



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:43 AM UTC

PDB ID : 5NOL / pdb_00005nol
EMDB ID : EMD-3667
Title : Ca²⁺-induced Movement of Tropomyosin on Native Cardiac Thin Filaments
- "Closed" state
Authors : Risi, C.; Eisner, J.; Belknap, B.; Heeley, D.H.; White, H.D.; Schroeder, G.F.;
Galkin, V.E.
Deposited on : 2017-04-12
Resolution : 8.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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

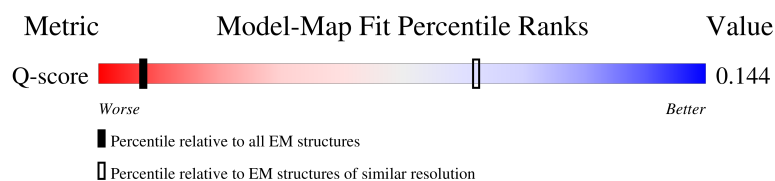
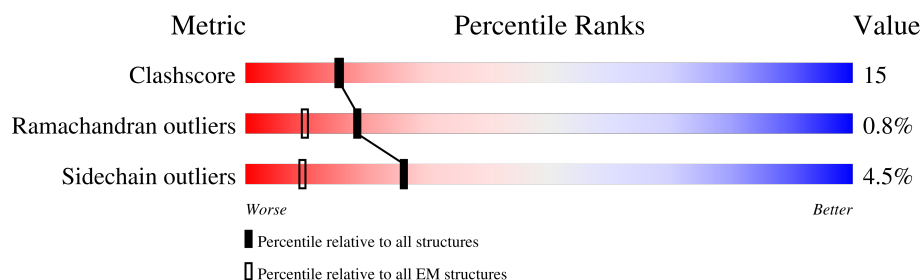
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	361 (7.50 - 8.50)

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	367	10% 61% 33% 5%
1	B	367	9% 61% 34% 5%
1	C	367	8% 60% 34% 5%
1	D	367	8% 60% 34% 5%

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Mol	Chain	Length	Quality of chain
1	E	367	8% 60% 35% 5%
2	F	135	99%
2	G	135	9% 99%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15790 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 Cardiac muscle alpha actin 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	0	0
			2860	1812	481	548	19		
1	B	367	Total	C	N	O	S	0	0
			2860	1812	481	548	19		
1	C	367	Total	C	N	O	S	0	0
			2860	1812	481	548	19		
1	D	367	Total	C	N	O	S	0	0
			2860	1812	481	548	19		
1	E	367	Total	C	N	O	S	0	0
			2860	1812	481	548	19		

- Molecule 2 is a protein called cardiac alpha tropomyosin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	135	Total	C	N	O	0	0
			675	405	135	135		
2	G	135	Total	C	N	O	0	0
			675	405	135	135		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0

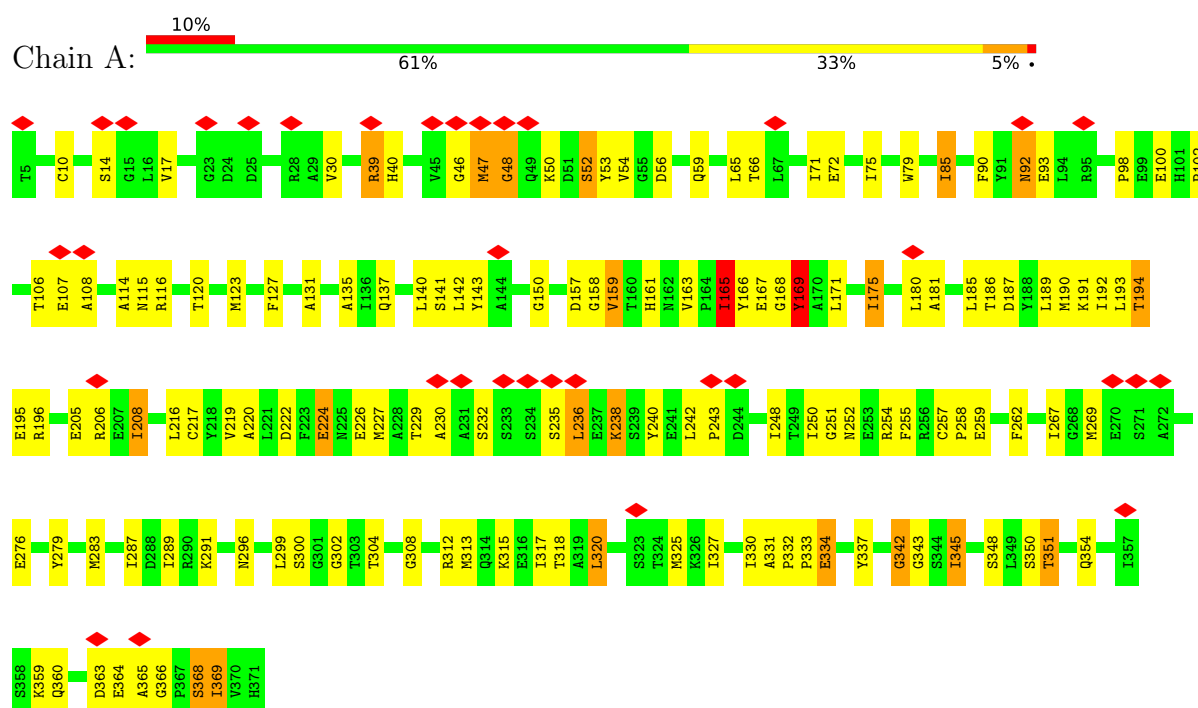
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

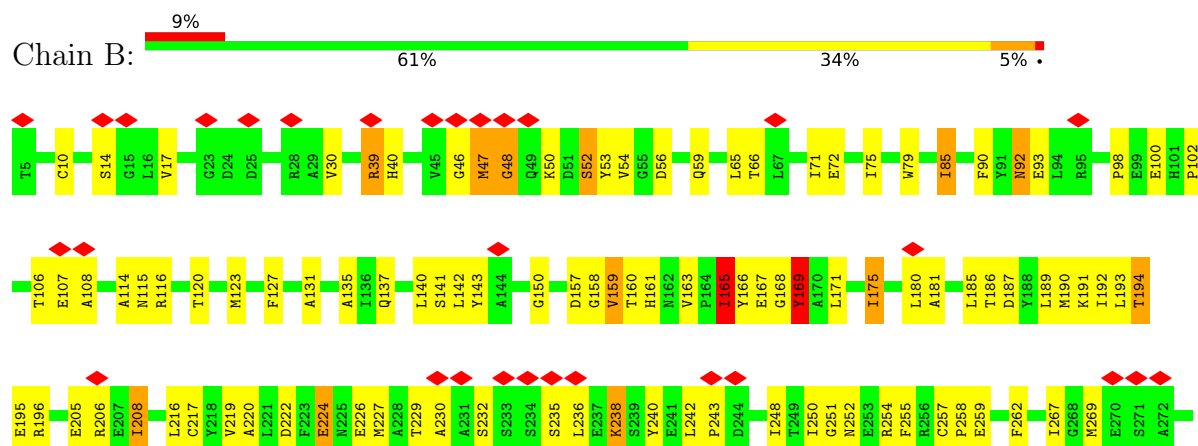
3 Residue-property plots

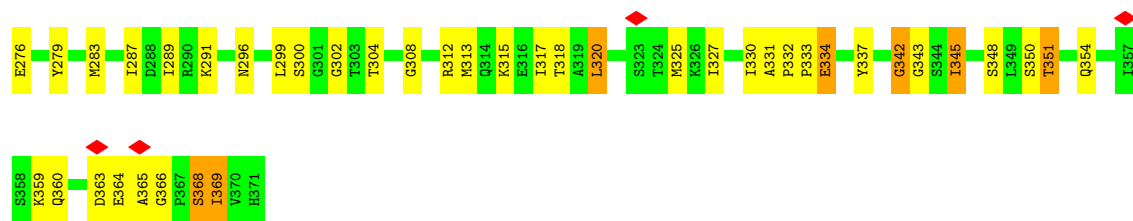
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cardiac muscle alpha actin 1

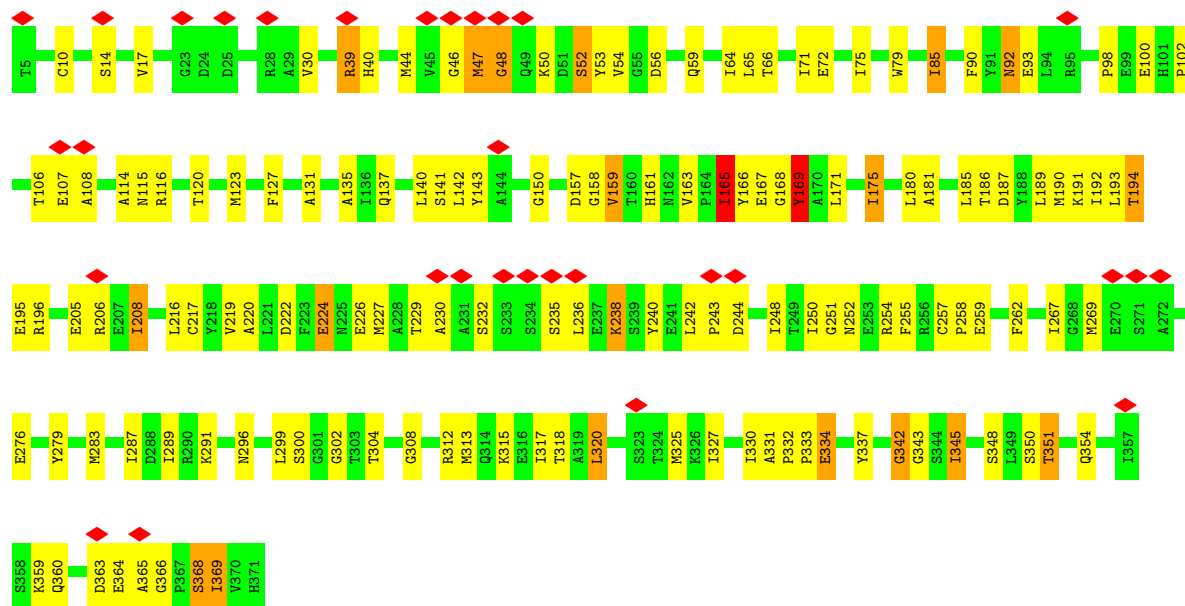


• Molecule 1: Cardiac muscle alpha actin 1

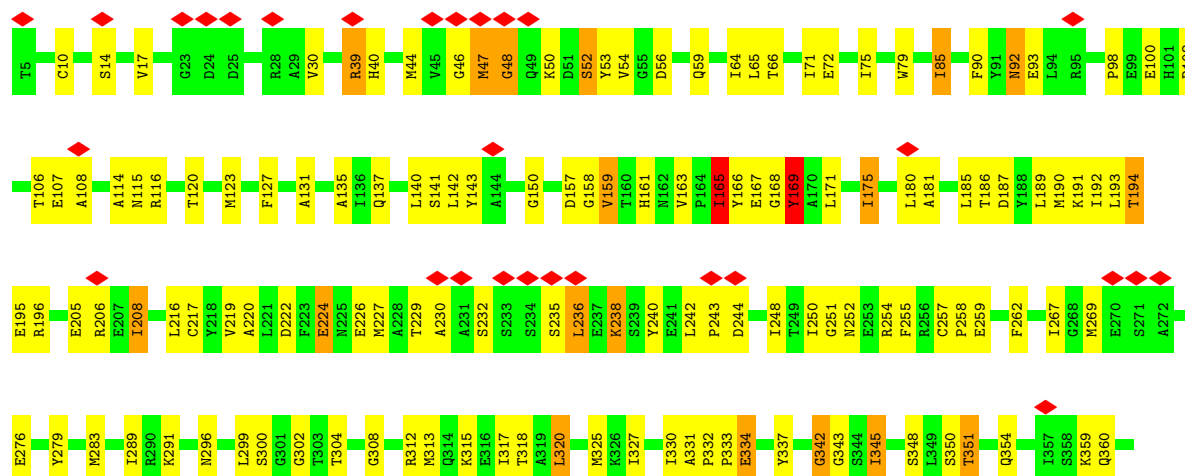




• Molecule 1: Cardiac muscle alpha actin 1

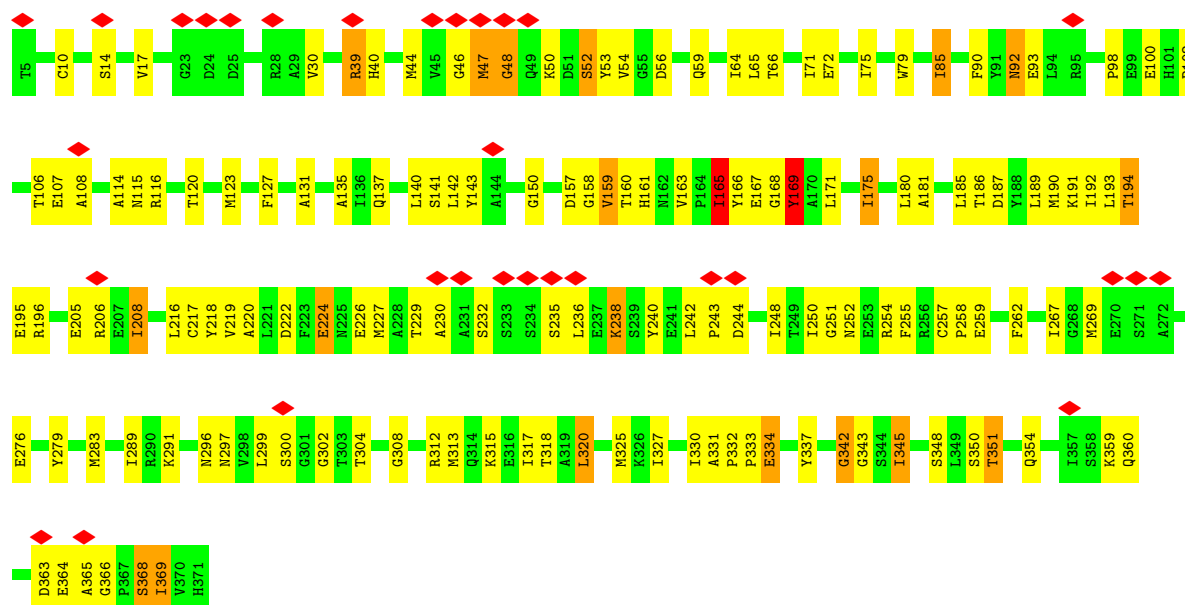


• Molecule 1: Cardiac muscle alpha actin 1

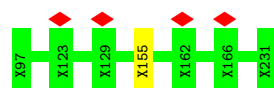




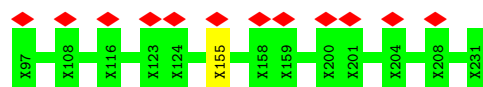
• Molecule 1: Cardiac muscle alpha actin 1



• Molecule 2: cardiac alpha tropomyosin



• Molecule 2: cardiac alpha tropomyosin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.8°, rise=27.4 Å, axial sym=C1	Depositor
Number of segments used	12356	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	123.085	Depositor
Minimum map value	-25.667	Depositor
Average map value	6.146	Depositor
Map value standard deviation	18.196	Depositor
Recommended contour level	50	Depositor
Map size (Å)	157.5, 157.5, 315.0	wwPDB
Map dimensions	150, 150, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.34	6/2922 (0.2%)	1.67	25/3962 (0.6%)
1	B	1.34	7/2922 (0.2%)	1.67	25/3962 (0.6%)
1	C	1.34	7/2922 (0.2%)	1.67	25/3962 (0.6%)
1	D	1.34	7/2922 (0.2%)	1.67	25/3962 (0.6%)
1	E	1.34	7/2922 (0.2%)	1.67	26/3962 (0.7%)
All	All	1.34	34/14610 (0.2%)	1.67	126/19810 (0.6%)

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	29
1	B	0	29
1	C	0	29
1	D	0	29
1	E	0	29
All	All	0	145

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	PRO	C-O	-7.09	1.15	1.24
1	C	243	PRO	C-O	-7.06	1.15	1.24
1	B	243	PRO	C-O	-7.05	1.15	1.24
1	E	243	PRO	C-O	-7.02	1.15	1.24
1	D	243	PRO	C-O	-7.02	1.15	1.24
1	A	165	ILE	C-O	6.79	1.30	1.24
1	B	165	ILE	C-O	6.78	1.30	1.24
1	D	165	ILE	C-O	6.77	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	ILE	C-O	6.72	1.30	1.24
1	E	165	ILE	C-O	6.71	1.30	1.24
1	D	30	VAL	C-O	-6.39	1.16	1.24
1	C	30	VAL	C-O	-6.35	1.16	1.24
1	B	30	VAL	C-O	-6.34	1.16	1.24
1	A	30	VAL	C-O	-6.34	1.16	1.24
1	E	30	VAL	C-O	-6.33	1.16	1.24
1	B	185	LEU	C-O	-5.42	1.17	1.24
1	D	185	LEU	C-O	-5.41	1.17	1.24
1	A	185	LEU	C-O	-5.40	1.17	1.24
1	C	185	LEU	C-O	-5.38	1.17	1.24
1	C	315	LYS	N-CA	-5.37	1.40	1.46
1	D	315	LYS	N-CA	-5.37	1.40	1.46
1	B	315	LYS	N-CA	-5.36	1.40	1.46
1	A	315	LYS	N-CA	-5.36	1.40	1.46
1	E	315	LYS	N-CA	-5.36	1.40	1.46
1	E	185	LEU	C-O	-5.35	1.17	1.24
1	D	123	MET	N-CA	-5.23	1.40	1.46
1	A	123	MET	N-CA	-5.23	1.40	1.46
1	B	123	MET	N-CA	-5.21	1.40	1.46
1	C	123	MET	N-CA	-5.21	1.40	1.46
1	E	123	MET	N-CA	-5.19	1.40	1.46
1	D	143	TYR	C-O	-5.06	1.18	1.24
1	B	143	TYR	C-O	-5.05	1.18	1.24
1	E	143	TYR	C-O	-5.05	1.18	1.24
1	C	143	TYR	C-O	-5.04	1.18	1.24

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	PHE	N-CA-C	-10.66	94.73	110.52
1	E	127	PHE	N-CA-C	-10.66	94.74	110.52
1	B	127	PHE	N-CA-C	-10.66	94.74	110.52
1	C	127	PHE	N-CA-C	-10.65	94.76	110.52
1	D	127	PHE	N-CA-C	-10.65	94.76	110.52
1	E	251	GLY	N-CA-C	7.87	117.37	110.21
1	A	251	GLY	N-CA-C	7.85	117.35	110.21
1	D	251	GLY	N-CA-C	7.84	117.35	110.21
1	C	251	GLY	N-CA-C	7.84	117.34	110.21
1	B	251	GLY	N-CA-C	7.82	117.33	110.21
1	D	320	LEU	N-CA-C	6.86	118.44	110.97
1	C	320	LEU	N-CA-C	6.82	118.40	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	LEU	N-CA-C	6.81	118.40	110.97
1	B	320	LEU	N-CA-C	6.79	118.38	110.97
1	E	320	LEU	N-CA-C	6.79	118.37	110.97
1	B	90	PHE	CA-CB-CG	6.24	120.04	113.80
1	C	90	PHE	CA-CB-CG	6.20	120.00	113.80
1	E	90	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	90	PHE	CA-CB-CG	6.18	119.98	113.80
1	D	90	PHE	CA-CB-CG	6.18	119.98	113.80
1	E	208	ILE	CA-C-O	-6.06	114.74	121.17
1	A	208	ILE	CA-C-O	-6.06	114.75	121.17
1	B	208	ILE	CA-C-O	-6.05	114.75	121.17
1	C	208	ILE	CA-C-O	-6.04	114.77	121.17
1	D	208	ILE	CA-C-O	-6.01	114.80	121.17
1	D	187	ASP	CA-C-O	-5.97	114.09	120.42
1	B	187	ASP	CA-C-O	-5.97	114.10	120.42
1	C	187	ASP	CA-C-O	-5.95	114.11	120.42
1	E	187	ASP	CA-C-O	-5.95	114.12	120.42
1	A	187	ASP	CA-C-O	-5.94	114.12	120.42
1	A	296	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	296	ASN	CA-CB-CG	5.76	118.36	112.60
1	D	296	ASN	CA-CB-CG	5.75	118.35	112.60
1	E	296	ASN	CA-CB-CG	5.74	118.34	112.60
1	C	296	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	39	ARG	N-CA-C	-5.59	103.99	112.04
1	C	39	ARG	N-CA-C	-5.59	104.00	112.04
1	A	39	ARG	N-CA-C	-5.58	104.00	112.04
1	D	39	ARG	N-CA-C	-5.58	104.00	112.04
1	E	39	ARG	N-CA-C	-5.58	104.01	112.04
1	B	354	GLN	O-C-N	-5.43	116.01	122.20
1	D	354	GLN	O-C-N	-5.43	116.01	122.20
1	C	354	GLN	O-C-N	-5.41	116.03	122.20
1	E	354	GLN	O-C-N	-5.40	116.04	122.20
1	A	354	GLN	O-C-N	-5.39	116.06	122.20
1	B	159	VAL	CA-C-O	-5.39	116.43	120.96
1	E	159	VAL	CA-C-O	-5.38	116.44	120.96
1	D	296	ASN	N-CA-C	5.38	119.36	112.26
1	D	143	TYR	CB-CA-C	-5.37	101.87	110.79
1	D	159	VAL	CA-C-O	-5.37	116.45	120.96
1	C	143	TYR	CB-CA-C	-5.37	101.88	110.79
1	C	159	VAL	CA-C-O	-5.37	116.45	120.96
1	E	143	TYR	CB-CA-C	-5.37	101.88	110.79
1	A	296	ASN	N-CA-C	5.37	119.34	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	SER	CA-C-N	-5.37	115.86	122.84
1	C	232	SER	C-N-CA	-5.37	115.86	122.84
1	B	232	SER	CA-C-N	-5.36	115.87	122.84
1	B	232	SER	C-N-CA	-5.36	115.87	122.84
1	A	159	VAL	CA-C-O	-5.36	116.46	120.96
1	E	296	ASN	N-CA-C	5.36	119.33	112.26
1	B	143	TYR	CB-CA-C	-5.36	101.90	110.79
1	C	296	ASN	N-CA-C	5.36	119.33	112.26
1	D	92	ASN	CA-CB-CG	5.36	117.95	112.60
1	E	232	SER	CA-C-N	-5.36	115.88	122.84
1	E	232	SER	C-N-CA	-5.36	115.88	122.84
1	E	359	LYS	O-C-N	5.36	127.59	122.07
1	B	296	ASN	N-CA-C	5.34	119.32	112.26
1	D	232	SER	CA-C-N	-5.34	115.89	122.84
1	D	232	SER	C-N-CA	-5.34	115.89	122.84
1	A	143	TYR	CB-CA-C	-5.34	101.93	110.79
1	A	232	SER	CA-C-N	-5.34	115.90	122.84
1	A	232	SER	C-N-CA	-5.34	115.90	122.84
1	A	92	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	236	LEU	CA-C-O	-5.33	114.77	120.42
1	C	236	LEU	CA-C-O	-5.32	114.78	120.42
1	C	92	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	343	GLY	CA-C-O	-5.32	115.02	120.66
1	B	236	LEU	CA-C-O	-5.32	114.79	120.42
1	D	236	LEU	CA-C-O	-5.32	114.78	120.42
1	E	236	LEU	CA-C-O	-5.32	114.79	120.42
1	D	343	GLY	CA-C-O	-5.31	115.03	120.66
1	C	359	LYS	O-C-N	5.31	127.54	122.07
1	D	359	LYS	O-C-N	5.31	127.54	122.07
1	A	359	LYS	O-C-N	5.30	127.53	122.07
1	B	343	GLY	CA-C-O	-5.30	115.04	120.66
1	E	343	GLY	CA-C-O	-5.30	115.04	120.66
1	C	343	GLY	CA-C-O	-5.30	115.05	120.66
1	E	92	ASN	CA-CB-CG	5.29	117.89	112.60
1	B	359	LYS	O-C-N	5.29	127.52	122.07
1	B	92	ASN	CA-CB-CG	5.29	117.89	112.60
1	B	114	ALA	CA-C-O	-5.24	114.33	120.20
1	E	114	ALA	CA-C-O	-5.24	114.33	120.20
1	B	66	THR	CA-C-O	-5.24	114.98	120.58
1	A	66	THR	CA-C-O	-5.23	114.99	120.58
1	D	66	THR	CA-C-O	-5.23	114.99	120.58
1	A	114	ALA	CA-C-O	-5.22	114.35	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	THR	CA-C-O	-5.22	115.00	120.58
1	A	72	GLU	N-CA-C	5.21	117.30	108.02
1	D	52	SER	CA-C-O	-5.21	114.67	120.66
1	A	52	SER	CA-C-O	-5.21	114.67	120.66
1	C	114	ALA	CA-C-O	-5.21	114.36	120.20
1	B	52	SER	CA-C-O	-5.21	114.67	120.66
1	C	52	SER	CA-C-O	-5.21	114.67	120.66
1	B	72	GLU	N-CA-C	5.21	117.29	108.02
1	E	72	GLU	N-CA-C	5.21	117.29	108.02
1	C	72	GLU	N-CA-C	5.21	117.29	108.02
1	D	72	GLU	N-CA-C	5.21	117.28	108.02
1	E	66	THR	CA-C-O	-5.20	115.01	120.58
1	D	114	ALA	CA-C-O	-5.19	114.39	120.20
1	E	52	SER	CA-C-O	-5.19	114.69	120.66
1	E	17	VAL	CB-CA-C	-5.14	103.94	110.98
1	A	17	VAL	CB-CA-C	-5.13	103.96	110.98
1	C	17	VAL	CB-CA-C	-5.13	103.96	110.98
1	C	85	ILE	CA-C-O	-5.12	115.62	120.95
1	A	85	ILE	CA-C-O	-5.12	115.63	120.95
1	E	85	ILE	CA-C-O	-5.12	115.63	120.95
1	B	85	ILE	CA-C-O	-5.12	115.63	120.95
1	E	345	ILE	CA-C-O	-5.11	115.73	121.05
1	D	17	VAL	CB-CA-C	-5.11	103.98	110.98
1	D	85	ILE	CA-C-O	-5.10	115.65	120.95
1	B	17	VAL	CB-CA-C	-5.09	104.00	110.98
1	A	345	ILE	CA-C-O	-5.09	115.76	121.05
1	C	345	ILE	CA-C-O	-5.06	115.79	121.05
1	D	345	ILE	CA-C-O	-5.04	115.81	121.05
1	B	345	ILE	CA-C-O	-5.04	115.81	121.05
1	E	297	ASN	N-CA-C	5.01	116.95	109.59

There are no chirality outliers.

All (145) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	120	THR	Mainchain
1	A	150	GLY	Mainchain
1	A	167	GLU	Mainchain
1	A	169	TYR	Mainchain
1	A	196	ARG	Mainchain
1	A	238	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	308	GLY	Mainchain
1	A	318	THR	Mainchain
1	A	332	PRO	Mainchain
1	A	334	GLU	Mainchain
1	A	337	TYR	Mainchain
1	A	342	GLY	Mainchain
1	A	348	SER	Mainchain
1	A	350	SER	Mainchain
1	A	351	THR	Mainchain
1	A	363	ASP	Sidechain
1	A	364	GLU	Mainchain
1	A	365	ALA	Mainchain
1	A	366	GLY	Mainchain
1	A	368	SER	Mainchain
1	A	46	GLY	Mainchain
1	A	50	LYS	Mainchain
1	A	52	SER	Mainchain
1	A	56	ASP	Mainchain
1	A	59	GLN	Mainchain
1	A	79	TRP	Mainchain
1	A	93	GLU	Mainchain
1	A	98	PRO	Mainchain
1	B	100	GLU	Mainchain
1	B	120	THR	Mainchain
1	B	150	GLY	Mainchain
1	B	167	GLU	Mainchain
1	B	169	TYR	Mainchain
1	B	196	ARG	Mainchain
1	B	238	LYS	Mainchain
1	B	308	GLY	Mainchain
1	B	318	THR	Mainchain
1	B	332	PRO	Mainchain
1	B	334	GLU	Mainchain
1	B	337	TYR	Mainchain
1	B	342	GLY	Mainchain
1	B	348	SER	Mainchain
1	B	350	SER	Mainchain
1	B	351	THR	Mainchain
1	B	363	ASP	Sidechain
1	B	364	GLU	Mainchain
1	B	365	ALA	Mainchain
1	B	366	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	B	368	SER	Mainchain
1	B	46	GLY	Mainchain
1	B	50	LYS	Mainchain
1	B	52	SER	Mainchain
1	B	56	ASP	Mainchain
1	B	59	GLN	Mainchain
1	B	79	TRP	Mainchain
1	B	93	GLU	Mainchain
1	B	98	PRO	Mainchain
1	C	100	GLU	Mainchain
1	C	120	THR	Mainchain
1	C	150	GLY	Mainchain
1	C	167	GLU	Mainchain
1	C	169	TYR	Mainchain
1	C	196	ARG	Mainchain
1	C	238	LYS	Mainchain
1	C	308	GLY	Mainchain
1	C	318	THR	Mainchain
1	C	332	PRO	Mainchain
1	C	334	GLU	Mainchain
1	C	337	TYR	Mainchain
1	C	342	GLY	Mainchain
1	C	348	SER	Mainchain
1	C	350	SER	Mainchain
1	C	351	THR	Mainchain
1	C	363	ASP	Sidechain
1	C	364	GLU	Mainchain
1	C	365	ALA	Mainchain
1	C	366	GLY	Mainchain
1	C	368	SER	Mainchain
1	C	46	GLY	Mainchain
1	C	50	LYS	Mainchain
1	C	52	SER	Mainchain
1	C	56	ASP	Mainchain
1	C	59	GLN	Mainchain
1	C	79	TRP	Mainchain
1	C	93	GLU	Mainchain
1	C	98	PRO	Mainchain
1	D	100	GLU	Mainchain
1	D	120	THR	Mainchain
1	D	150	GLY	Mainchain
1	D	167	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	169	TYR	Mainchain
1	D	196	ARG	Mainchain
1	D	238	LYS	Mainchain
1	D	308	GLY	Mainchain
1	D	318	THR	Mainchain
1	D	332	PRO	Mainchain
1	D	334	GLU	Mainchain
1	D	337	TYR	Mainchain
1	D	342	GLY	Mainchain
1	D	348	SER	Mainchain
1	D	350	SER	Mainchain
1	D	351	THR	Mainchain
1	D	363	ASP	Sidechain
1	D	364	GLU	Mainchain
1	D	365	ALA	Mainchain
1	D	366	GLY	Mainchain
1	D	368	SER	Mainchain
1	D	46	GLY	Mainchain
1	D	50	LYS	Mainchain
1	D	52	SER	Mainchain
1	D	56	ASP	Mainchain
1	D	59	GLN	Mainchain
1	D	79	TRP	Mainchain
1	D	93	GLU	Mainchain
1	D	98	PRO	Mainchain
1	E	100	GLU	Mainchain
1	E	120	THR	Mainchain
1	E	150	GLY	Mainchain
1	E	167	GLU	Mainchain
1	E	169	TYR	Mainchain
1	E	196	ARG	Mainchain
1	E	238	LYS	Mainchain
1	E	308	GLY	Mainchain
1	E	318	THR	Mainchain
1	E	332	PRO	Mainchain
1	E	334	GLU	Mainchain
1	E	337	TYR	Mainchain
1	E	342	GLY	Mainchain
1	E	348	SER	Mainchain
1	E	350	SER	Mainchain
1	E	351	THR	Mainchain
1	E	363	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	E	364	GLU	Mainchain
1	E	365	ALA	Mainchain
1	E	366	GLY	Mainchain
1	E	368	SER	Mainchain
1	E	46	GLY	Mainchain
1	E	50	LYS	Mainchain
1	E	52	SER	Mainchain
1	E	56	ASP	Mainchain
1	E	59	GLN	Mainchain
1	E	79	TRP	Mainchain
1	E	93	GLU	Mainchain
1	E	98	PRO	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	2860	0	2830	90	0
1	B	2860	0	2831	90	0
1	C	2860	0	2831	92	0
1	D	2860	0	2830	90	0
1	E	2860	0	2831	91	0
2	F	675	0	137	1	0
2	G	675	0	137	1	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	15790	0	14487	445	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 15.

All (445) 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:D:226:GLU:HB3	1:D:255:PHE:CZ	1.49	1.48
1:C:226:GLU:HB3	1:C:255:PHE:CZ	1.49	1.45
1:B:226:GLU:HB3	1:B:255:PHE:CZ	1.49	1.44
1:A:226:GLU:HB3	1:A:255:PHE:CZ	1.49	1.44
1:E:226:GLU:HB3	1:E:255:PHE:CZ	1.49	1.44
1:E:226:GLU:HB3	1:E:255:PHE:CE1	1.75	1.22
1:C:226:GLU:HB3	1:C:255:PHE:CE1	1.75	1.22
1:A:226:GLU:HB3	1:A:255:PHE:CE1	1.75	1.21
1:B:226:GLU:HB3	1:B:255:PHE:CE1	1.75	1.19
1:D:226:GLU:HB3	1:D:255:PHE:CE1	1.75	1.18
1:A:226:GLU:CB	1:A:255:PHE:CZ	2.29	1.16
1:B:226:GLU:CB	1:B:255:PHE:CZ	2.29	1.15
1:C:226:GLU:CB	1:C:255:PHE:CZ	2.29	1.15
1:D:226:GLU:CB	1:D:255:PHE:CZ	2.29	1.14
1:E:226:GLU:CB	1:E:255:PHE:CZ	2.29	1.14
1:A:226:GLU:CB	1:A:255:PHE:CE1	2.32	1.12
1:C:226:GLU:CB	1:C:255:PHE:CE1	2.32	1.12
1:D:226:GLU:CB	1:D:255:PHE:CE1	2.32	1.12
1:E:226:GLU:CB	1:E:255:PHE:CE1	2.32	1.12
1:B:226:GLU:CB	1:B:255:PHE:CE1	2.32	1.11
1:C:226:GLU:HB3	1:C:255:PHE:CE2	1.98	0.99
1:D:226:GLU:HB3	1:D:255:PHE:CE2	1.98	0.98
1:A:226:GLU:HB3	1:A:255:PHE:CE2	1.98	0.98
1:E:226:GLU:HB3	1:E:255:PHE:CE2	1.98	0.98
1:B:226:GLU:HB3	1:B:255:PHE:CE2	1.98	0.97
1:C:220:ALA:HB2	1:C:226:GLU:HG3	1.54	0.90
1:D:220:ALA:HB2	1:D:226:GLU:HG3	1.53	0.90
1:A:220:ALA:HB2	1:A:226:GLU:HG3	1.54	0.90
1:B:220:ALA:HB2	1:B:226:GLU:HG3	1.54	0.89
1:E:220:ALA:HB2	1:E:226:GLU:HG3	1.54	0.88
1:A:226:GLU:O	1:A:229:THR:HG22	1.75	0.86
1:C:226:GLU:HB2	1:C:255:PHE:CE1	2.11	0.86
1:D:226:GLU:O	1:D:229:THR:HG22	1.75	0.86
1:C:226:GLU:O	1:C:229:THR:HG22	1.75	0.85
1:B:226:GLU:O	1:B:229:THR:HG22	1.75	0.85
1:C:222:ASP:OD1	1:C:224:GLU:CD	2.20	0.84
1:E:226:GLU:O	1:E:229:THR:HG22	1.75	0.84
1:B:216:LEU:HD12	1:B:250:ILE:HD11	1.58	0.84
1:B:222:ASP:OD1	1:B:224:GLU:CD	2.20	0.84
1:D:216:LEU:HD12	1:D:250:ILE:HD11	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ASP:OD1	1:E:224:GLU:CD	2.20	0.84
1:E:226:GLU:HB2	1:E:255:PHE:CE1	2.11	0.84
1:A:226:GLU:HB2	1:A:255:PHE:CE1	2.11	0.84
1:D:222:ASP:OD1	1:D:224:GLU:CD	2.20	0.84
1:A:216:LEU:HD12	1:A:250:ILE:HD11	1.58	0.84
1:D:226:GLU:HB2	1:D:255:PHE:CE1	2.11	0.84
1:A:222:ASP:OD1	1:A:224:GLU:CD	2.20	0.83
1:C:216:LEU:HD12	1:C:250:ILE:HD11	1.58	0.83
1:B:226:GLU:HB2	1:B:255:PHE:CE1	2.11	0.83
1:E:216:LEU:HD12	1:E:250:ILE:HD11	1.58	0.83
1:C:220:ALA:HB2	1:C:226:GLU:CG	2.09	0.82
1:E:220:ALA:HB2	1:E:226:GLU:CG	2.09	0.82
1:B:220:ALA:HB2	1:B:226:GLU:CG	2.09	0.82
1:A:220:ALA:HB2	1:A:226:GLU:CG	2.09	0.82
1:D:220:ALA:HB2	1:D:226:GLU:CG	2.09	0.81
1:D:291:LYS:HA	1:D:325:MET:HE1	1.62	0.81
1:A:163:VAL:HG22	1:A:175:ILE:HD13	1.63	0.81
1:E:163:VAL:HG22	1:E:175:ILE:HD13	1.63	0.81
1:B:291:LYS:HA	1:B:325:MET:HE1	1.62	0.81
1:C:163:VAL:HG22	1:C:175:ILE:HD13	1.63	0.81
1:E:291:LYS:HA	1:E:325:MET:HE1	1.62	0.79
1:A:291:LYS:HA	1:A:325:MET:HE1	1.62	0.79
1:C:291:LYS:HA	1:C:325:MET:HE1	1.62	0.79
1:D:75:ILE:HA	1:D:115:ASN:HD21	1.48	0.79
1:B:163:VAL:HG22	1:B:175:ILE:HD13	1.63	0.79
1:D:163:VAL:HG22	1:D:175:ILE:HD13	1.63	0.78
1:D:220:ALA:CB	1:D:226:GLU:CG	2.61	0.78
1:A:220:ALA:CB	1:A:226:GLU:CG	2.61	0.78
1:C:220:ALA:CB	1:C:226:GLU:CG	2.61	0.78
1:E:220:ALA:CB	1:E:226:GLU:CG	2.61	0.78
1:B:220:ALA:CB	1:B:226:GLU:CG	2.61	0.78
1:B:75:ILE:HA	1:B:115:ASN:HD21	1.48	0.78
1:A:75:ILE:HA	1:A:115:ASN:HD21	1.47	0.78
1:E:75:ILE:HA	1:E:115:ASN:HD21	1.48	0.78
1:C:75:ILE:HA	1:C:115:ASN:HD21	1.48	0.77
1:C:142:LEU:HD22	1:C:165:ILE:HG21	1.68	0.76
1:B:142:LEU:HD22	1:B:165:ILE:HG21	1.68	0.76
1:E:142:LEU:HD22	1:E:165:ILE:HG21	1.68	0.75
1:A:142:LEU:HD22	1:A:165:ILE:HG21	1.68	0.75
1:D:142:LEU:HD22	1:D:165:ILE:HG21	1.68	0.75
1:B:230:ALA:HB2	1:B:252:ASN:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:HB2	1:A:252:ASN:HB3	1.72	0.70
1:D:230:ALA:HB2	1:D:252:ASN:HB3	1.72	0.70
1:C:230:ALA:HB2	1:C:252:ASN:HB3	1.72	0.69
1:E:230:ALA:HB2	1:E:252:ASN:HB3	1.72	0.69
1:E:226:GLU:HB3	1:E:255:PHE:CD1	2.29	0.68
1:B:369:ILE:HD12	1:B:369:ILE:C	2.19	0.68
1:C:226:GLU:HB3	1:C:255:PHE:CD1	2.29	0.67
1:D:369:ILE:C	1:D:369:ILE:HD12	2.19	0.67
1:A:226:GLU:HB3	1:A:255:PHE:CD1	2.29	0.67
1:C:369:ILE:C	1:C:369:ILE:HD12	2.19	0.67
1:E:369:ILE:HD12	1:E:369:ILE:C	2.20	0.67
1:A:369:ILE:C	1:A:369:ILE:HD12	2.19	0.67
1:A:190:MET:CE	1:A:206:ARG:HG2	2.25	0.67
1:B:190:MET:CE	1:B:206:ARG:HG2	2.25	0.67
1:C:190:MET:CE	1:C:206:ARG:HG2	2.25	0.67
1:D:190:MET:CE	1:D:206:ARG:HG2	2.25	0.67
1:E:190:MET:CE	1:E:206:ARG:HG2	2.25	0.66
1:D:226:GLU:HB3	1:D:255:PHE:CD1	2.29	0.66
1:C:216:LEU:HD11	1:C:240:TYR:HB2	1.78	0.66
1:A:216:LEU:HD11	1:A:240:TYR:HB2	1.78	0.65
1:D:216:LEU:HD11	1:D:240:TYR:HB2	1.78	0.65
1:E:216:LEU:HD11	1:E:240:TYR:HB2	1.78	0.65
1:B:216:LEU:HD11	1:B:240:TYR:HB2	1.78	0.65
1:B:226:GLU:HB3	1:B:255:PHE:CD1	2.29	0.65
1:E:299:LEU:HB3	1:E:304:THR:HG21	1.78	0.65
1:B:299:LEU:HB3	1:B:304:THR:HG21	1.78	0.64
1:A:299:LEU:HB3	1:A:304:THR:HG21	1.78	0.64
1:B:189:LEU:O	1:B:193:LEU:HB2	1.98	0.64
1:C:299:LEU:HB3	1:C:304:THR:HG21	1.78	0.64
1:D:54:VAL:HG23	1:D:85:ILE:HG22	1.79	0.64
1:E:189:LEU:O	1:E:193:LEU:HB2	1.98	0.64
1:C:54:VAL:HG23	1:C:85:ILE:HG22	1.79	0.64
1:C:189:LEU:O	1:C:193:LEU:HB2	1.98	0.63
1:A:54:VAL:HG23	1:A:85:ILE:HG22	1.79	0.63
1:E:54:VAL:HG23	1:E:85:ILE:HG22	1.79	0.63
1:D:299:LEU:HB3	1:D:304:THR:HG21	1.78	0.63
1:B:54:VAL:HG23	1:B:85:ILE:HG22	1.79	0.63
1:B:220:ALA:CB	1:B:226:GLU:HG2	2.29	0.63
1:D:189:LEU:O	1:D:193:LEU:HB2	1.98	0.63
1:B:304:THR:O	1:B:304:THR:HG22	1.99	0.63
1:A:189:LEU:O	1:A:193:LEU:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:THR:HG22	1:D:304:THR:O	1.99	0.62
1:A:220:ALA:CB	1:A:226:GLU:HG2	2.29	0.62
1:C:220:ALA:CB	1:C:226:GLU:HG2	2.29	0.62
1:A:220:ALA:CB	1:A:226:GLU:HG3	2.28	0.61
1:D:220:ALA:CB	1:D:226:GLU:HG2	2.29	0.61
1:E:304:THR:O	1:E:304:THR:HG22	1.99	0.61
1:E:220:ALA:CB	1:E:226:GLU:HG2	2.29	0.61
1:B:166:TYR:HB3	1:D:64:ILE:HD11	1.83	0.61
1:D:317:ILE:HG22	1:D:327:ILE:HD13	1.83	0.61
1:B:317:ILE:HG22	1:B:327:ILE:HD13	1.83	0.61
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.83	0.61
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.83	0.60
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.83	0.60
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.83	0.60
1:C:304:THR:HG22	1:C:304:THR:O	1.99	0.60
1:A:304:THR:HG22	1:A:304:THR:O	1.99	0.60
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.83	0.60
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.83	0.60
1:C:166:TYR:HB3	1:E:64:ILE:HD11	1.83	0.59
1:C:317:ILE:HG22	1:C:327:ILE:HD13	1.83	0.59
1:E:317:ILE:HG22	1:E:327:ILE:HD13	1.83	0.59
1:A:166:TYR:HB3	1:C:64:ILE:HD11	1.82	0.59
1:E:226:GLU:CB	1:E:255:PHE:CD1	2.86	0.59
1:A:226:GLU:CB	1:A:255:PHE:CD1	2.86	0.58
1:C:226:GLU:CB	1:C:255:PHE:CD1	2.86	0.58
1:E:142:LEU:CD2	1:E:165:ILE:HG21	2.33	0.58
1:A:106:THR:CG2	1:A:137:GLN:HG2	2.34	0.58
1:C:142:LEU:CD2	1:C:165:ILE:HG21	2.33	0.58
1:B:142:LEU:CD2	1:B:165:ILE:HG21	2.33	0.58
1:B:106:THR:CG2	1:B:137:GLN:HG2	2.34	0.58
1:D:106:THR:CG2	1:D:137:GLN:HG2	2.34	0.58
1:D:142:LEU:CD2	1:D:165:ILE:HG21	2.33	0.58
1:A:142:LEU:CD2	1:A:165:ILE:HG21	2.33	0.58
1:C:106:THR:CG2	1:C:137:GLN:HG2	2.34	0.58
1:E:106:THR:CG2	1:E:137:GLN:HG2	2.34	0.58
1:D:220:ALA:HB1	1:D:226:GLU:HG2	1.87	0.57
1:C:220:ALA:HB1	1:C:226:GLU:HG2	1.87	0.57
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.87	0.57
1:C:219:VAL:HG22	1:C:258:PRO:HB2	1.87	0.57
1:A:219:VAL:HG22	1:A:258:PRO:HB2	1.87	0.57
1:A:220:ALA:HB1	1:A:226:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ALA:HB1	1:B:226:GLU:HG2	1.87	0.56
1:B:219:VAL:HG22	1:B:258:PRO:HB2	1.87	0.56
1:D:219:VAL:HG22	1:D:258:PRO:HB2	1.87	0.56
1:D:220:ALA:CB	1:D:226:GLU:HG3	2.28	0.56
1:D:189:LEU:HA	1:D:192:ILE:HG22	1.88	0.56
1:E:220:ALA:HB1	1:E:226:GLU:HG2	1.87	0.56
1:E:158:GLY:C	1:E:159:VAL:HG23	2.32	0.55
1:B:158:GLY:C	1:B:159:VAL:HG23	2.32	0.55
1:B:189:LEU:HA	1:B:192:ILE:HG22	1.88	0.55
1:D:299:LEU:HD12	1:D:331:ALA:HB2	1.89	0.55
1:E:189:LEU:HA	1:E:192:ILE:HG22	1.88	0.55
1:B:220:ALA:CB	1:B:226:GLU:HG3	2.28	0.55
1:B:299:LEU:HD12	1:B:331:ALA:HB2	1.89	0.55
1:E:279:TYR:CE1	1:E:283:MET:HE3	2.42	0.55
1:A:158:GLY:C	1:A:159:VAL:HG23	2.32	0.55
1:A:279:TYR:CE1	1:A:283:MET:HE3	2.42	0.54
1:C:189:LEU:HA	1:C:192:ILE:HG22	1.88	0.54
1:C:279:TYR:CE1	1:C:283:MET:HE3	2.42	0.54
1:E:220:ALA:CB	1:E:226:GLU:HG3	2.28	0.54
1:A:299:LEU:HD12	1:A:331:ALA:HB2	1.89	0.54
1:B:226:GLU:CB	1:B:255:PHE:CD1	2.86	0.54
1:C:158:GLY:C	1:C:159:VAL:HG23	2.32	0.54
1:B:279:TYR:CE1	1:B:283:MET:HE3	2.42	0.54
1:D:53:TYR:CD2	1:D:65:LEU:HD11	2.43	0.54
1:D:158:GLY:C	1:D:159:VAL:HG23	2.32	0.54
1:D:226:GLU:CB	1:D:255:PHE:CD1	2.86	0.54
1:B:53:TYR:CD2	1:B:65:LEU:HD11	2.43	0.54
1:C:299:LEU:HD12	1:C:331:ALA:HB2	1.89	0.54
1:D:279:TYR:CE1	1:D:283:MET:HE3	2.42	0.54
1:A:189:LEU:HA	1:A:192:ILE:HG22	1.88	0.54
1:A:53:TYR:CD2	1:A:65:LEU:HD11	2.43	0.54
1:A:226:GLU:HG3	1:A:255:PHE:CD1	2.43	0.54
1:E:226:GLU:HG3	1:E:255:PHE:CD1	2.43	0.54
1:C:53:TYR:CD2	1:C:65:LEU:HD11	2.43	0.53
1:E:299:LEU:HD12	1:E:331:ALA:HB2	1.89	0.53
1:A:226:GLU:HB3	1:A:255:PHE:CD2	2.44	0.53
1:E:205:GLU:HA	1:E:208:ILE:HD12	1.91	0.53
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.91	0.53
1:C:226:GLU:HB3	1:C:255:PHE:CD2	2.44	0.53
1:E:53:TYR:CD2	1:E:65:LEU:HD11	2.43	0.53
1:C:190:MET:HE3	1:C:206:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:GLU:HA	1:C:208:ILE:HD12	1.91	0.53
1:A:190:MET:HE3	1:A:206:ARG:HG2	1.91	0.53
1:C:226:GLU:HG3	1:C:255:PHE:CD1	2.43	0.53
1:E:190:MET:HE3	1:E:206:ARG:HG2	1.91	0.53
1:E:218:TYR:OH	1:E:226:GLU:OE1	2.22	0.53
1:B:190:MET:HE3	1:B:206:ARG:HG2	1.91	0.53
1:B:226:GLU:HG3	1:B:255:PHE:CD1	2.43	0.53
1:D:190:MET:HE3	1:D:206:ARG:HG2	1.91	0.53
1:D:192:ILE:O	1:D:195:GLU:HG2	2.09	0.53
1:D:226:GLU:C	1:D:255:PHE:CZ	2.87	0.52
1:B:192:ILE:O	1:B:195:GLU:HG2	2.09	0.52
1:D:222:ASP:OD1	1:D:224:GLU:CG	2.57	0.52
1:B:222:ASP:OD1	1:B:224:GLU:CG	2.58	0.52
1:B:226:GLU:C	1:B:255:PHE:CZ	2.87	0.52
1:D:226:GLU:HG3	1:D:255:PHE:CD1	2.43	0.52
1:C:53:TYR:HD2	1:C:65:LEU:HD21	1.75	0.52
1:E:226:GLU:C	1:E:255:PHE:CZ	2.87	0.52
1:B:205:GLU:HA	1:B:208:ILE:HD12	1.90	0.52
1:C:220:ALA:CB	1:C:226:GLU:HG3	2.28	0.52
1:C:226:GLU:C	1:C:255:PHE:CZ	2.87	0.52
1:E:53:TYR:HD2	1:E:65:LEU:HD21	1.75	0.52
1:A:53:TYR:HD2	1:A:65:LEU:HD21	1.75	0.52
1:D:205:GLU:HA	1:D:208:ILE:HD12	1.90	0.52
1:C:192:ILE:O	1:C:195:GLU:HG2	2.09	0.52
1:D:53:TYR:HD2	1:D:65:LEU:HD21	1.75	0.52
1:A:226:GLU:C	1:A:255:PHE:CZ	2.87	0.52
1:E:192:ILE:O	1:E:195:GLU:HG2	2.09	0.51
1:E:222:ASP:OD1	1:E:224:GLU:CG	2.58	0.51
1:A:192:ILE:O	1:A:195:GLU:HG2	2.09	0.51
1:B:53:TYR:HD2	1:B:65:LEU:HD21	1.75	0.51
1:A:222:ASP:OD1	1:A:224:GLU:CG	2.58	0.51
1:C:222:ASP:OD1	1:C:224:GLU:CG	2.58	0.51
1:B:171:LEU:HD11	1:B:289:ILE:HD11	1.93	0.51
1:D:171:LEU:HD11	1:D:289:ILE:HD11	1.93	0.51
1:E:14:SER:HA	1:E:71:ILE:HG23	1.93	0.51
1:D:14:SER:HA	1:D:71:ILE:HG23	1.93	0.50
1:C:14:SER:HA	1:C:71:ILE:HG23	1.93	0.50
1:B:14:SER:HA	1:B:71:ILE:HG23	1.93	0.50
1:B:220:ALA:HB1	1:B:226:GLU:CG	2.42	0.50
1:B:226:GLU:HB3	1:B:255:PHE:CD2	2.44	0.50
1:A:14:SER:HA	1:A:71:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:GLY:HA3	3:D:401:ADP:O5'	2.12	0.50
1:B:242:LEU:HD13	1:B:248:ILE:HG12	1.94	0.50
1:D:226:GLU:HB3	1:D:255:PHE:CD2	2.44	0.50
1:A:171:LEU:HD11	1:A:289:ILE:HD11	1.93	0.50
1:B:302:GLY:HA3	3:B:401:ADP:O5'	2.12	0.50
1:D:242:LEU:HD13	1:D:248:ILE:HG12	1.94	0.50
1:C:171:LEU:HD11	1:C:289:ILE:HD11	1.93	0.49
1:E:171:LEU:HD11	1:E:289:ILE:HD11	1.93	0.49
1:E:302:GLY:HA3	3:E:401:ADP:O5'	2.12	0.49
1:C:242:LEU:HD13	1:C:248:ILE:HG12	1.94	0.49
1:E:242:LEU:HD13	1:E:248:ILE:HG12	1.94	0.49
1:A:108:ALA:HB1	1:A:161:HIS:HE2	1.78	0.49
1:A:242:LEU:HD13	1:A:248:ILE:HG12	1.94	0.49
1:C:108:ALA:HB1	1:C:161:HIS:HE2	1.78	0.49
1:C:302:GLY:HA3	3:C:401:ADP:O5'	2.12	0.49
1:A:302:GLY:HA3	3:A:401:ADP:O5'	2.12	0.48
1:E:226:GLU:HB3	1:E:255:PHE:CD2	2.44	0.48
1:E:220:ALA:HB1	1:E:226:GLU:CG	2.42	0.48
1:A:107:GLU:OE2	1:A:116:ARG:NE	2.47	0.48
1:D:216:LEU:O	1:D:254:ARG:HD3	2.14	0.48
1:E:107:GLU:OE2	1:E:116:ARG:NE	2.47	0.48
1:E:108:ALA:HB1	1:E:161:HIS:HE2	1.78	0.48
1:E:168:GLY:O	1:E:169:TYR:C	2.57	0.48
1:A:168:GLY:O	1:A:169:TYR:C	2.57	0.48
1:D:107:GLU:OE2	1:D:116:ARG:NE	2.47	0.48
1:B:168:GLY:HA2	1:D:44:MET:HG3	1.97	0.47
1:B:107:GLU:OE2	1:B:116:ARG:NE	2.47	0.47
1:D:108:ALA:HB1	1:D:161:HIS:HE2	1.78	0.47
1:A:217:CYS:HA	1:A:254:ARG:HG2	1.97	0.47
1:B:216:LEU:O	1:B:254:ARG:HD3	2.14	0.47
1:B:108:ALA:HB1	1:B:161:HIS:HE2	1.78	0.47
1:E:217:CYS:HA	1:E:254:ARG:HG2	1.97	0.47
1:C:107:GLU:OE2	1:C:116:ARG:NE	2.47	0.47
1:C:168:GLY:O	1:C:169:TYR:C	2.57	0.47
1:A:216:LEU:O	1:A:254:ARG:HD3	2.14	0.47
1:B:168:GLY:O	1:B:169:TYR:C	2.57	0.47
1:C:216:LEU:O	1:C:254:ARG:HD3	2.14	0.47
1:A:47:MET:O	1:A:48:GLY:C	2.58	0.47
1:A:222:ASP:OD1	1:A:224:GLU:HG2	2.16	0.46
1:E:47:MET:O	1:E:48:GLY:C	2.58	0.46
1:E:267:ILE:HG22	1:E:267:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLY:HA2	1:C:44:MET:HG3	1.97	0.46
1:A:276:GLU:HG3	1:A:320:LEU:HD11	1.98	0.46
1:B:47:MET:O	1:B:48:GLY:C	2.58	0.46
1:B:267:ILE:O	1:B:267:ILE:HG22	2.16	0.46
1:C:276:GLU:HG3	1:C:320:LEU:HD11	1.98	0.46
1:E:276:GLU:HG3	1:E:320:LEU:HD11	1.98	0.46
1:B:222:ASP:OD1	1:B:224:GLU:HG2	2.16	0.46
1:C:168:GLY:HA2	1:E:44:MET:HG3	1.97	0.46
1:D:47:MET:O	1:D:48:GLY:C	2.58	0.46
1:E:166:TYR:HB2	1:E:289:ILE:HD12	1.98	0.46
1:A:166:TYR:HB2	1:A:289:ILE:HD12	1.98	0.46
1:B:166:TYR:HB2	1:B:289:ILE:HD12	1.98	0.46
1:C:166:TYR:HB2	1:C:289:ILE:HD12	1.98	0.46
1:C:217:CYS:HA	1:C:254:ARG:HG2	1.97	0.46
1:E:216:LEU:O	1:E:254:ARG:HD3	2.14	0.46
1:B:276:GLU:HG3	1:B:320:LEU:HD11	1.98	0.46
1:D:168:GLY:O	1:D:169:TYR:C	2.57	0.46
1:E:157:ASP:C	1:E:181:ALA:HB1	2.41	0.46
1:E:222:ASP:OD1	1:E:224:GLU:HG2	2.16	0.46
1:C:157:ASP:C	1:C:181:ALA:HB1	2.41	0.46
1:D:157:ASP:C	1:D:181:ALA:HB1	2.41	0.46
1:D:166:TYR:HB2	1:D:289:ILE:HD12	1.98	0.46
1:D:276:GLU:HG3	1:D:320:LEU:HD11	1.98	0.46
1:C:47:MET:O	1:C:48:GLY:C	2.58	0.46
1:E:304:THR:O	1:E:304:THR:CG2	2.64	0.46
1:E:369:ILE:C	1:E:369:ILE:CD1	2.87	0.46
1:B:217:CYS:HA	1:B:254:ARG:HG2	1.97	0.46
1:C:267:ILE:HG22	1:C:267:ILE:O	2.16	0.46
1:A:267:ILE:HG22	1:A:267:ILE:O	2.16	0.45
1:C:180:LEU:HG	1:C:269:MET:HE1	1.99	0.45
1:C:222:ASP:OD1	1:C:224:GLU:HG2	2.16	0.45
1:E:180:LEU:HG	1:E:269:MET:HE1	1.99	0.45
1:A:180:LEU:HG	1:A:269:MET:HE1	1.98	0.45
1:A:267:ILE:O	1:A:267:ILE:CG2	2.64	0.45
1:D:217:CYS:HA	1:D:254:ARG:HG2	1.97	0.45
2:F:155:UNK:HA	2:G:155:UNK:HA	1.98	0.45
1:A:157:ASP:C	1:A:181:ALA:HB1	2.41	0.45
1:D:267:ILE:O	1:D:267:ILE:HG22	2.16	0.45
1:D:222:ASP:OD1	1:D:224:GLU:HG2	2.16	0.45
1:B:180:LEU:HG	1:B:269:MET:HE1	1.99	0.45
1:D:180:LEU:HG	1:D:269:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TYR:CD2	1:A:65:LEU:HD21	2.52	0.45
1:B:157:ASP:C	1:B:181:ALA:HB1	2.41	0.45
1:B:190:MET:HE1	1:B:206:ARG:HG2	1.98	0.45
1:C:53:TYR:CD2	1:C:65:LEU:HD21	2.52	0.45
1:B:369:ILE:C	1:B:369:ILE:CD1	2.87	0.45
1:E:53:TYR:CD2	1:E:65:LEU:HD21	2.52	0.45
1:A:216:LEU:HD22	1:A:238:LYS:HD2	1.99	0.45
1:A:342:GLY:HA2	1:A:345:ILE:HG22	1.99	0.45
1:B:267:ILE:O	1:B:267:ILE:CG2	2.64	0.45
1:C:216:LEU:HD22	1:C:238:LYS:HD2	1.99	0.45
1:A:190:MET:HE1	1:A:206:ARG:HG2	1.98	0.44
1:B:53:TYR:CD2	1:B:65:LEU:HD21	2.52	0.44
1:D:190:MET:HE1	1:D:206:ARG:HG2	1.98	0.44
1:E:267:ILE:O	1:E:267:ILE:CG2	2.64	0.44
1:A:304:THR:O	1:A:304:THR:CG2	2.64	0.44
1:C:342:GLY:HA2	1:C:345:ILE:HG22	1.99	0.44
1:E:216:LEU:HD22	1:E:238:LYS:HD2	1.99	0.44
1:C:135:ALA:HB1	1:C:140:LEU:HD11	2.00	0.44
1:C:190:MET:HE1	1:C:206:ARG:HG2	1.98	0.44
1:C:267:ILE:O	1:C:267:ILE:CG2	2.64	0.44
1:D:267:ILE:O	1:D:267:ILE:CG2	2.64	0.44
1:E:135:ALA:HB1	1:E:140:LEU:HD11	2.00	0.44
1:E:190:MET:HE1	1:E:206:ARG:HG2	1.98	0.44
1:D:53:TYR:CD2	1:D:65:LEU:HD21	2.52	0.44
1:E:342:GLY:HA2	1:E:345:ILE:HG22	1.99	0.44
1:A:135:ALA:HB1	1:A:140:LEU:HD11	2.00	0.44
1:A:313:MET:O	1:A:317:ILE:HD12	2.18	0.44
1:A:333:PRO:O	1:A:334:GLU:HB2	2.18	0.44
1:D:102:PRO:HA	1:D:131:ALA:O	2.18	0.44
1:E:333:PRO:O	1:E:334:GLU:HB2	2.18	0.44
1:B:304:THR:O	1:B:304:THR:CG2	2.64	0.44
1:E:313:MET:O	1:E:317:ILE:HD12	2.18	0.44
1:A:54:VAL:CG2	1:A:85:ILE:HG22	2.47	0.44
1:A:220:ALA:HB1	1:A:226:GLU:CG	2.42	0.44
1:B:216:LEU:HD22	1:B:238:LYS:HD2	1.99	0.44
1:B:342:GLY:HA2	1:B:345:ILE:HG22	1.99	0.44
1:C:313:MET:O	1:C:317:ILE:HD12	2.18	0.44
1:D:333:PRO:O	1:D:334:GLU:HB2	2.18	0.44
1:D:216:LEU:HD22	1:D:238:LYS:HD2	1.99	0.43
1:D:342:GLY:HA2	1:D:345:ILE:HG22	1.99	0.43
1:D:369:ILE:C	1:D:369:ILE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HA	1:A:131:ALA:O	2.18	0.43
1:B:262:PHE:CE2	1:B:312:ARG:HD3	2.54	0.43
1:C:333:PRO:O	1:C:334:GLU:HB2	2.18	0.43
1:D:313:MET:O	1:D:317:ILE:HD12	2.18	0.43
1:D:262:PHE:CE2	1:D:312:ARG:HD3	2.54	0.43
1:E:102:PRO:HA	1:E:131:ALA:O	2.18	0.43
1:E:191:LYS:O	1:E:194:THR:HG22	2.18	0.43
1:A:369:ILE:HD12	1:A:369:ILE:O	2.19	0.43
1:B:313:MET:O	1:B:317:ILE:HD12	2.18	0.43
1:B:333:PRO:O	1:B:334:GLU:HB2	2.18	0.43
1:D:54:VAL:CG2	1:D:85:ILE:HG22	2.47	0.43
1:D:191:LYS:O	1:D:194:THR:HG22	2.18	0.43
1:E:54:VAL:CG2	1:E:85:ILE:HG22	2.47	0.43
1:E:163:VAL:HG13	1:E:175:ILE:HD11	2.01	0.43
1:A:262:PHE:CE2	1:A:312:ARG:HD3	2.54	0.43
1:C:304:THR:O	1:C:304:THR:CG2	2.64	0.43
1:C:102:PRO:HA	1:C:131:ALA:O	2.18	0.43
1:E:369:ILE:HD12	1:E:369:ILE:O	2.19	0.43
1:A:163:VAL:HG13	1:A:175:ILE:HD11	2.01	0.43
1:B:191:LYS:O	1:B:194:THR:HG22	2.18	0.43
1:C:262:PHE:CE2	1:C:312:ARG:HD3	2.54	0.43
1:D:369:ILE:HD12	1:D:369:ILE:O	2.19	0.43
1:B:102:PRO:HA	1:B:131:ALA:O	2.18	0.43
1:B:135:ALA:HB1	1:B:140:LEU:HD11	1.99	0.43
1:C:163:VAL:HG13	1:C:175:ILE:HD11	2.01	0.43
1:D:220:ALA:HB1	1:D:226:GLU:CG	2.42	0.43
1:D:304:THR:O	1:D:304:THR:CG2	2.64	0.43
1:E:262:PHE:CE2	1:E:312:ARG:HD3	2.54	0.43
1:A:191:LYS:O	1:A:194:THR:HG22	2.19	0.43
1:B:54:VAL:CG2	1:B:85:ILE:HG22	2.47	0.42
1:B:190:MET:HE2	1:B:190:MET:HB2	1.97	0.42
1:D:135:ALA:HB1	1:D:140:LEU:HD11	2.00	0.42
1:C:369:ILE:C	1:C:369:ILE:CD1	2.87	0.42
1:A:141:SER:HB2	1:A:300:SER:OG	2.20	0.42
1:C:369:ILE:HD12	1:C:369:ILE:O	2.19	0.42
1:D:39:ARG:HD2	1:D:40:HIS:NE2	2.35	0.42
1:A:39:ARG:HD2	1:A:40:HIS:NE2	2.35	0.42
1:A:287:ILE:HG23	1:C:244:ASP:HB2	2.02	0.42
1:B:39:ARG:HD2	1:B:40:HIS:NE2	2.35	0.42
1:C:39:ARG:HD2	1:C:40:HIS:NE2	2.35	0.42
1:C:54:VAL:CG2	1:C:85:ILE:HG22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:SER:HB2	1:D:300:SER:OG	2.20	0.42
1:D:259:GLU:OE2	1:D:312:ARG:NH2	2.53	0.42
1:E:190:MET:HE1	1:E:206:ARG:HA	2.02	0.42
1:A:229:THR:HG21	1:A:236:LEU:HD22	1.87	0.42
1:B:369:ILE:HD12	1:B:369:ILE:O	2.19	0.42
1:C:141:SER:HB2	1:C:300:SER:OG	2.20	0.42
1:C:190:MET:HE1	1:C:206:ARG:HA	2.02	0.42
1:C:220:ALA:HB1	1:C:226:GLU:CG	2.42	0.42
1:C:287:ILE:HG23	1:E:244:ASP:HB2	2.02	0.42
1:E:39:ARG:HD2	1:E:40:HIS:NE2	2.35	0.42
1:B:163:VAL:HG13	1:B:175:ILE:HD11	2.01	0.41
1:D:163:VAL:HG13	1:D:175:ILE:HD11	2.01	0.41
1:A:369:ILE:C	1:A:369:ILE:CD1	2.87	0.41
1:B:158:GLY:C	1:B:159:VAL:CG2	2.93	0.41
1:C:191:LYS:O	1:C:194:THR:HG22	2.19	0.41
1:E:259:GLU:OE2	1:E:312:ARG:NH2	2.53	0.41
1:B:259:GLU:OE2	1:B:312:ARG:NH2	2.53	0.41
1:B:141:SER:HB2	1:B:300:SER:OG	2.20	0.41
1:C:259:GLU:OE2	1:C:312:ARG:NH2	2.53	0.41
1:D:158:GLY:C	1:D:159:VAL:CG2	2.93	0.41
1:D:291:LYS:CA	1:D:325:MET:HE1	2.43	0.41
1:E:141:SER:HB2	1:E:300:SER:OG	2.20	0.41
1:A:190:MET:HE1	1:A:206:ARG:HA	2.02	0.41
1:D:190:MET:HE1	1:D:206:ARG:HA	2.02	0.41
1:A:158:GLY:C	1:A:159:VAL:CG2	2.93	0.41
1:B:190:MET:HE1	1:B:206:ARG:HA	2.02	0.41
1:C:158:GLY:C	1:C:159:VAL:CG2	2.93	0.41
1:A:259:GLU:OE2	1:A:312:ARG:NH2	2.53	0.41
1:D:229:THR:HG21	1:D:236:LEU:HD22	1.87	0.41
1:B:160:THR:OG1	1:B:180:LEU:O	2.37	0.41
1:E:158:GLY:C	1:E:159:VAL:CG2	2.93	0.41
1:B:287:ILE:HG23	1:D:244:ASP:HB2	2.02	0.40
1:C:226:GLU:HB3	1:C:255:PHE:CG	2.56	0.40
1:E:226:GLU:HB3	1:E:255:PHE:CG	2.56	0.40
1:E:160:THR:OG1	1:E:180:LEU:O	2.37	0.40
1:A:226:GLU:HB3	1:A:255:PHE:CG	2.56	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	365/367 (100%)	351 (96%)	11 (3%)	3 (1%)	16	54
1	B	365/367 (100%)	351 (96%)	11 (3%)	3 (1%)	16	54
1	C	365/367 (100%)	351 (96%)	11 (3%)	3 (1%)	16	54
1	D	365/367 (100%)	351 (96%)	11 (3%)	3 (1%)	16	54
1	E	365/367 (100%)	351 (96%)	11 (3%)	3 (1%)	16	54
All	All	1825/1835 (100%)	1755 (96%)	55 (3%)	15 (1%)	18	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TYR
1	B	169	TYR
1	C	169	TYR
1	D	169	TYR
1	E	169	TYR
1	A	47	MET
1	A	48	GLY
1	B	47	MET
1	B	48	GLY
1	C	47	MET
1	C	48	GLY
1	D	47	MET
1	D	48	GLY
1	E	47	MET
1	E	48	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/310 (100%)	296 (96%)	14 (4%)	24	46
1	B	310/310 (100%)	296 (96%)	14 (4%)	24	46
1	C	310/310 (100%)	296 (96%)	14 (4%)	24	46
1	D	310/310 (100%)	296 (96%)	14 (4%)	24	46
1	E	310/310 (100%)	296 (96%)	14 (4%)	24	46
All	All	1550/1550 (100%)	1480 (96%)	70 (4%)	26	46

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	92	ASN
1	A	165	ILE
1	A	175	ILE
1	A	186	THR
1	A	194	THR
1	A	224	GLU
1	A	227	MET
1	A	235	SER
1	A	330	ILE
1	A	351	THR
1	A	360	GLN
1	A	368	SER
1	A	369	ILE
1	B	10	CYS
1	B	92	ASN
1	B	165	ILE
1	B	175	ILE
1	B	186	THR
1	B	194	THR
1	B	224	GLU
1	B	227	MET
1	B	235	SER
1	B	330	ILE
1	B	351	THR
1	B	360	GLN
1	B	368	SER
1	B	369	ILE

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Mol	Chain	Res	Type
1	C	10	CYS
1	C	92	ASN
1	C	165	ILE
1	C	175	ILE
1	C	186	THR
1	C	194	THR
1	C	224	GLU
1	C	227	MET
1	C	235	SER
1	C	330	ILE
1	C	351	THR
1	C	360	GLN
1	C	368	SER
1	C	369	ILE
1	D	10	CYS
1	D	92	ASN
1	D	165	ILE
1	D	175	ILE
1	D	186	THR
1	D	194	THR
1	D	224	GLU
1	D	227	MET
1	D	235	SER
1	D	330	ILE
1	D	351	THR
1	D	360	GLN
1	D	368	SER
1	D	369	ILE
1	E	10	CYS
1	E	92	ASN
1	E	165	ILE
1	E	175	ILE
1	E	186	THR
1	E	194	THR
1	E	224	GLU
1	E	227	MET
1	E	235	SER
1	E	330	ILE
1	E	351	THR
1	E	360	GLN
1	E	368	SER
1	E	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	92	ASN
1	A	121	GLN
1	A	128	ASN
1	A	371	HIS
1	B	88	HIS
1	B	92	ASN
1	B	121	GLN
1	B	128	ASN
1	B	371	HIS
1	C	88	HIS
1	C	92	ASN
1	C	121	GLN
1	C	128	ASN
1	C	371	HIS
1	D	88	HIS
1	D	92	ASN
1	D	121	GLN
1	D	371	HIS
1	E	88	HIS
1	E	92	ASN
1	E	121	GLN
1	E	371	HIS

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
3	ADP	B	401	4	28,29,29	1.62	4 (14%)	43,45,45	2.12	10 (23%)
3	ADP	D	401	4	28,29,29	1.62	4 (14%)	43,45,45	2.12	10 (23%)
3	ADP	C	401	4	28,29,29	1.61	4 (14%)	43,45,45	2.12	10 (23%)
3	ADP	E	401	4	28,29,29	1.61	4 (14%)	43,45,45	2.12	10 (23%)
3	ADP	A	401	4	28,29,29	1.61	4 (14%)	43,45,45	2.12	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
3	ADP	B	401	4	-	0/16/32/32	0/3/3/3
3	ADP	D	401	4	-	0/16/32/32	0/3/3/3
3	ADP	C	401	4	-	0/16/32/32	0/3/3/3
3	ADP	E	401	4	-	0/16/32/32	0/3/3/3
3	ADP	A	401	4	-	0/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	C5-C4	6.14	1.50	1.39
3	B	401	ADP	C5-C4	6.14	1.50	1.39
3	C	401	ADP	C5-C4	6.14	1.50	1.39
3	A	401	ADP	C5-C4	6.13	1.50	1.39
3	E	401	ADP	C5-C4	6.11	1.50	1.39
3	D	401	ADP	C5-C6	2.44	1.47	1.41
3	C	401	ADP	C5-C6	2.43	1.47	1.41
3	B	401	ADP	C5-C6	2.43	1.47	1.41
3	A	401	ADP	C5-C6	2.42	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ADP	C5-C6	2.42	1.47	1.41
3	E	401	ADP	C2-N1	2.30	1.38	1.33
3	B	401	ADP	C2-N1	2.29	1.38	1.33
3	A	401	ADP	C2-N1	2.28	1.38	1.33
3	C	401	ADP	C2-N1	2.28	1.38	1.33
3	D	401	ADP	C2-N1	2.26	1.37	1.33
3	A	401	ADP	C4-N9	-2.09	1.33	1.37
3	D	401	ADP	C4-N9	-2.08	1.33	1.37
3	B	401	ADP	C4-N9	-2.08	1.33	1.37
3	E	401	ADP	C4-N9	-2.07	1.33	1.37
3	C	401	ADP	C4-N9	-2.06	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-C4-N3	-6.74	117.43	126.72
3	B	401	ADP	C5-C4-N3	-6.74	117.44	126.72
3	D	401	ADP	C5-C4-N3	-6.74	117.44	126.72
3	C	401	ADP	C5-C4-N3	-6.73	117.45	126.72
3	E	401	ADP	C5-C4-N3	-6.72	117.46	126.72
3	C	401	ADP	N3-C4-N9	6.57	138.34	127.17
3	E	401	ADP	N3-C4-N9	6.56	138.33	127.17
3	B	401	ADP	N3-C4-N9	6.56	138.32	127.17
3	D	401	ADP	N3-C4-N9	6.56	138.32	127.17
3	A	401	ADP	N3-C4-N9	6.55	138.31	127.17
3	C	401	ADP	C4-N9-C8	3.70	109.63	105.74
3	E	401	ADP	C4-N9-C8	3.70	109.63	105.74
3	A	401	ADP	C4-N9-C8	3.69	109.61	105.74
3	B	401	ADP	C4-N9-C8	3.68	109.61	105.74
3	D	401	ADP	C4-N9-C8	3.67	109.60	105.74
3	A	401	ADP	C2-N3-C4	3.63	120.70	111.83
3	E	401	ADP	C2-N3-C4	3.63	120.69	111.83
3	C	401	ADP	C2-N3-C4	3.62	120.67	111.83
3	D	401	ADP	C2-N3-C4	3.62	120.67	111.83
3	B	401	ADP	C2-N3-C4	3.61	120.65	111.83
3	B	401	ADP	C4-C5-N7	-3.23	106.89	110.58
3	A	401	ADP	C4-C5-N7	-3.22	106.89	110.58
3	E	401	ADP	C4-C5-N7	-3.22	106.89	110.58
3	D	401	ADP	C4-C5-N7	-3.22	106.91	110.58
3	C	401	ADP	C4-C5-N7	-3.20	106.92	110.58
3	E	401	ADP	N3-C2-N1	-3.04	123.97	128.58
3	A	401	ADP	N3-C2-N1	-3.02	124.00	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ADP	N3-C2-N1	-3.02	124.01	128.58
3	D	401	ADP	N3-C2-N1	-3.01	124.03	128.58
3	B	401	ADP	N3-C2-N1	-2.98	124.07	128.58
3	E	401	ADP	N9-C8-N7	-2.57	110.30	113.94
3	A	401	ADP	N9-C8-N7	-2.56	110.30	113.94
3	D	401	ADP	N9-C8-N7	-2.55	110.32	113.94
3	C	401	ADP	N9-C8-N7	-2.55	110.32	113.94
3	B	401	ADP	N9-C8-N7	-2.54	110.33	113.94
3	B	401	ADP	O3A-PB-O1B	-2.41	98.37	111.04
3	A	401	ADP	O3A-PB-O1B	-2.41	98.37	111.04
3	E	401	ADP	O3A-PB-O1B	-2.41	98.37	111.04
3	C	401	ADP	O3A-PB-O1B	-2.41	98.38	111.04
3	D	401	ADP	O3A-PB-O1B	-2.40	98.39	111.04
3	D	401	ADP	C2'-C3'-C4'	2.24	106.95	102.61
3	C	401	ADP	C2'-C3'-C4'	2.24	106.94	102.61
3	E	401	ADP	C5-N7-C8	2.24	106.97	103.45
3	A	401	ADP	C2'-C3'-C4'	2.24	106.93	102.61
3	B	401	ADP	C2'-C3'-C4'	2.23	106.93	102.61
3	E	401	ADP	C2'-C3'-C4'	2.22	106.90	102.61
3	A	401	ADP	C5-N7-C8	2.22	106.94	103.45
3	D	401	ADP	C5-N7-C8	2.22	106.94	103.45
3	B	401	ADP	C5-N7-C8	2.21	106.93	103.45
3	C	401	ADP	C5-N7-C8	2.21	106.93	103.45

There are no chirality outliers.

There are no torsion outliers.

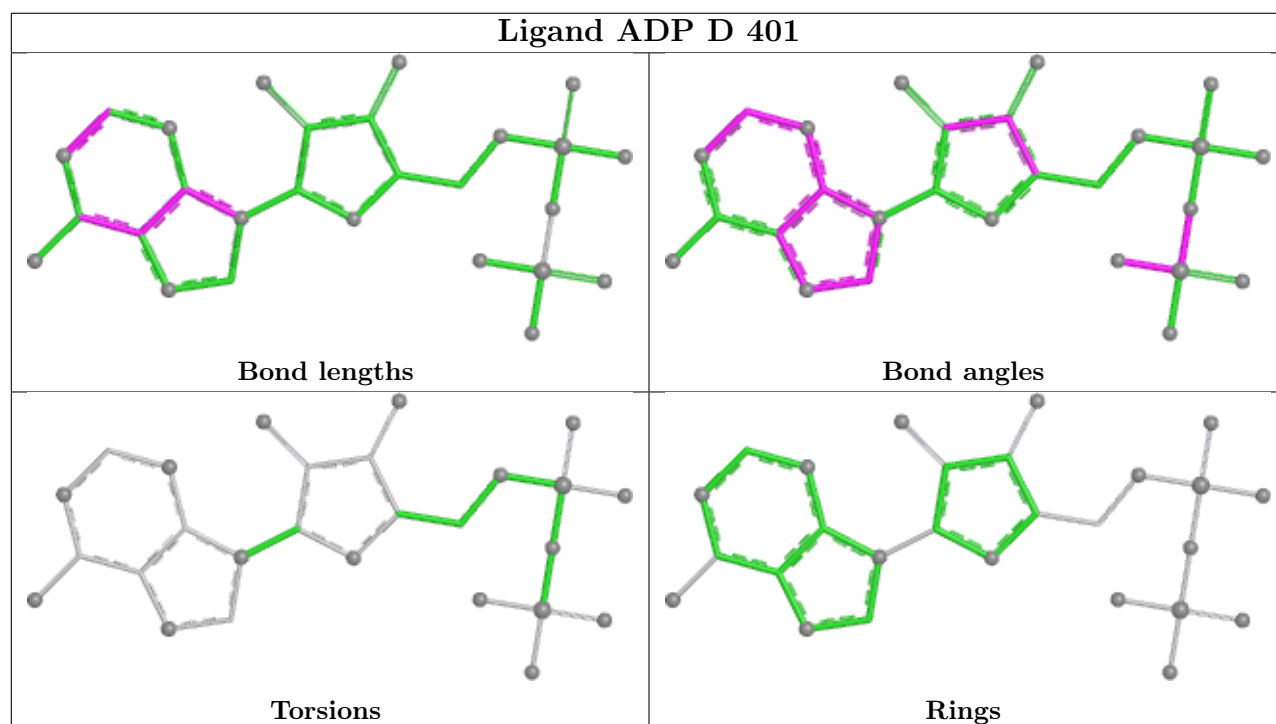
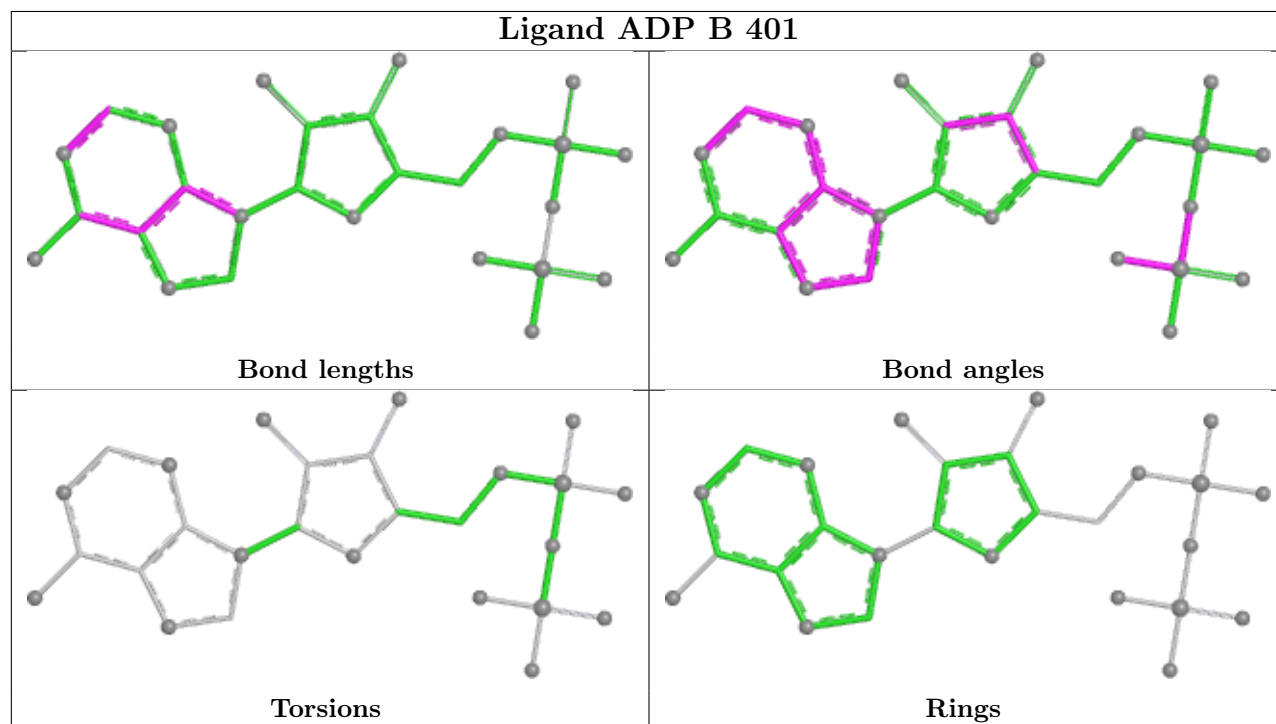
There are no ring outliers.

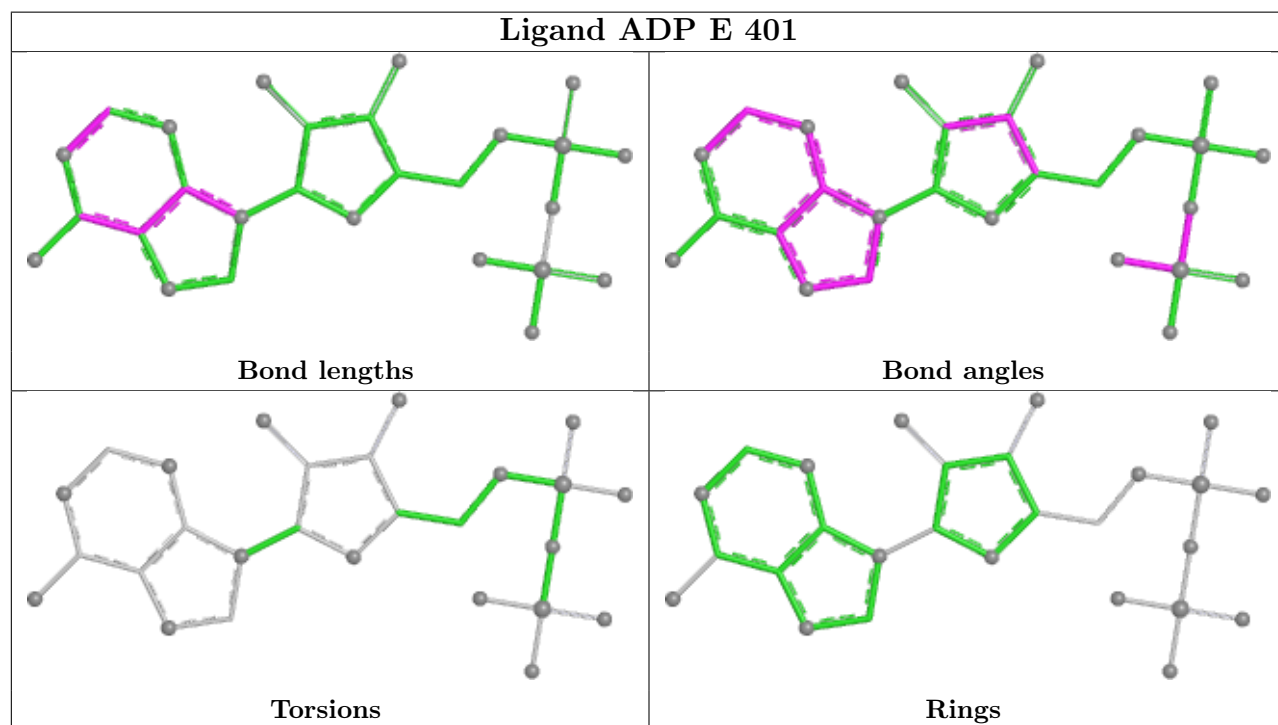
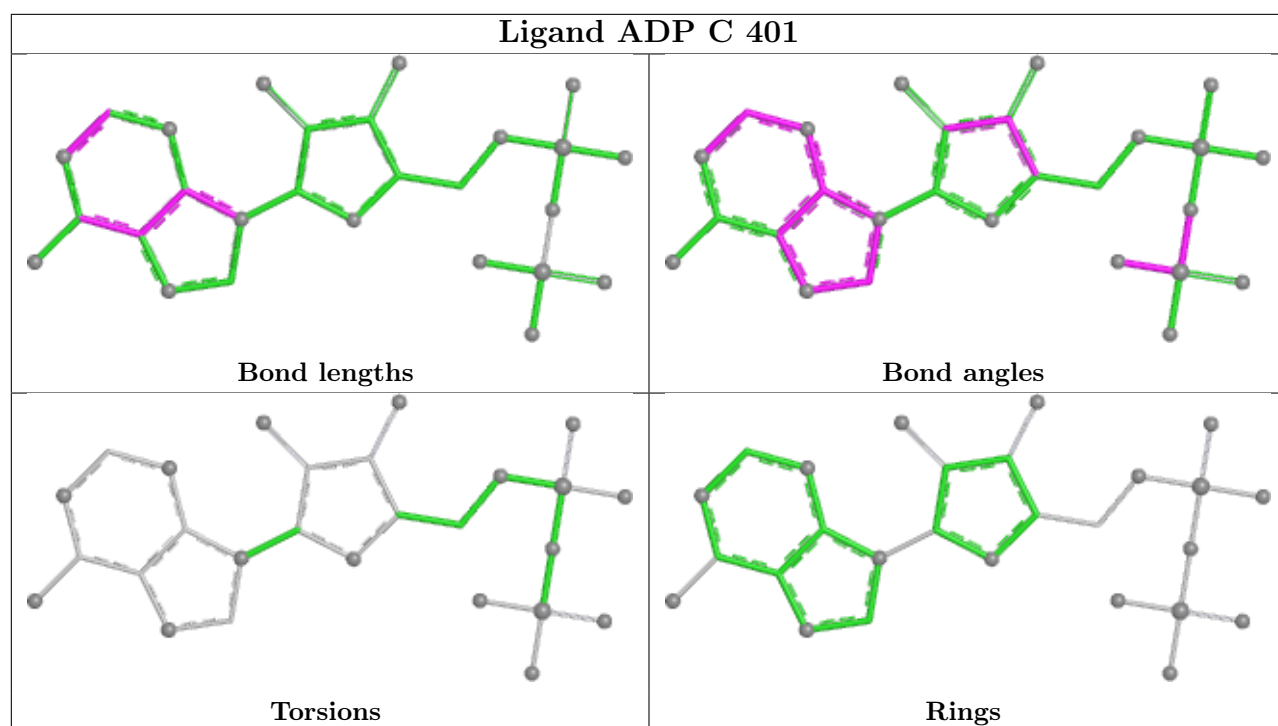
5 monomers are involved in 5 short contacts:

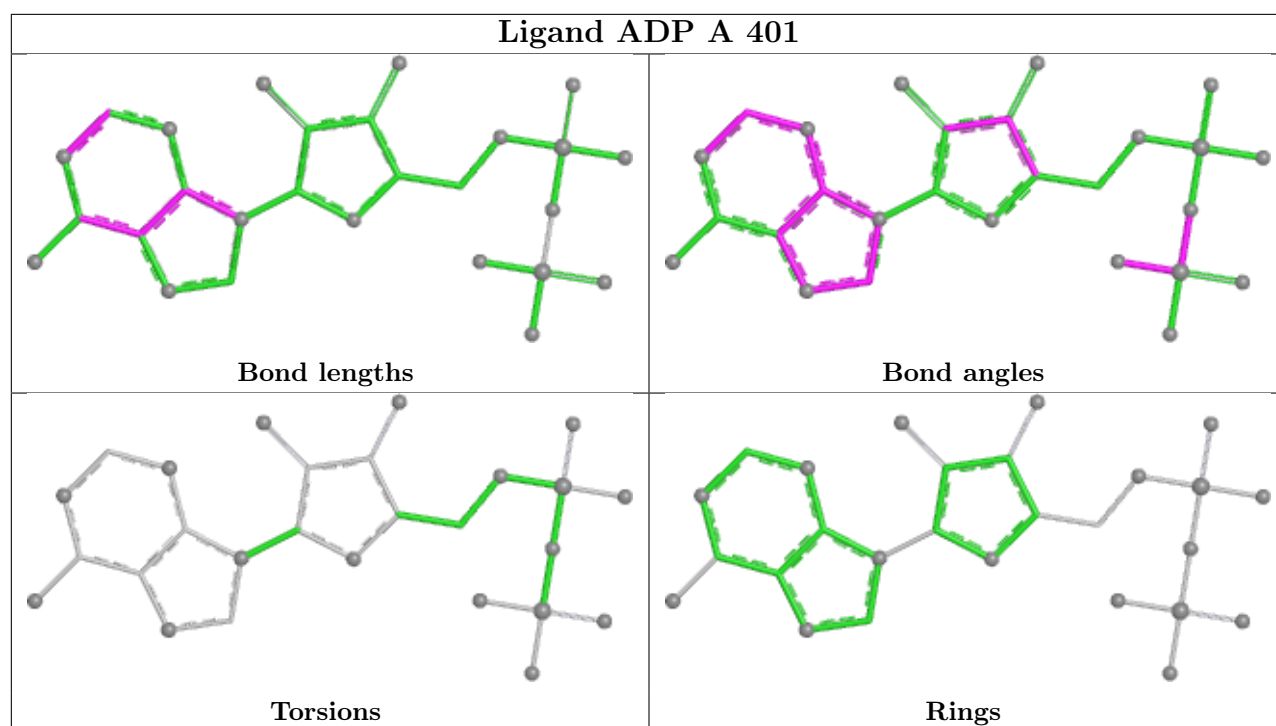
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ADP	1	0
3	D	401	ADP	1	0
3	C	401	ADP	1	0
3	E	401	ADP	1	0
3	A	401	ADP	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

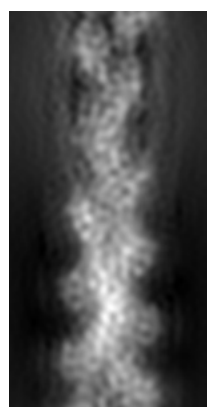
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3667. These allow visual inspection of the internal detail of the map and identification of artifacts.

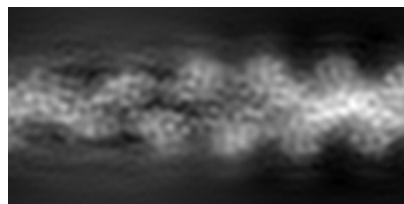
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

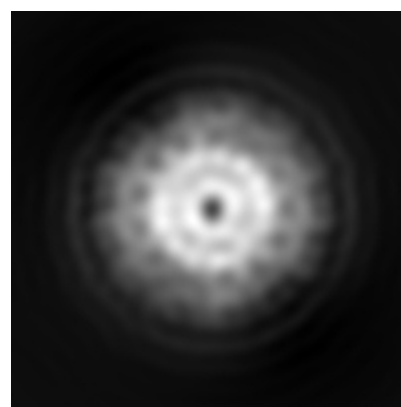
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

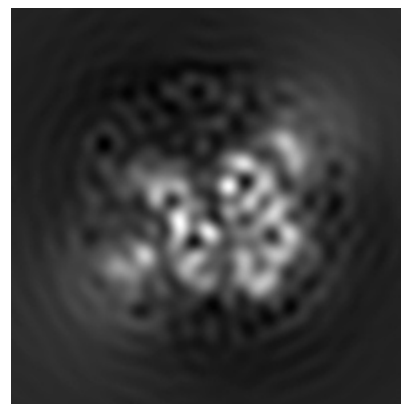
6.2.1 Primary map



X Index: 75



Y Index: 75



Z Index: 150

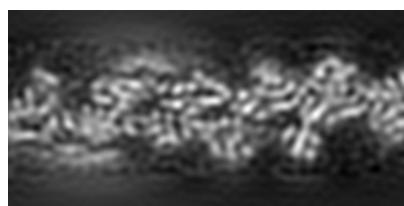
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

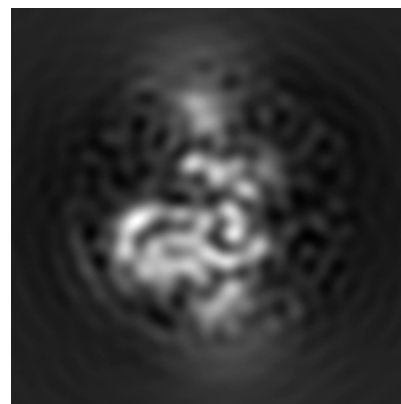
6.3.1 Primary map



X Index: 68



Y Index: 83

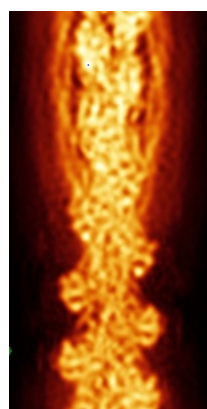


Z Index: 269

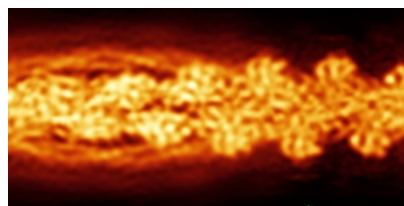
The images above show the largest variance slices of the map in three orthogonal directions.

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

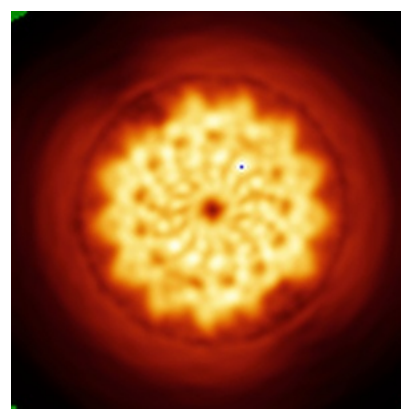
6.4.1 Primary map



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

This section was not generated.

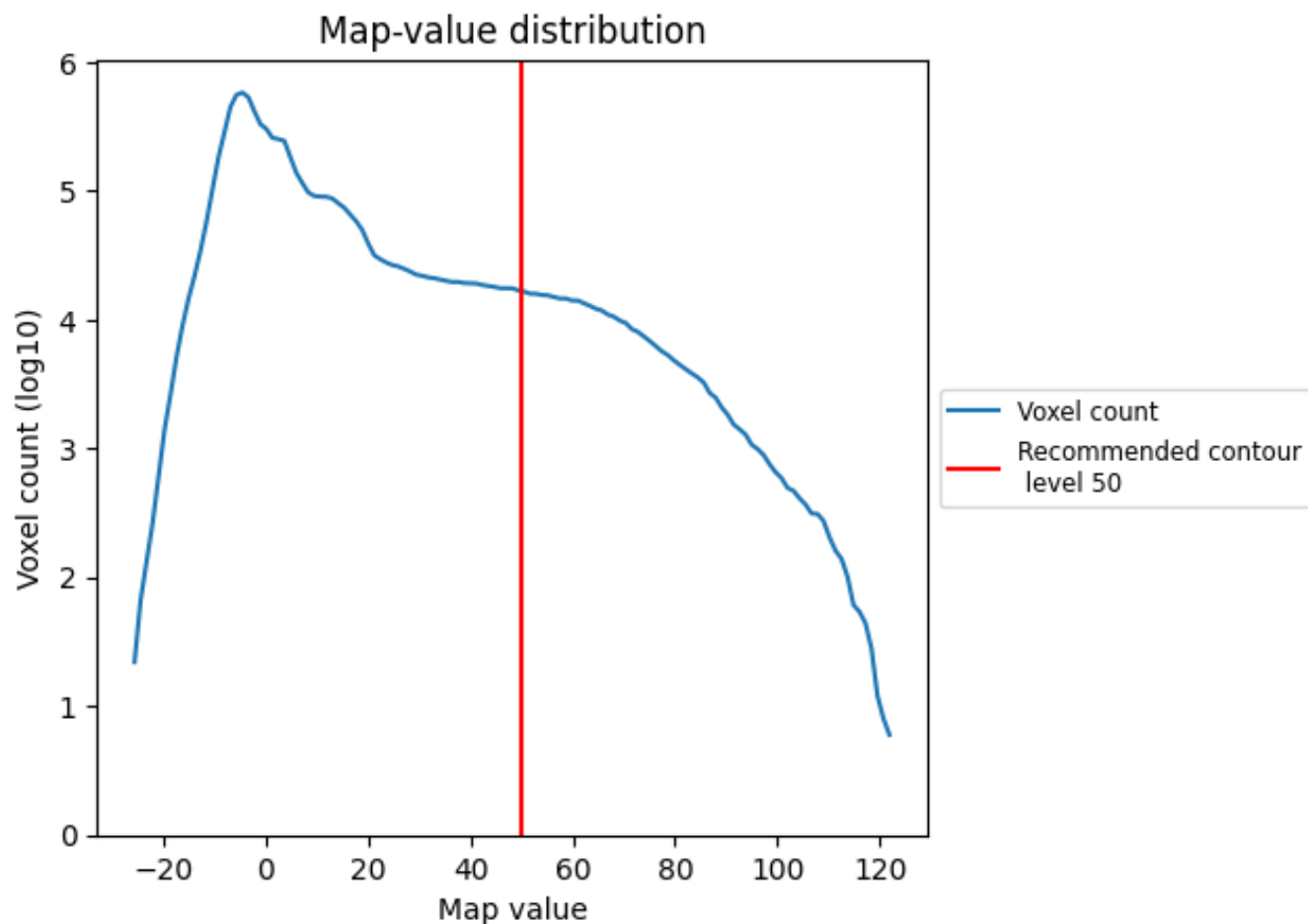
6.6 Mask visualisation

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

7 Map analysis [i](#)

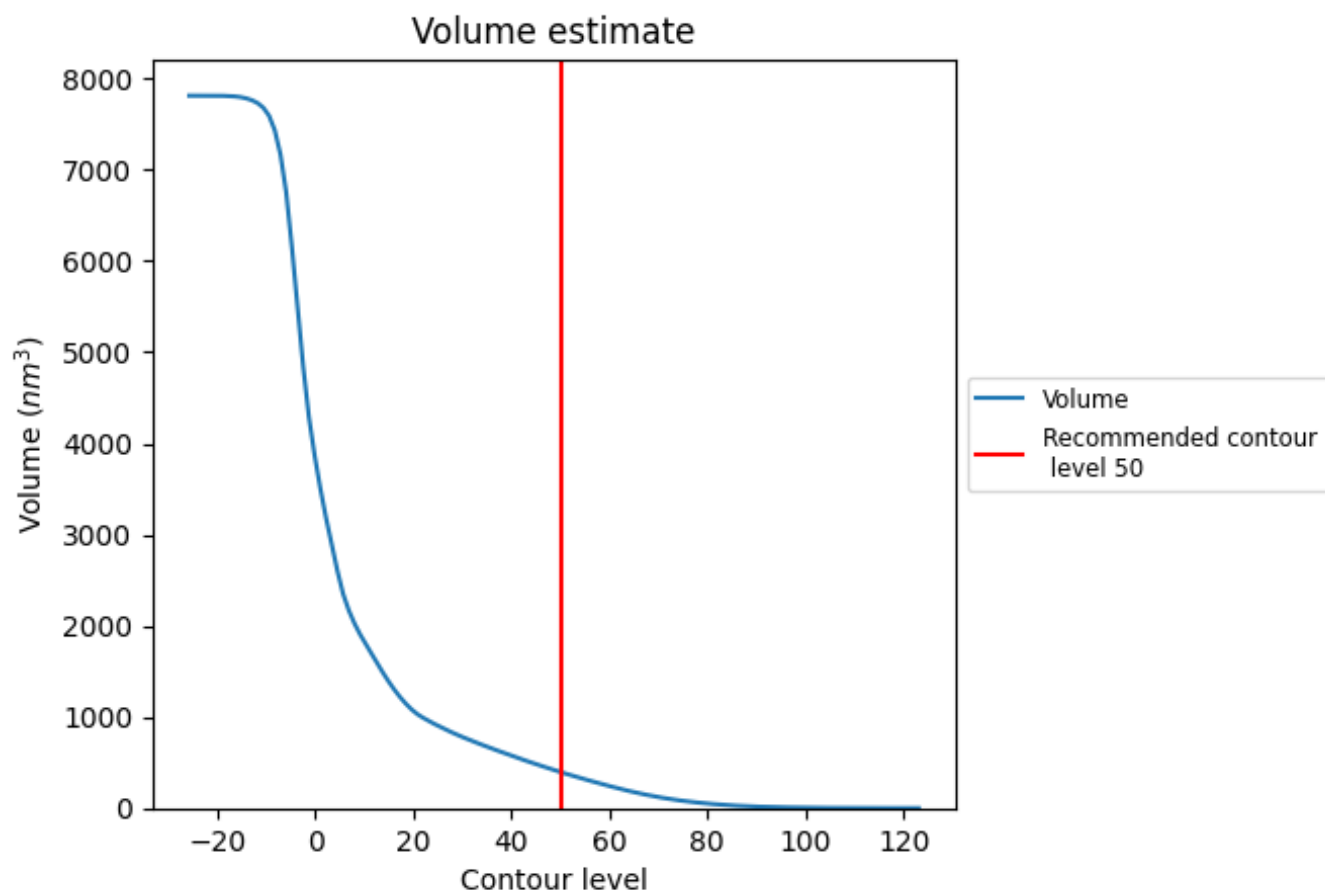
This section contains the results of statistical analysis of the map.

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 396 nm³; this corresponds to an approximate mass of 358 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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

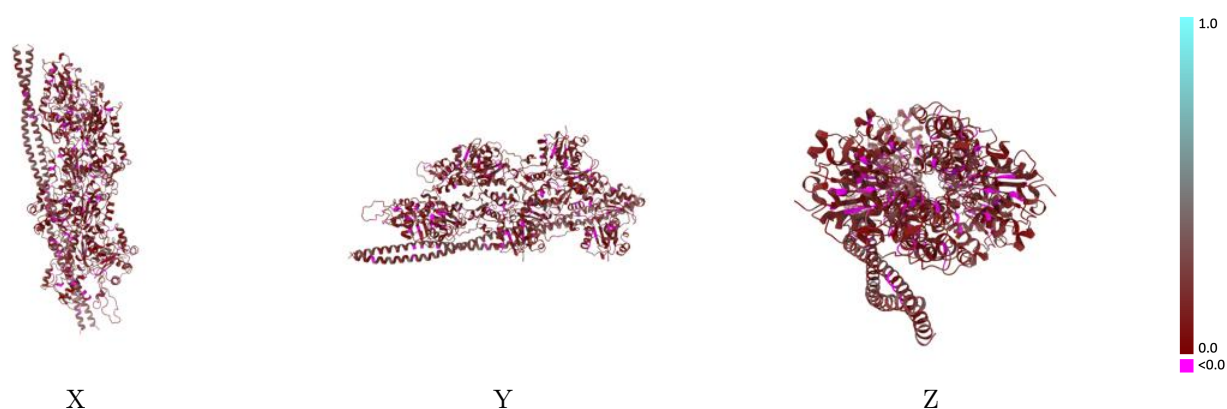
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3667 and PDB model 5NOL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

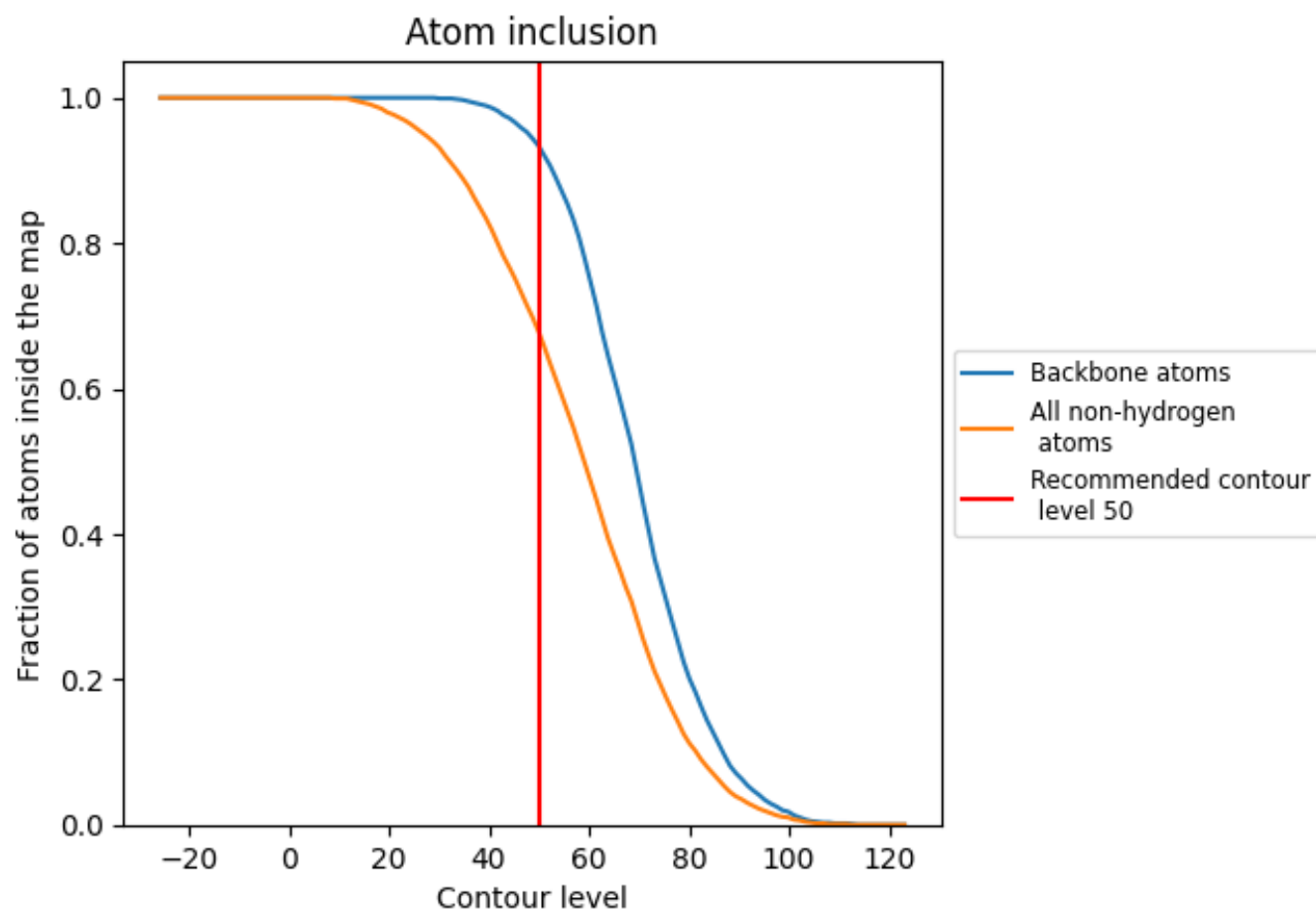


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 68% 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 (50) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.1440
A	0.6520	0.1380
B	0.6510	0.1370
C	0.6550	0.1380
D	0.6590	0.1380
E	0.6620	0.1380
F	0.9050	0.2240
G	0.8920	0.2060

1.0

0.0

<0.0