0.42
2:G:523:ILE:HD13	2:G:779:ARG:CB	2.50	0.42
1:A:215:LEU:HD11	1:A:239:TYR:HB2	2.01	0.41
1:A:305:TYR:CE1	4:A:401:ADP:C2	3.08	0.41
1:B:95:VAL:O	1:B:97:PRO:HD3	2.20	0.41
1:C:364:SER:CB	1:C:368:ILE:HG21	2.50	0.41
1:E:60:LYS:O	1:E:64:LEU:HD13	2.19	0.41
2:F:336:SER:HA	2:F:338:PRO:HD2	2.02	0.41
2:F:358:SER:O	2:F:362:ILE:HG12	2.19	0.41
2:G:141:PHE:HE1	2:G:694:ARG:CZ	2.33	0.41
1:A:55:ASP:N	1:A:55:ASP:OD1	2.53	0.41
1:A:289:ARG:HD2	1:C:243:ASP:OD1	2.20	0.41
1:C:12:GLY:HA3	4:C:401:ADP:O1B	2.21	0.41
1:C:271:CYS:HB3	1:C:275:GLU:HB2	2.01	0.41
1:E:12:GLY:HA3	4:E:401:ADP:O1B	2.20	0.41
2:F:72:ASP:HB3	2:F:79:GLU:HB3	2.02	0.41
2:F:214:TYR:CZ	2:F:218:VAL:HG21	2.55	0.41
2:F:242:ASN:HB2	2:F:243:PRO:HD3	2.01	0.41
2:F:303:ILE:HG23	2:F:304:PHE:N	2.35	0.41
2:G:284:TYR:CD1	2:G:681:LEU:HD13	2.56	0.41
2:G:423:GLY:HA2	2:G:424:ARG:HA	1.79	0.41
1:E:10:ASP:HA	1:E:105:THR:HG22	2.02	0.41
2:G:389:ALA:O	2:G:390:THR:HB	2.20	0.41
1:A:145:GLY:C	2:F:561:PRO:HB3	2.45	0.41
1:B:12:GLY:HA3	4:B:401:ADP:O1B	2.21	0.41
1:C:17:LYS:NZ	1:C:335:LYS:O	2.53	0.41
1:E:64:LEU:CD1	1:E:64:LEU:N	2.82	0.41
1:E:162:VAL:HG22	1:E:174:ILE:HG12	2.01	0.41
1:E:334:ARG:HA	1:E:337:SER:OG	2.20	0.41
1:A:12:GLY:HA3	4:A:401:ADP:O1B	2.20	0.41
1:A:122:MET:O	1:A:128:THR:HG22	2.21	0.41
1:B:341:GLY:O	1:B:344:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:HB2	1:D:202:THR:HG21	2.02	0.41
1:E:9:ILE:HB	1:E:104:LEU:HD23	2.02	0.41
1:E:332:PRO:O	1:E:333:GLU:CB	2.68	0.41
2:F:68:ALA:CB	2:F:82:LEU:HD23	2.50	0.41
2:F:253:THR:HA	2:F:298:GLU:HG2	2.02	0.41
2:F:316:LYS:O	2:F:320:LEU:N	2.49	0.41
2:G:489:SER:O	2:G:492:GLN:HB3	2.19	0.41
1:A:66:LEU:HB2	1:A:202:THR:HG21	2.01	0.41
2:G:551:LEU:HD23	2:G:551:LEU:HA	1.82	0.41
1:A:364:SER:CB	1:A:368:ILE:HG21	2.51	0.41
1:D:289:ARG:HD2	1:E:243:ASP:OD1	2.21	0.41
1:D:334:ARG:HA	1:D:337:SER:OG	2.20	0.41
2:G:616:ASP:O	2:G:616:ASP:CG	2.64	0.41
1:E:107:ALA:HB1	1:E:160:HIS:NE2	2.35	0.41
2:F:141:PHE:HE1	2:F:694:ARG:CZ	2.33	0.41
2:F:175:TYR:CE1	2:F:214:TYR:HB2	2.55	0.41
1:B:66:LEU:HB2	1:B:202:THR:HG21	2.02	0.41
1:C:55:ASP:N	1:C:55:ASP:OD1	2.53	0.41
1:D:55:ASP:N	1:D:55:ASP:OD1	2.54	0.41
1:E:66:LEU:HB2	1:E:202:THR:HG21	2.02	0.41
2:F:110:MET:HG3	2:F:137:TYR:O	2.21	0.41
2:F:778:TYR:CD1	2:F:778:TYR:C	2.99	0.41
1:B:10:ASP:OD1	1:B:10:ASP:C	2.64	0.41
1:D:17:LYS:NZ	1:D:335:LYS:O	2.54	0.41
1:D:271:CYS:HB3	1:D:275:GLU:HB2	2.03	0.41
1:E:26:PRO:HD3	1:E:339:TRP:CE3	2.56	0.41
2:G:335:SER:O	2:G:337:SER:HB2	2.20	0.41
1:A:356:ILE:CG2	1:A:368:ILE:HD11	2.52	0.40
1:B:269:GLU:O	1:B:270:SER:C	2.64	0.40
1:C:11:ASN:OD1	1:C:16:CYS:SG	2.61	0.40
1:C:66:LEU:HB2	1:C:202:THR:HG21	2.03	0.40
1:D:12:GLY:HA3	4:D:401:ADP:O1B	2.21	0.40
2:F:335:SER:O	2:F:337:SER:HB2	2.21	0.40
2:F:390:THR:OG1	2:F:391:MET:N	2.54	0.40
2:F:420:ILE:HD13	2:F:429:LYS:HB2	2.02	0.40
1:A:64:LEU:N	1:A:64:LEU:CD1	2.84	0.40
1:C:269:GLU:O	1:C:270:SER:C	2.64	0.40
1:D:3:GLU:OE1	2:G:663:ARG:NH1	2.55	0.40
1:E:29:VAL:O	1:E:29:VAL:HG23	2.21	0.40
1:E:269:GLU:O	1:E:270:SER:C	2.63	0.40
2:F:68:ALA:HB1	2:F:80:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:528:LEU:HG	2:F:529:ASP:N	2.36	0.40
2:G:546:ASN:OD1	2:G:546:ASN:N	2.53	0.40
1:A:271:CYS:HB3	1:A:275:GLU:HB2	2.03	0.40
1:E:10:ASP:OD1	1:E:10:ASP:C	2.64	0.40
1:E:33:ILE:HD13	1:E:58:GLN:HE21	1.87	0.40
2:F:284:TYR:CD1	2:F:681:LEU:HD13	2.56	0.40
2:F:738:PHE:CE2	2:F:785:ILE:HD11	2.56	0.40
2:G:352:LEU:CD1	2:G:362:ILE:HD12	2.32	0.40
1:A:9:ILE:HB	1:A:104:LEU:HD23	2.02	0.40
1:C:332:PRO:O	1:C:333:GLU:CB	2.70	0.40
1:D:148:THR:HG23	1:D:165:TYR:HA	2.03	0.40
1:D:332:PRO:HD2	2:G:430:ALA:HB2	2.02	0.40
2:F:497:TYR:O	2:F:500:GLU:HB3	2.22	0.40
2:F:529:ASP:HB3	2:F:532:LEU:HG	2.04	0.40
2:G:488:ASN:HB2	2:G:604:ASP:O	2.21	0.40
1:A:341:GLY:O	1:A:344:ILE:HG22	2.21	0.40
1:C:9:ILE:HB	1:C:104:LEU:HD23	2.03	0.40
1:C:75:VAL:CG2	1:C:78:TRP:CE2	3.04	0.40
1:D:341:GLY:O	1:D:344:ILE:HG22	2.22	0.40
1:E:52:TYR:HD2	1:E:64:LEU:HD21	1.86	0.40
2:F:775:PRO:O	2:F:779:ARG:NH1	2.55	0.40
2:G:791:VAL:HG23	2:G:792:LEU:N	2.37	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	372/374 (100%)	346 (93%)	21 (6%)	5 (1%)	9	40
1	B	372/374 (100%)	349 (94%)	17 (5%)	6 (2%)	7	36
1	C	372/374 (100%)	348 (94%)	18 (5%)	6 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	372/374 (100%)	349 (94%)	17 (5%)	6 (2%)	7	36
1	E	372/374 (100%)	347 (93%)	19 (5%)	6 (2%)	7	36
2	F	731/1039 (70%)	680 (93%)	39 (5%)	12 (2%)	7	36
2	G	731/1039 (70%)	679 (93%)	40 (6%)	12 (2%)	7	36
All	All	3322/3948 (84%)	3098 (93%)	171 (5%)	53 (2%)	10	36

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ALA
2	F	337	SER
2	F	466	SER
2	F	667	PHE
2	F	668	ARG
2	G	337	SER
2	G	466	SER
2	G	667	PHE
2	G	668	ARG
1	A	49	LYS
1	B	169	ALA
1	C	49	LYS
1	C	169	ALA
1	D	169	ALA
1	E	49	LYS
1	E	169	ALA
2	F	340	GLN
2	G	340	GLN
1	A	4	ILE
1	B	4	ILE
1	B	49	LYS
1	B	168	TYR
1	D	4	ILE
1	D	49	LYS
1	D	168	TYR
1	E	168	TYR
2	F	71	ARG
2	F	385	ASN
2	F	561	PRO
2	F	758	MET
2	G	71	ARG
2	G	385	ASN

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Mol	Chain	Res	Type
2	G	758	MET
1	A	47	GLY
1	A	168	TYR
1	B	47	GLY
1	C	4	ILE
1	C	47	GLY
1	C	168	TYR
1	D	47	GLY
1	E	4	ILE
1	E	47	GLY
2	F	284	TYR
2	G	284	TYR
2	G	561	PRO
2	F	662	PRO
2	G	662	PRO
2	F	546	ASN
2	G	546	ASN
1	C	157	GLY
1	B	157	GLY
1	D	157	GLY
1	E	157	GLY

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%)	311 (98%)	6 (2%)	50	66
1	B	317/317 (100%)	312 (98%)	5 (2%)	55	69
1	C	317/317 (100%)	312 (98%)	5 (2%)	55	69
1	D	317/317 (100%)	311 (98%)	6 (2%)	50	66
1	E	317/317 (100%)	311 (98%)	6 (2%)	50	66
2	F	613/888 (69%)	605 (99%)	8 (1%)	61	71
2	G	613/888 (69%)	605 (99%)	8 (1%)	61	71
All	All	2811/3361 (84%)	2767 (98%)	44 (2%)	54	69

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASP
1	A	158	VAL
1	A	164	ILE
1	A	278	PHE
1	A	345	LEU
1	A	363	GLU
1	B	158	VAL
1	B	164	ILE
1	B	278	PHE
1	B	345	LEU
1	B	363	GLU
1	C	158	VAL
1	C	164	ILE
1	C	278	PHE
1	C	345	LEU
1	C	363	GLU
1	D	153	ASP
1	D	158	VAL
1	D	164	ILE
1	D	278	PHE
1	D	345	LEU
1	D	363	GLU
1	E	153	ASP
1	E	158	VAL
1	E	164	ILE
1	E	278	PHE
1	E	345	LEU
1	E	363	GLU
2	F	140	LEU
2	F	215	LEU
2	F	417	THR
2	F	422	VAL
2	F	569	VAL
2	F	696	ILE
2	F	718	CYS
2	F	771	LEU
2	G	140	LEU
2	G	215	LEU
2	G	417	THR
2	G	422	VAL
2	G	569	VAL
2	G	696	ILE

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Mol	Chain	Res	Type
2	G	718	CYS
2	G	771	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	87	HIS
1	A	91	ASN
1	A	114	ASN
1	B	58	GLN
1	B	87	HIS
1	B	114	ASN
1	C	58	GLN
1	C	87	HIS
1	C	114	ASN
1	D	58	GLN
1	D	87	HIS
1	D	91	ASN
1	D	114	ASN
1	E	58	GLN
1	E	87	HIS
1	E	114	ASN
2	F	63	HIS
2	F	237	GLN
2	F	250	ASN
2	F	377	ASN
2	F	385	ASN
2	F	388	GLN
2	F	431	GLN
2	F	496	ASN
2	F	583	GLN
2	F	687	ASN
2	F	700	HIS
2	F	715	GLN
2	G	63	HIS
2	G	237	GLN
2	G	250	ASN
2	G	377	ASN
2	G	385	ASN
2	G	388	GLN
2	G	431	GLN

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Mol	Chain	Res	Type
2	G	496	ASN
2	G	583	GLN
2	G	687	ASN
2	G	700	HIS
2	G	715	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	D	401	5	28,29,29	1.47	4 (14%)	43,45,45	1.84	10 (23%)
4	ADP	A	401	5	28,29,29	1.46	4 (14%)	43,45,45	1.83	9 (20%)
4	ADP	C	401	5	28,29,29	1.46	4 (14%)	43,45,45	1.84	10 (23%)
4	ADP	E	401	5	28,29,29	1.47	4 (14%)	43,45,45	1.85	10 (23%)
4	ADP	B	401	5	28,29,29	1.47	4 (14%)	43,45,45	1.84	10 (23%)

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	D	401	5	-	3/16/32/32	0/3/3/3
4	ADP	A	401	5	-	3/16/32/32	0/3/3/3
4	ADP	C	401	5	-	3/16/32/32	0/3/3/3
4	ADP	E	401	5	-	3/16/32/32	0/3/3/3
4	ADP	B	401	5	-	3/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-C4	5.30	1.48	1.39
4	A	401	ADP	C5-C4	5.28	1.48	1.39
4	B	401	ADP	C5-C4	5.27	1.48	1.39
4	C	401	ADP	C5-C4	5.24	1.48	1.39
4	E	401	ADP	C5-C4	5.23	1.48	1.39
4	D	401	ADP	C5-C6	2.95	1.49	1.41
4	E	401	ADP	C5-C6	2.95	1.49	1.41
4	A	401	ADP	C5-C6	2.94	1.49	1.41
4	B	401	ADP	C5-C6	2.94	1.49	1.41
4	C	401	ADP	C5-C6	2.93	1.49	1.41
4	D	401	ADP	C5-N7	-2.53	1.34	1.39
4	B	401	ADP	C5-N7	-2.51	1.34	1.39
4	E	401	ADP	C5-N7	-2.48	1.34	1.39
4	C	401	ADP	C5-N7	-2.46	1.34	1.39
4	A	401	ADP	C5-N7	-2.44	1.34	1.39
4	E	401	ADP	C4-N9	-2.26	1.33	1.37
4	D	401	ADP	C4-N9	-2.24	1.33	1.37
4	B	401	ADP	C4-N9	-2.21	1.33	1.37
4	C	401	ADP	C4-N9	-2.20	1.33	1.37
4	A	401	ADP	C4-N9	-2.19	1.33	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	401	ADP	C5-C4-N3	-5.86	118.64	126.72
4	D	401	ADP	C5-C4-N3	-5.84	118.68	126.72
4	C	401	ADP	C5-C4-N3	-5.84	118.68	126.72
4	B	401	ADP	C5-C4-N3	-5.82	118.70	126.72
4	A	401	ADP	C5-C4-N3	-5.78	118.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	401	ADP	N3-C4-N9	5.11	135.86	127.17
4	B	401	ADP	N3-C4-N9	5.11	135.86	127.17
4	D	401	ADP	N3-C4-N9	5.09	135.82	127.17
4	C	401	ADP	N3-C4-N9	5.08	135.80	127.17
4	A	401	ADP	N3-C4-N9	5.06	135.77	127.17
4	A	401	ADP	O3B-PB-O2B	3.25	119.98	107.80
4	D	401	ADP	O3B-PB-O2B	3.24	119.97	107.80
4	C	401	ADP	O3B-PB-O2B	3.24	119.94	107.80
4	B	401	ADP	O3B-PB-O2B	3.23	119.93	107.80
4	E	401	ADP	O3B-PB-O2B	3.23	119.93	107.80
4	E	401	ADP	C4-N9-C8	3.18	109.08	105.74
4	B	401	ADP	C4-N9-C8	3.17	109.06	105.74
4	C	401	ADP	C4-C5-N7	-3.15	106.98	110.58
4	C	401	ADP	C4-N9-C8	3.15	109.04	105.74
4	D	401	ADP	C4-N9-C8	3.14	109.03	105.74
4	D	401	ADP	C4-C5-N7	-3.11	107.02	110.58
4	A	401	ADP	C4-N9-C8	3.10	108.99	105.74
4	E	401	ADP	C4-C5-N7	-3.08	107.06	110.58
4	A	401	ADP	C4-C5-N7	-3.03	107.11	110.58
4	B	401	ADP	C4-C5-N7	-3.03	107.12	110.58
4	B	401	ADP	C2-N3-C4	3.01	119.19	111.83
4	E	401	ADP	C2-N3-C4	3.00	119.16	111.83
4	D	401	ADP	C2-N3-C4	2.97	119.08	111.83
4	C	401	ADP	C2-N3-C4	2.96	119.06	111.83
4	A	401	ADP	C2-N3-C4	2.95	119.05	111.83
4	C	401	ADP	C5-N7-C8	2.56	107.47	103.45
4	D	401	ADP	C5-N7-C8	2.52	107.42	103.45
4	E	401	ADP	C5-N7-C8	2.50	107.38	103.45
4	B	401	ADP	C5-N7-C8	2.46	107.31	103.45
4	A	401	ADP	C5-N7-C8	2.45	107.30	103.45
4	A	401	ADP	C3'-C2'-C1'	2.40	106.00	101.46
4	D	401	ADP	C3'-C2'-C1'	2.36	105.92	101.46
4	E	401	ADP	C3'-C2'-C1'	2.36	105.92	101.46
4	C	401	ADP	C3'-C2'-C1'	2.36	105.92	101.46
4	B	401	ADP	C3'-C2'-C1'	2.30	105.82	101.46
4	C	401	ADP	N9-C8-N7	-2.08	110.98	113.94
4	E	401	ADP	N9-C8-N7	-2.08	110.98	113.94
4	C	401	ADP	O2A-PA-O1A	2.05	121.98	112.44
4	D	401	ADP	N9-C8-N7	-2.05	111.03	113.94
4	B	401	ADP	O2A-PA-O1A	2.05	121.96	112.44
4	A	401	ADP	O2A-PA-O1A	2.04	121.95	112.44
4	D	401	ADP	O2A-PA-O1A	2.04	121.94	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	N9-C8-N7	-2.03	111.06	113.94
4	E	401	ADP	O2A-PA-O1A	2.03	121.88	112.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	C5'-O5'-PA-O3A
4	C	401	ADP	C5'-O5'-PA-O3A
4	D	401	ADP	C5'-O5'-PA-O3A
4	E	401	ADP	C5'-O5'-PA-O3A
4	A	401	ADP	C5'-O5'-PA-O1A
4	B	401	ADP	C5'-O5'-PA-O1A
4	C	401	ADP	C5'-O5'-PA-O1A
4	D	401	ADP	C5'-O5'-PA-O1A
4	E	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C3'-C4'-C5'-O5'
4	B	401	ADP	C3'-C4'-C5'-O5'
4	C	401	ADP	C3'-C4'-C5'-O5'
4	D	401	ADP	C3'-C4'-C5'-O5'
4	E	401	ADP	C3'-C4'-C5'-O5'

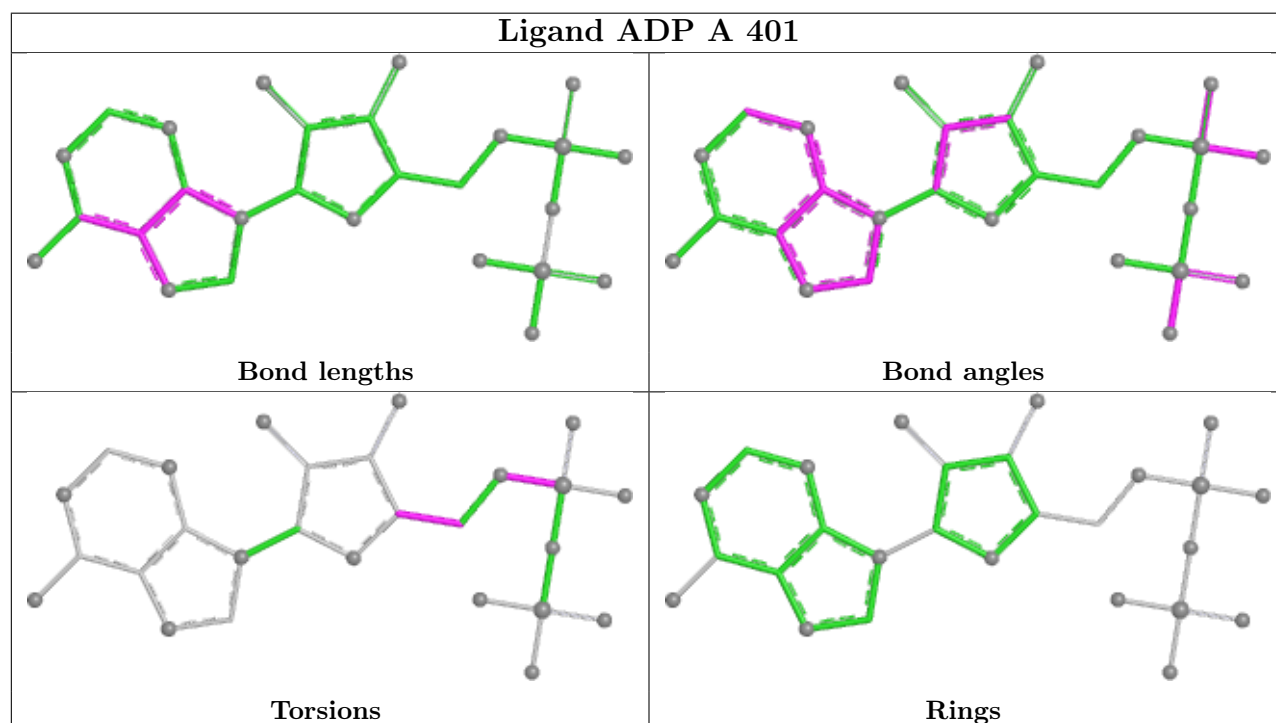
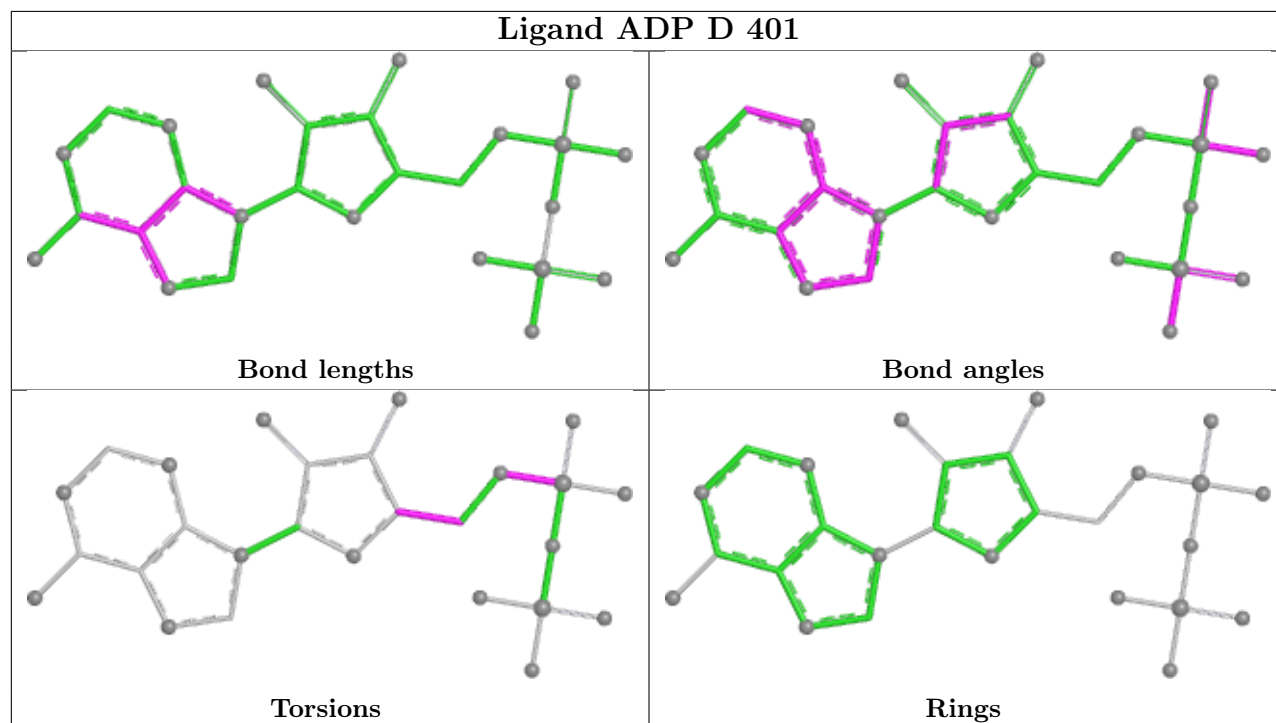
There are no ring outliers.

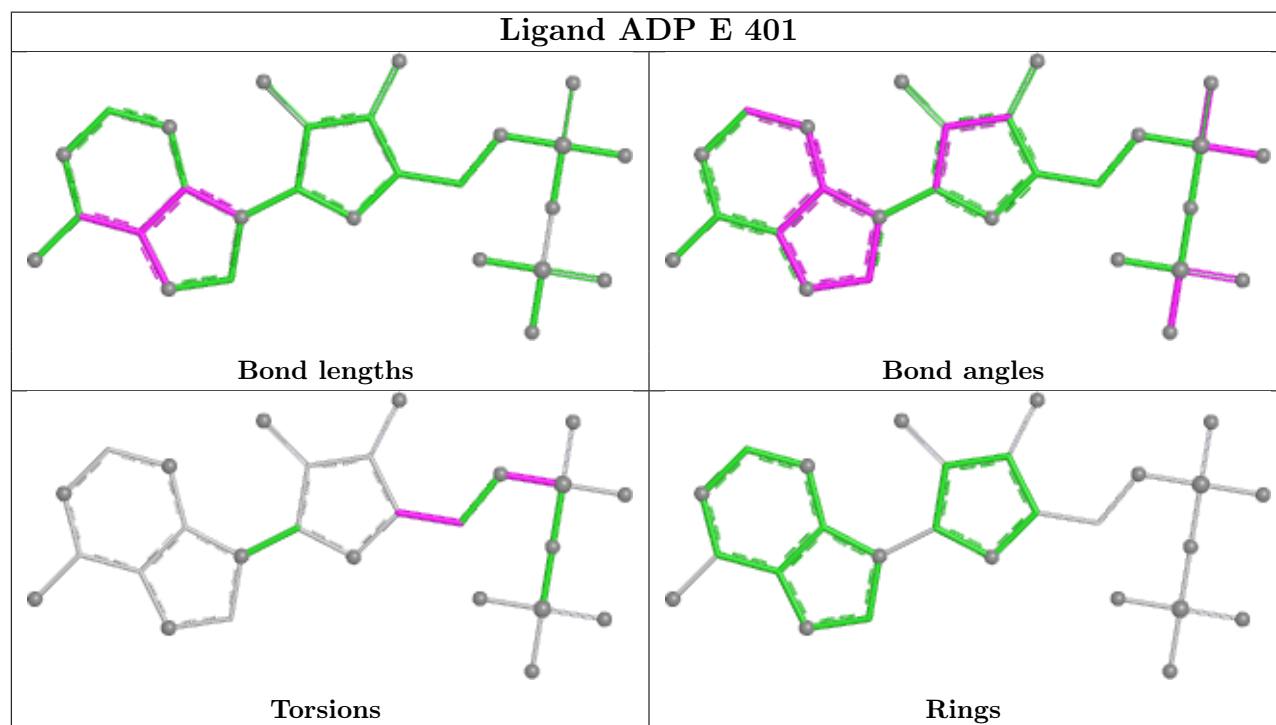
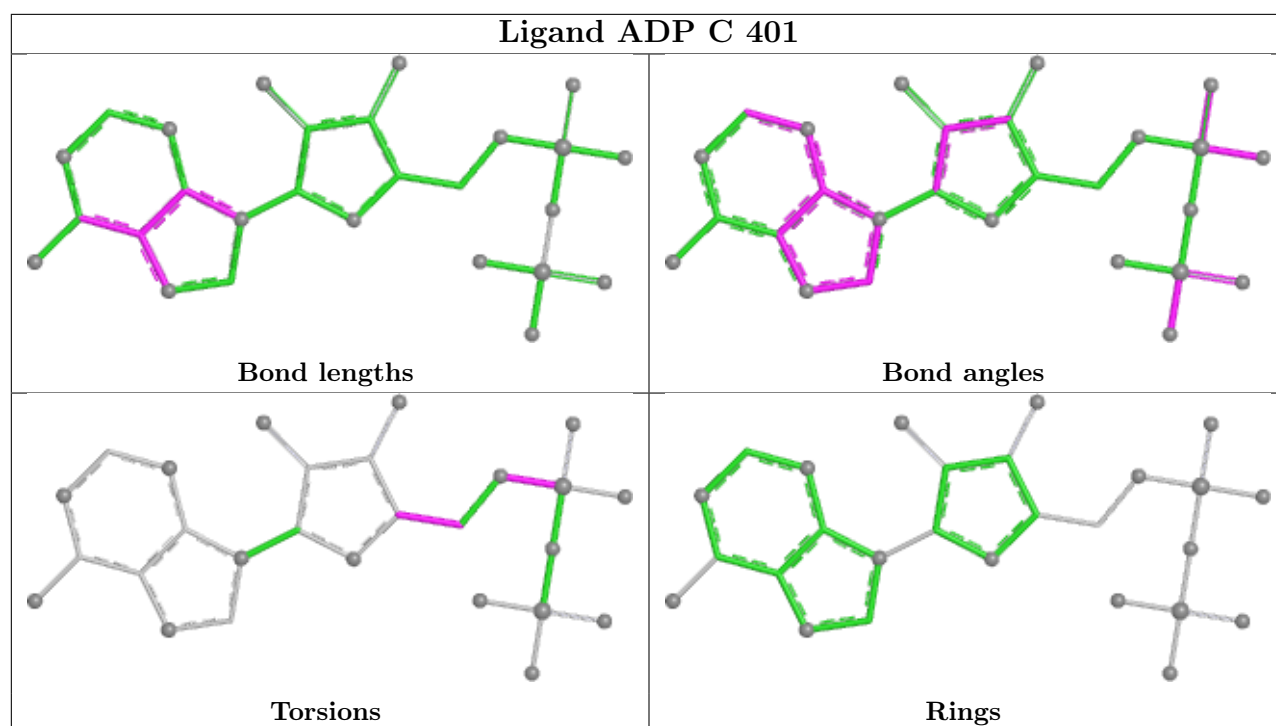
5 monomers are involved in 11 short contacts:

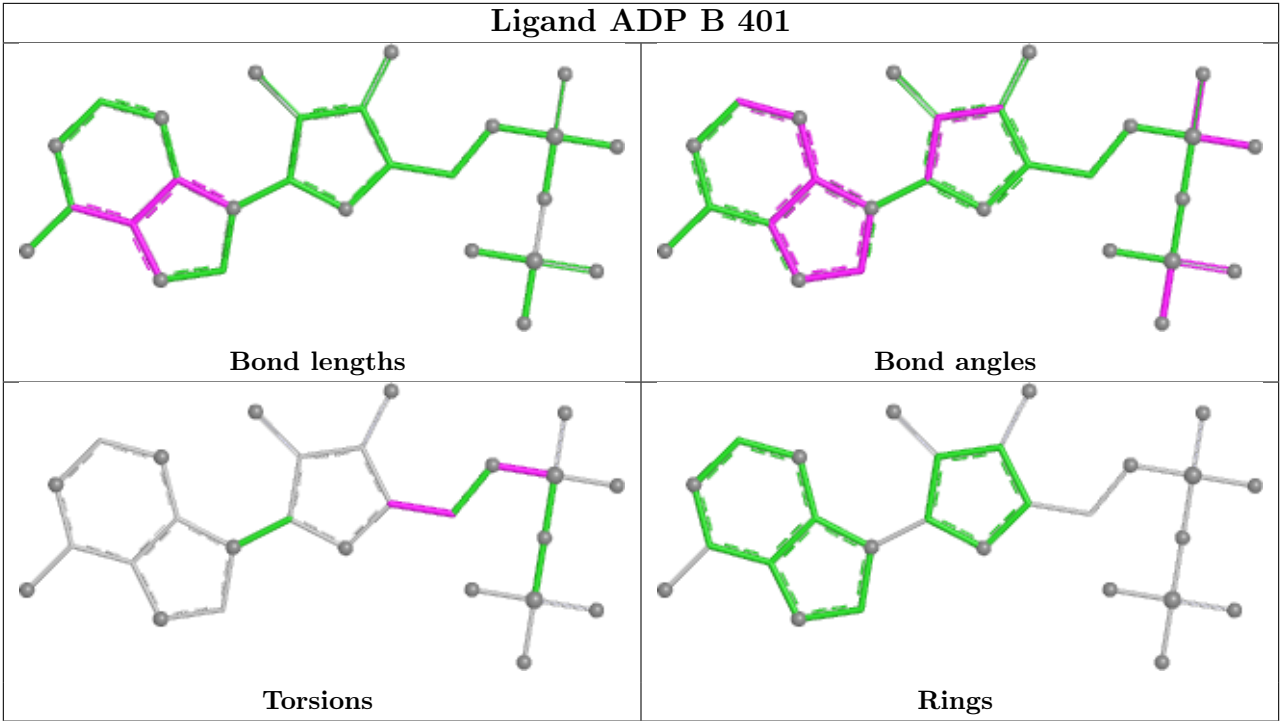
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	2	0
4	A	401	ADP	3	0
4	C	401	ADP	2	0
4	E	401	ADP	2	0
4	B	401	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	195:UNK	C	196:UNK	N	1.14

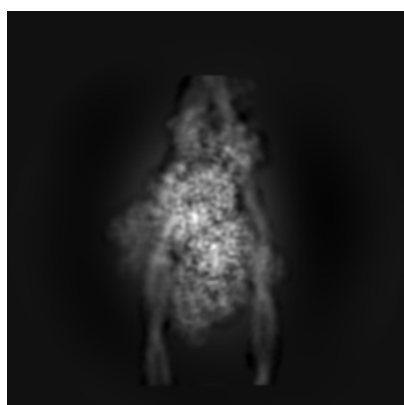
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8164. These allow visual inspection of the internal detail of the map and identification of artifacts.

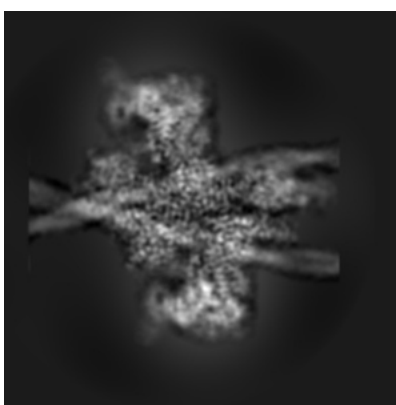
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

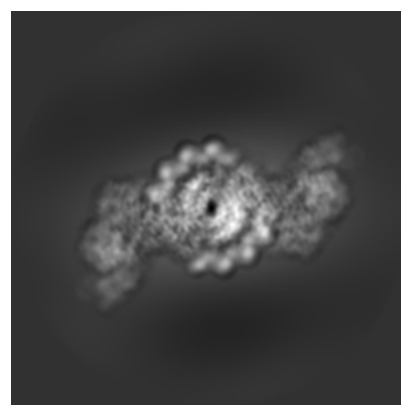
6.1.1 Primary map



X



Y



Z

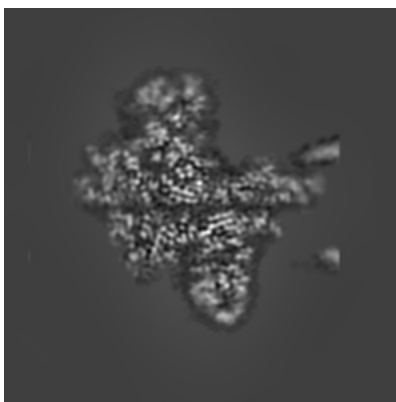
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

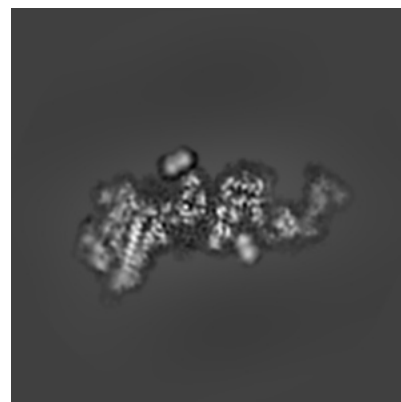
6.2.1 Primary map



X Index: 128



Y Index: 128

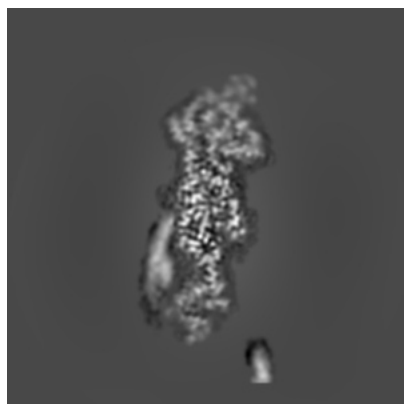


Z Index: 128

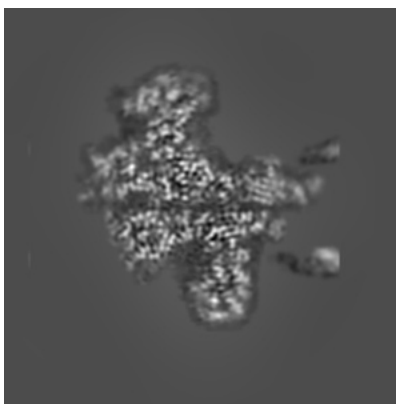
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

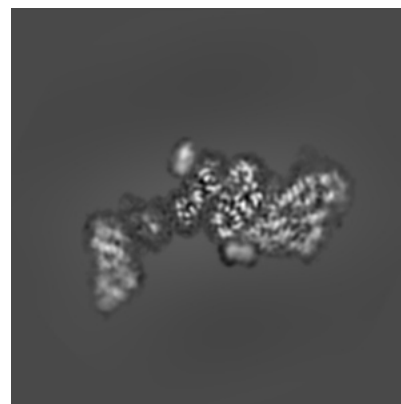
6.3.1 Primary map



X Index: 141



Y Index: 131



Z Index: 113

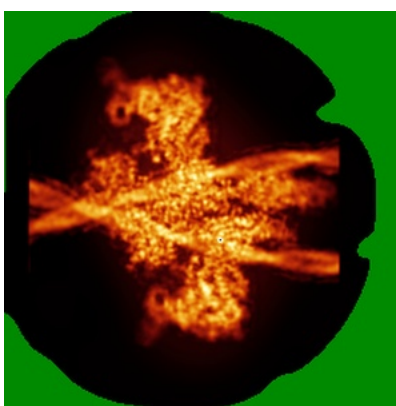
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

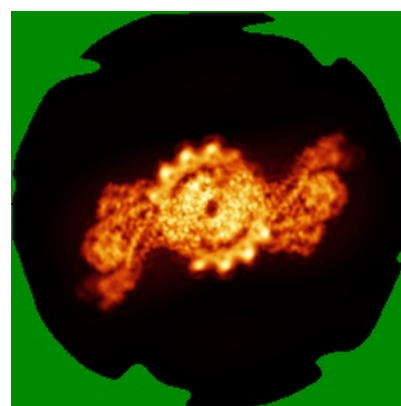
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.049. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

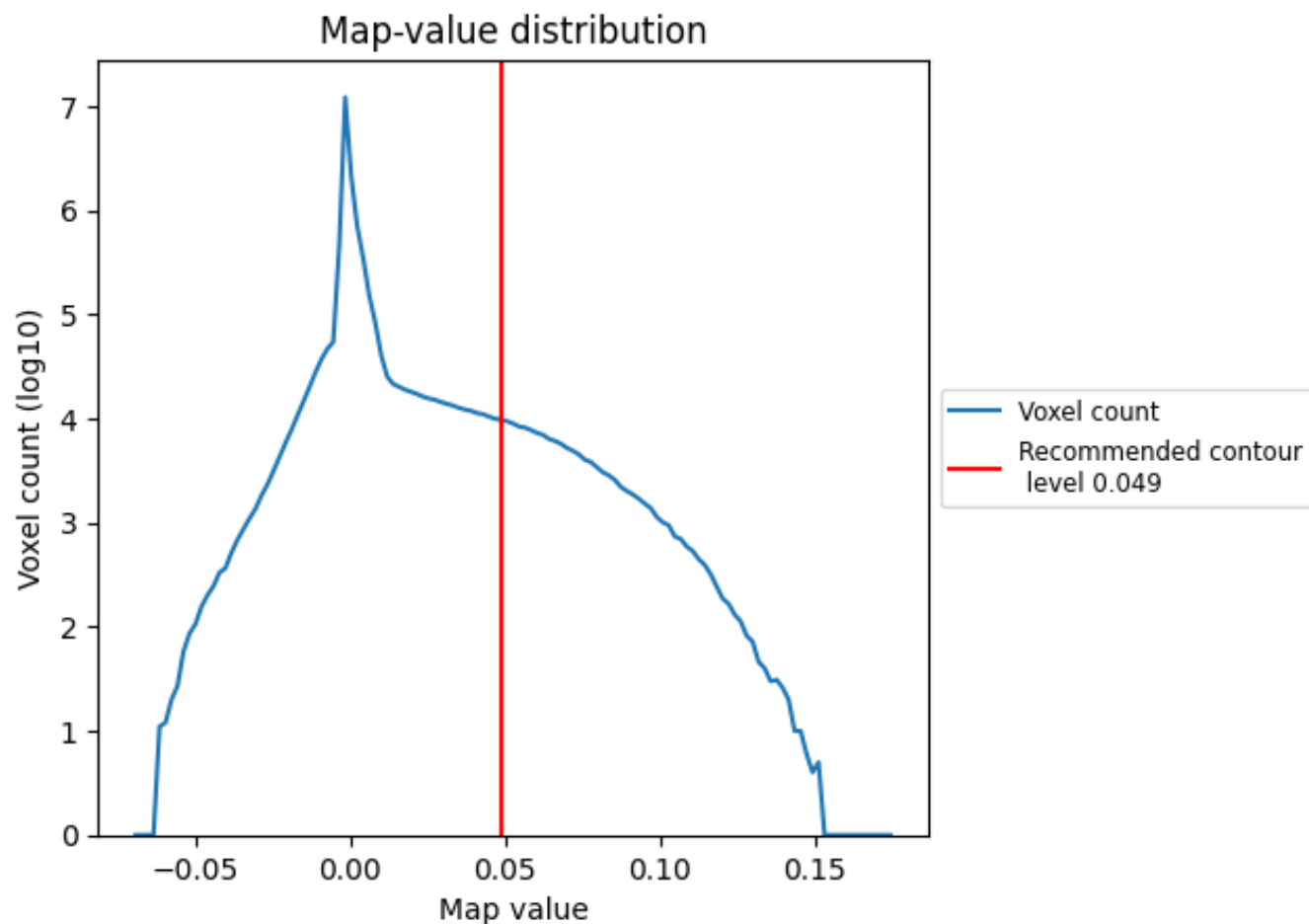
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

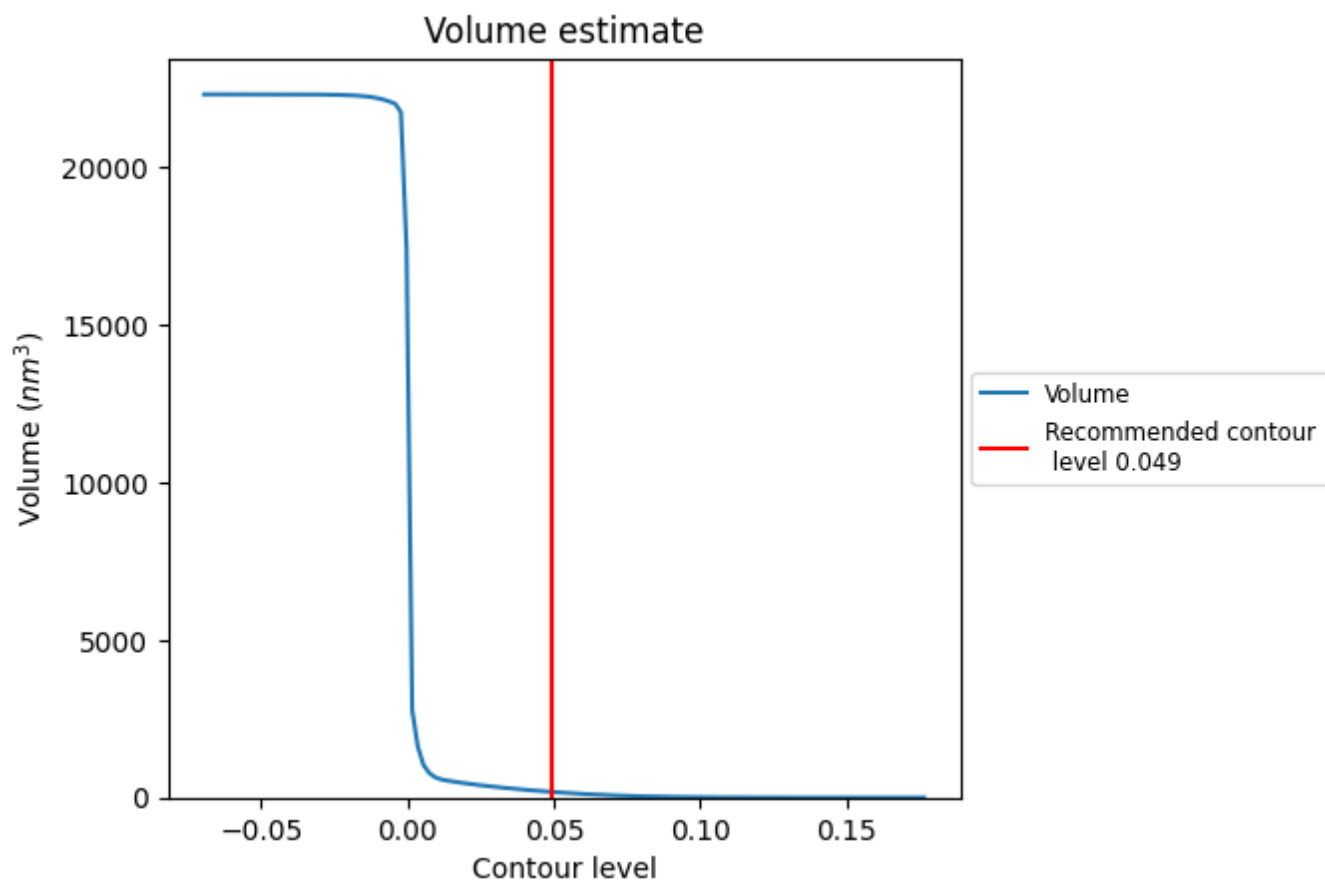
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

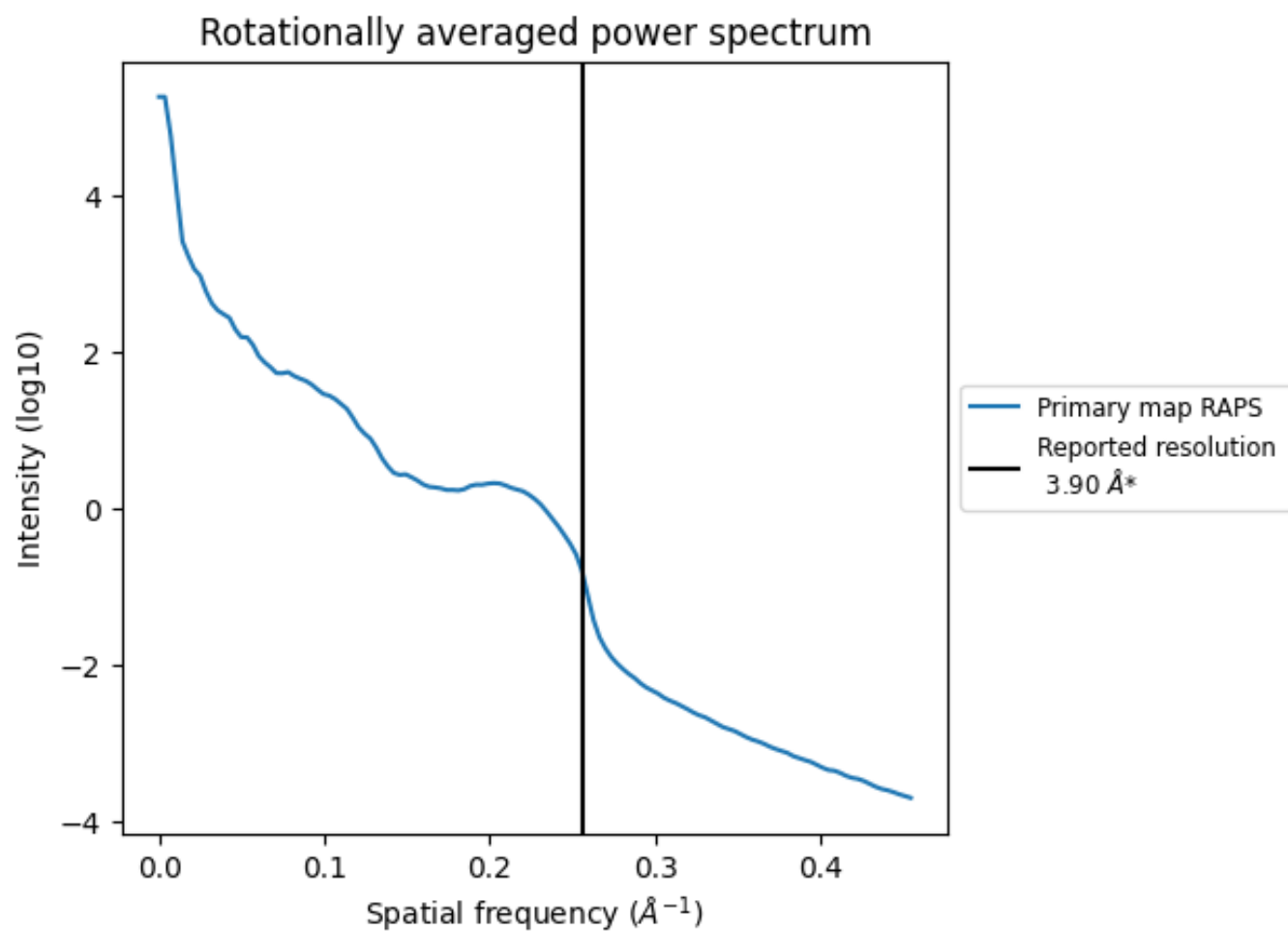
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm^3 ; this corresponds to an approximate mass of 164 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

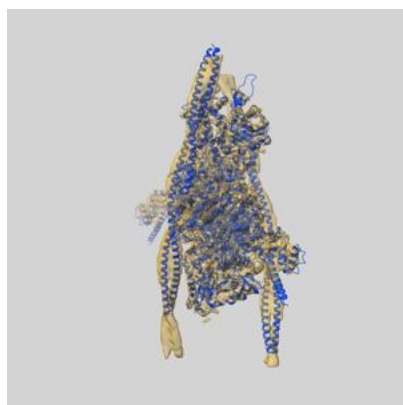
8 Fourier-Shell correlation

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

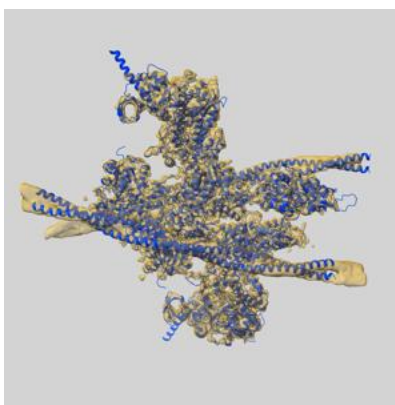
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8164 and PDB model 5JLH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

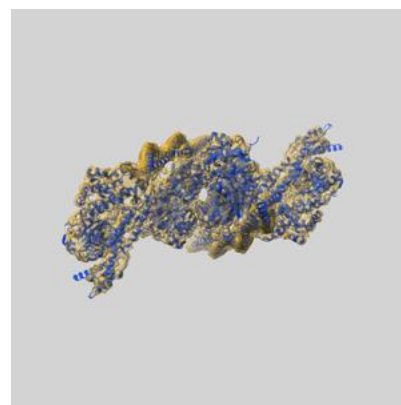
9.1 Map-model overlay [i](#)



X



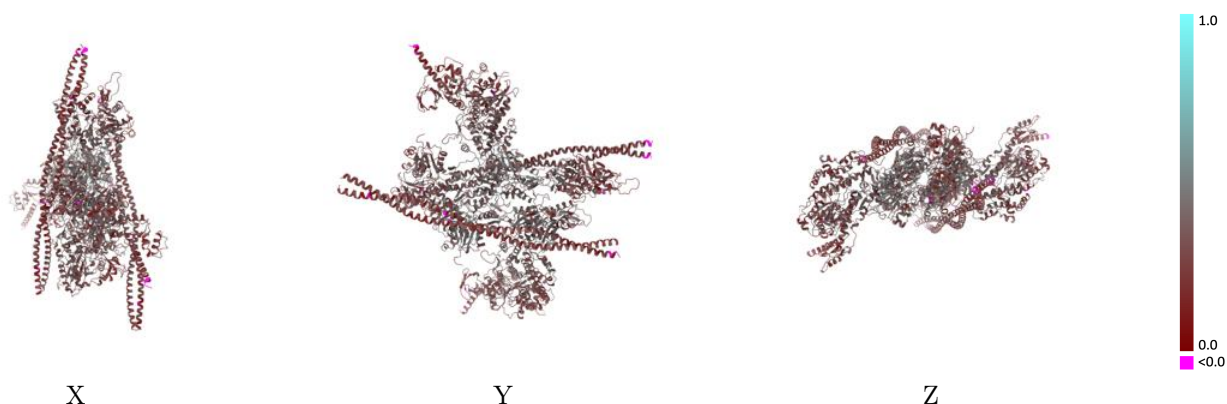
Y



Z

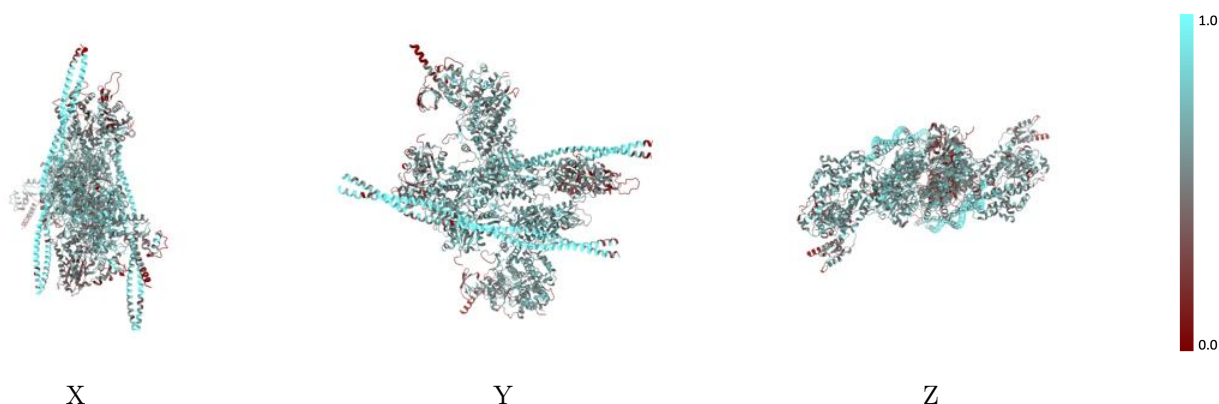
The images above show the 3D surface view of the map at the recommended contour level 0.049 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



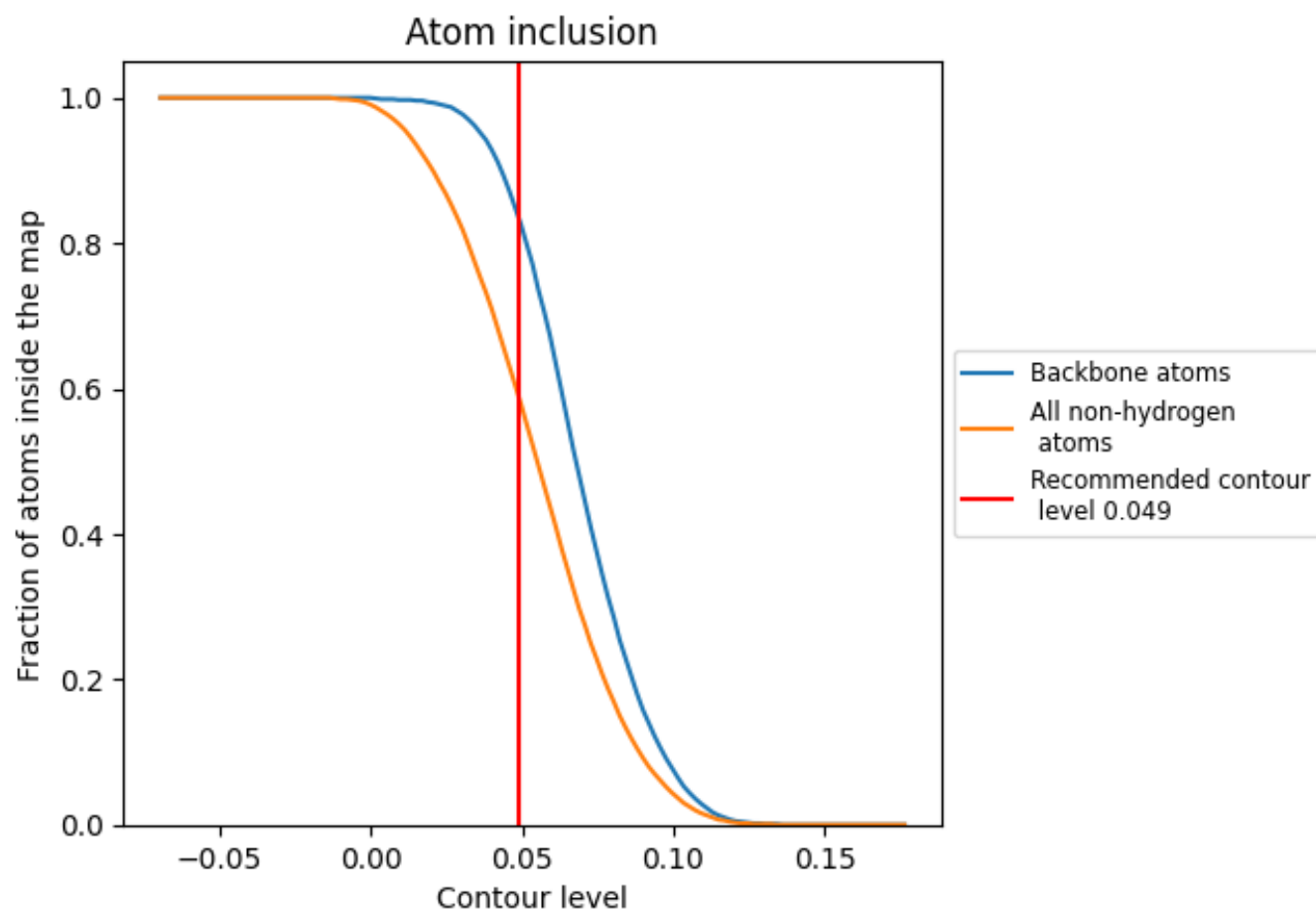
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.049).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5870	0.3410
A	0.6430	0.4160
B	0.4340	0.3140
C	0.5000	0.3480
D	0.6260	0.4000
E	0.6430	0.4110
F	0.5550	0.3190
G	0.5490	0.3170
H	0.8270	0.2390
I	0.8370	0.2440
J	0.8550	0.2480
K	0.8160	0.2460

1.0

0.0

<0.0