



## Full wwPDB EM Validation Report ⓘ

Oct 5, 2025 – 02:31 PM JST

PDB ID : 9KQN / pdb\_00009kqn  
EMDB ID : EMD-62508  
Title : Hsp90-Cdc37-PINK1 complex  
Authors : Tian, X.Y.; Su, J.Y.  
Deposited on : 2024-11-26  
Resolution : 2.84 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

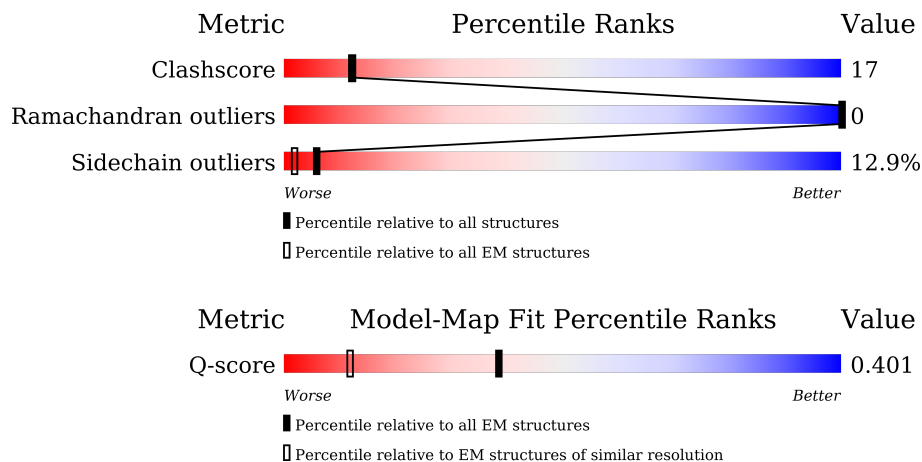
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11884 ( 2.34 - 3.34 )

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  $\geq 3$ , 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	732	
1	B	732	
2	C	494	
3	E	378	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14292 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	632	Total	C	N	O	S	0	0
			5141	3261	865	992	23		
1	B	633	Total	C	N	O	S	0	0
			5150	3267	867	993	23		

- Molecule 2 is a protein called Serine/threonine-protein kinase PINK1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	234	Total	C	N	O	S	0	0
			1821	1166	318	322	15		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	582	ASP	-	expression tag	UNP Q9BXM7
C	583	TYR	-	expression tag	UNP Q9BXM7
C	584	LYS	-	expression tag	UNP Q9BXM7
C	585	ASP	-	expression tag	UNP Q9BXM7
C	586	HIS	-	expression tag	UNP Q9BXM7
C	587	ASP	-	expression tag	UNP Q9BXM7
C	588	GLY	-	expression tag	UNP Q9BXM7
C	589	GLY	-	expression tag	UNP Q9BXM7
C	590	TYR	-	expression tag	UNP Q9BXM7
C	591	LYS	-	expression tag	UNP Q9BXM7
C	592	ASP	-	expression tag	UNP Q9BXM7
C	593	HIS	-	expression tag	UNP Q9BXM7
C	594	ASP	-	expression tag	UNP Q9BXM7
C	595	ILE	-	expression tag	UNP Q9BXM7
C	596	ASP	-	expression tag	UNP Q9BXM7
C	597	TYR	-	expression tag	UNP Q9BXM7
C	598	LYS	-	expression tag	UNP Q9BXM7
C	599	ASP	-	expression tag	UNP Q9BXM7
C	600	ASP	-	expression tag	UNP Q9BXM7

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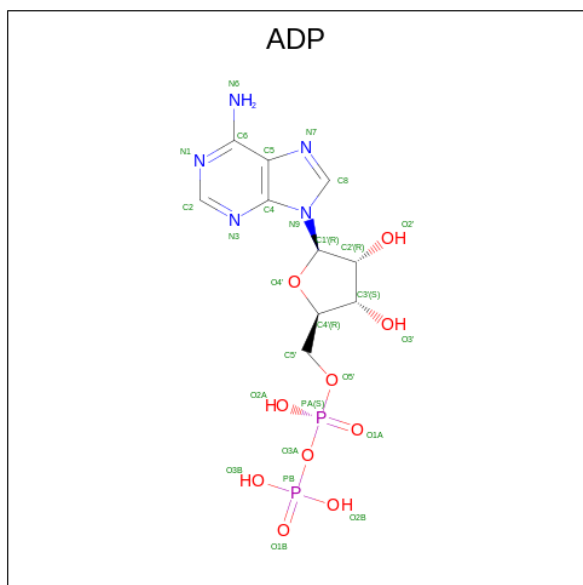
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Chain	Residue	Modelled	Actual	Comment	Reference
C	601	ASP	-	expression tag	UNP Q9BXM7
C	602	ASP	-	expression tag	UNP Q9BXM7
C	603	LYS	-	expression tag	UNP Q9BXM7

- Molecule 3 is a protein called Hsp90 co-chaperone Cdc37.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	253	Total	C	N	O	P	S	0	0
			2126	1325	382	403	1	15		

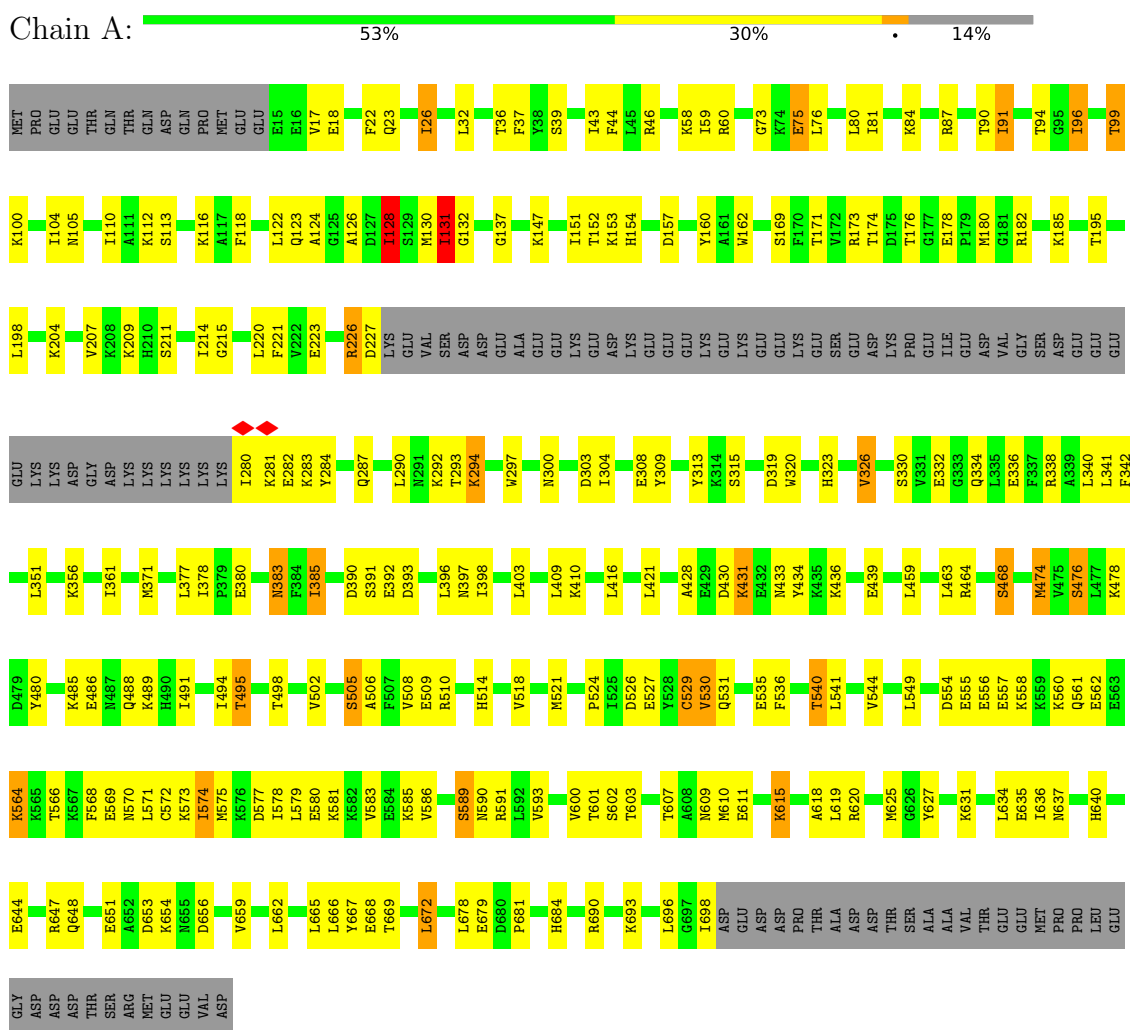
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



### 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.

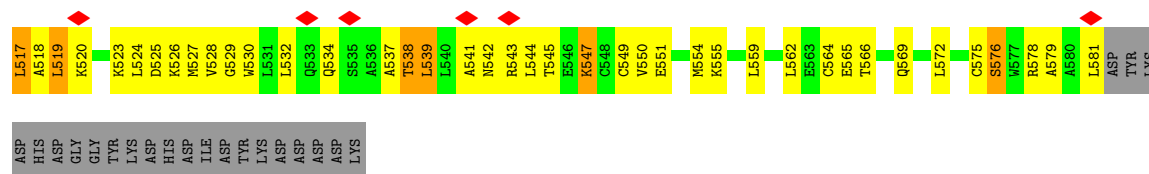
#### • Molecule 1: Heat shock protein HSP 90-alpha



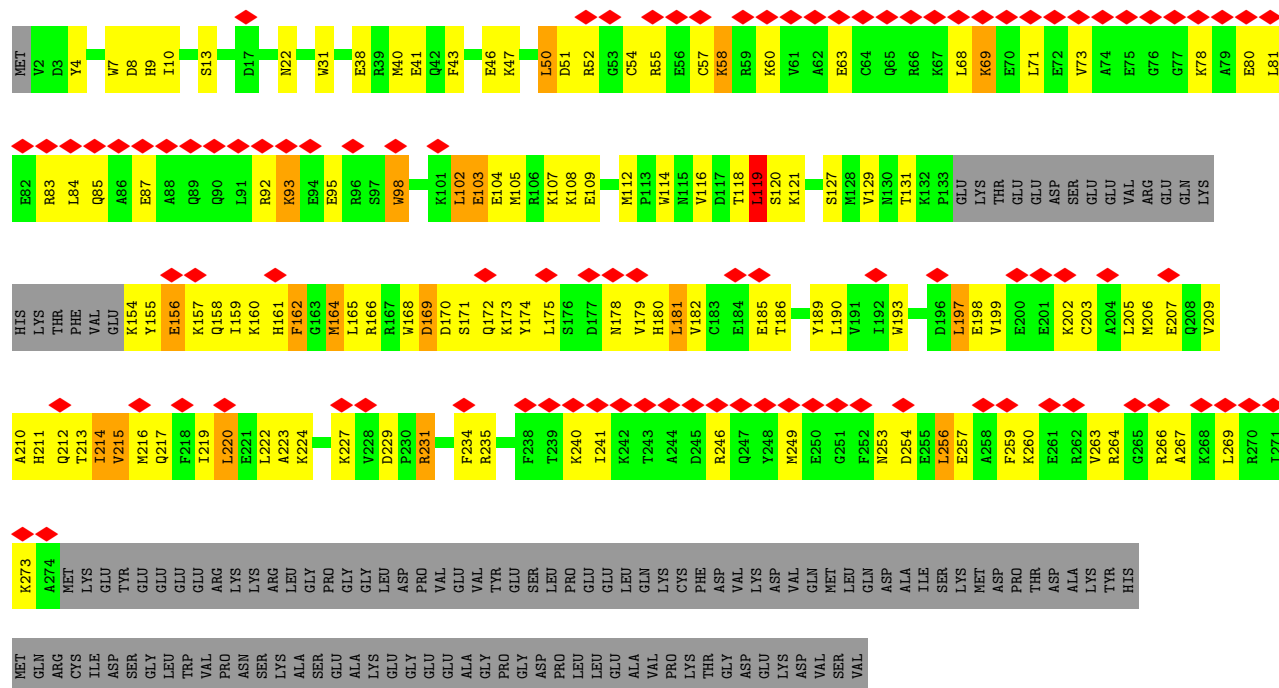
#### • Molecule 1: Heat shock protein HSP 90-alpha







• Molecule 3: Hsp90 co-chaperone Cdc37



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1324869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	40.239	Depositor
Minimum map value	-17.762	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.059	Depositor
Recommended contour level	4.62	Depositor
Map size ( $\text{\AA}$ )	243.516, 243.516, 243.516	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8697, 0.8697, 0.8697	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, 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	0.68	0/5224	0.88	23/7021 (0.3%)
1	B	0.67	0/5233	0.83	15/7032 (0.2%)
2	C	0.84	5/1858 (0.3%)	1.02	21/2521 (0.8%)
3	E	0.57	1/2150 (0.0%)	0.79	5/2872 (0.2%)
All	All	0.68	6/14465 (0.0%)	0.87	64/19446 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	321	TYR	CA-C	-6.37	1.45	1.53
2	C	538	THR	CA-C	-5.72	1.44	1.52
2	C	360	HIS	CA-C	-5.72	1.45	1.52
2	C	326	ARG	CA-C	-5.55	1.45	1.52
2	C	351	ASP	CA-C	-5.38	1.46	1.52
3	E	119	LEU	CA-C	-5.16	1.46	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ILE	N-CA-C	10.67	120.65	110.30
1	A	36	THR	N-CA-C	9.81	122.05	111.36
2	C	444	TYR	N-CA-C	-9.61	100.66	111.71
1	A	137	GLY	N-CA-C	8.20	122.56	112.73
1	A	75	GLU	N-CA-C	7.91	119.54	111.07
1	B	547	GLU	N-CA-C	7.82	119.80	111.28
2	C	539	LEU	N-CA-C	-7.70	102.97	111.36
3	E	178	ASN	N-CA-C	7.51	120.88	109.23
1	B	195	THR	N-CA-C	-7.31	104.37	113.28
1	A	37	PHE	N-CA-C	7.20	118.81	110.97
1	A	211	SER	N-CA-C	6.87	121.02	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	547	LYS	N-CA-C	-6.80	105.26	113.97
1	B	96	ILE	N-CA-C	-6.58	100.15	109.63
1	A	39	SER	N-CA-C	6.53	118.48	111.36
2	C	308	LEU	N-CA-C	6.46	120.22	109.95
2	C	456	GLN	N-CA-C	6.42	118.28	111.28
1	B	303	ASP	N-CA-C	-6.41	104.15	114.09
2	C	465	SER	N-CA-C	6.29	118.20	109.15
1	A	627	TYR	N-CA-C	6.28	118.21	111.36
1	A	132	GLY	N-CA-C	6.27	122.98	111.12
2	C	321	TYR	CA-C-N	-6.19	112.10	119.84
2	C	321	TYR	C-N-CA	-6.19	112.10	119.84
1	B	108	GLY	N-CA-C	6.13	120.08	112.73
1	B	618	ALA	N-CA-C	6.12	117.95	111.28
1	A	309	TYR	N-CA-C	-6.12	104.61	111.28
2	C	532	LEU	N-CA-C	-6.03	104.64	112.23
1	A	334	GLN	N-CA-C	-6.00	104.74	111.28
2	C	528	VAL	N-CA-C	-6.00	104.66	110.72
3	E	120	SER	N-CA-C	5.96	119.18	109.06
1	A	169	SER	N-CA-C	5.93	118.19	109.24
2	C	368	ILE	N-CA-C	5.92	116.05	108.12
2	C	362	ASP	CA-C-N	-5.91	114.66	123.00
2	C	362	ASP	C-N-CA	-5.91	114.66	123.00
1	A	128	ILE	N-CA-C	5.89	118.11	109.63
2	C	470	GLN	N-CA-C	-5.89	106.08	113.20
1	A	300	ASN	CA-C-N	-5.88	114.21	120.03
1	A	300	ASN	C-N-CA	-5.88	114.21	120.03
1	A	60	ARG	N-CA-C	-5.85	104.82	111.14
1	A	488	GLN	N-CA-C	5.74	118.02	111.02
1	A	485	LYS	N-CA-C	-5.72	103.38	110.41
1	A	618	ALA	N-CA-C	5.67	117.46	111.28
1	A	215	GLY	N-CA-C	5.53	119.37	112.73
1	B	169	SER	N-CA-C	5.46	118.29	109.40
1	B	285	ILE	N-CA-C	-5.41	100.45	108.45
3	E	58	LYS	N-CA-C	-5.40	105.55	111.82
1	B	378	ILE	CA-C-N	-5.39	114.07	120.11
1	B	378	ILE	C-N-CA	-5.39	114.07	120.11
1	B	347	ALA	CA-C-N	-5.37	115.05	120.31
1	B	347	ALA	C-N-CA	-5.37	115.05	120.31
2	C	442	ILE	N-CA-C	-5.29	105.22	110.62
2	C	323	CYS	N-CA-C	5.28	117.09	109.07
1	A	356	LYS	N-CA-C	5.26	117.02	111.28
1	B	309	TYR	N-CA-C	-5.21	105.60	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ALA	N-CA-C	5.17	117.58	111.33
1	A	303	ASP	N-CA-C	-5.16	106.39	113.30
2	C	351	ASP	N-CA-C	-5.15	105.58	111.14
2	C	458	LYS	N-CA-C	5.12	118.39	111.17
1	B	128	ILE	N-CA-C	5.11	116.27	109.37
2	C	373	ASP	CA-C-N	-5.06	114.00	120.23
2	C	373	ASP	C-N-CA	-5.06	114.00	120.23
2	C	454	TYR	N-CA-C	-5.06	105.89	111.71
3	E	269	LEU	N-CA-C	-5.06	105.76	111.28
3	E	98	TRP	N-CA-C	-5.05	105.66	111.07
1	B	423	LEU	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5141	0	5189	167	0
1	B	5150	0	5202	148	0
2	C	1821	0	1866	88	0
3	E	2126	0	2098	116	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
All	All	14292	0	14379	485	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 17.

All (485) 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:B:628:MET:HG3	2:C:374:PRO:HB2	1.52	0.90
3:E:246:ARG:O	3:E:249:MET:HG3	1.72	0.88
2:C:520:LYS:HG3	2:C:578:ARG:HE	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:HG2	1:A:336:GLU:OE2	1.78	0.82
2:C:514:GLU:H	2:C:537:ALA:HB1	1.43	0.82
1:A:105:ASN:HB3	1:A:112:LYS:NZ	1.93	0.82
2:C:458:LYS:HB3	2:C:464:ARG:HB3	1.59	0.82
1:A:128:ILE:HD13	1:A:130:MET:HE3	1.62	0.81
1:A:99:THR:HG23	1:A:154:HIS:HD2	1.46	0.81
1:A:118:PHE:CD2	1:A:130:MET:HE1	2.17	0.80
3:E:229:ASP:HB3	3:E:231:ARG:HG2	1.65	0.79
3:E:162:PHE:CD2	3:E:171:SER:HB3	2.18	0.79
1:A:283:LYS:HE3	2:C:526:LYS:NZ	1.98	0.78
1:A:463:LEU:O	1:A:464:ARG:NH1	2.17	0.78
1:A:586:VAL:HG12	1:A:634:LEU:HB3	1.66	0.77
3:E:168:TRP:O	3:E:172:GLN:HB2	1.84	0.77
1:B:463:LEU:O	1:B:464:ARG:NH1	2.17	0.77
1:A:80:LEU:HD21	1:A:91:ILE:HD13	1.68	0.76
1:B:226:ARG:HD2	1:B:282:GLU:OE1	1.86	0.76
3:E:175:LEU:HD12	3:E:181:LEU:HB2	1.66	0.75
1:B:586:VAL:HG12	1:B:634:LEU:HB3	1.66	0.75
1:A:171:THR:HG22	1:B:19:THR:HG22	1.69	0.75
1:A:433:ASN:OD1	1:A:436:LYS:NZ	2.20	0.75
1:B:433:ASN:OD1	1:B:436:LYS:NZ	2.20	0.75
1:A:380:GLU:O	1:A:383:ASN:ND2	2.20	0.74
3:E:162:PHE:HD2	3:E:171:SER:HB3	1.50	0.74
1:B:361:ILE:HD11	1:B:377:LEU:HB3	1.68	0.74
3:E:162:PHE:HA	3:E:165:LEU:HD12	1.69	0.73
1:A:361:ILE:HD11	1:A:377:LEU:HB3	1.70	0.73
2:C:527:MET:HB3	2:C:530:TRP:HB2	1.70	0.72
1:A:403:LEU:HD22	1:A:409:LEU:CD1	2.19	0.72
3:E:10:ILE:HG12	3:E:114:TRP:HB2	1.73	0.71
1:B:607:THR:HG22	1:B:610:MET:HB2	1.73	0.71
2:C:527:MET:HG2	2:C:529:GLY:H	1.56	0.70
1:A:226:ARG:O	1:A:280:ILE:HG22	1.91	0.70
1:A:656:ASP:HB3	1:A:659:VAL:HG22	1.75	0.69
1:A:544:VAL:O	1:A:591:ARG:NH2	2.25	0.69
3:E:104:GLU:HA	3:E:107:LYS:HD2	1.73	0.69
1:B:544:VAL:O	1:B:591:ARG:NH2	2.25	0.69
2:C:433:LYS:NZ	2:C:494:ALA:O	2.25	0.69
1:A:602:SER:HB3	1:A:631:LYS:HB2	1.74	0.68
1:B:693:LYS:HB3	1:B:698:ILE:HG12	1.75	0.68
1:B:81:ILE:HG22	1:B:81:ILE:O	1.93	0.68
1:B:529:CYS:SG	1:B:530:VAL:N	2.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PHE:HB3	1:B:295:PRO:HG3	1.76	0.68
2:C:329:LEU:HD11	2:C:446:ILE:HA	1.77	0.67
1:A:529:CYS:SG	1:A:530:VAL:N	2.67	0.67
3:E:160:LYS:HA	3:E:193:TRP:CH2	2.30	0.67
1:A:403:LEU:HD22	1:A:409:LEU:HD11	1.77	0.66
2:C:517:LEU:HB3	2:C:523:LYS:NZ	2.09	0.66
1:B:320:TRP:HB3	3:E:182:VAL:HG21	1.76	0.66
1:B:226:ARG:CD	1:B:282:GLU:OE1	2.44	0.66
1:A:105:ASN:HB3	1:A:112:LYS:HZ3	1.58	0.66
1:B:564:LYS:HD3	1:B:638:PRO:HG3	1.78	0.66
1:B:564:LYS:HD3	1:B:638:PRO:CG	2.25	0.65
2:C:541:ALA:HA	2:C:544:LEU:HB2	1.76	0.65
2:C:358:ILE:O	2:C:358:ILE:HG13	1.96	0.65
1:A:468:SER:HG	1:A:518:VAL:H	1.42	0.64
1:B:212:GLN:O	1:B:291:ASN:ND2	2.22	0.64
2:C:575:CYS:SG	2:C:576:SER:N	2.71	0.64
1:A:619:LEU:HB2	2:C:313:THR:HG21	1.79	0.64
1:A:26:ILE:HG21	1:B:22:PHE:HB2	1.79	0.64
1:A:22:PHE:HB2	1:B:26:ILE:HG21	1.79	0.64
3:E:175:LEU:HB3	3:E:181:LEU:HD13	1.80	0.63
1:A:105:ASN:HB3	1:A:112:LYS:HZ2	1.61	0.63
1:B:571:LEU:HA	1:B:574:ILE:HD11	1.80	0.63
1:A:570:ASN:OD1	1:A:571:LEU:N	2.31	0.63
1:A:607:THR:H	1:A:610:MET:HE2	1.62	0.63
1:B:297:TRP:O	1:B:338:ARG:NH2	2.30	0.62
2:C:527:MET:HG2	2:C:529:GLY:N	2.12	0.62
1:A:118:PHE:CE2	1:A:130:MET:HE1	2.33	0.62
1:A:123:GLN:HE22	1:A:126:ALA:HA	1.63	0.62
3:E:58:LYS:HG3	3:E:95:GLU:CD	2.23	0.62
1:A:122:LEU:HD12	1:A:128:ILE:HD11	1.80	0.62
1:A:123:GLN:NE2	1:A:126:ALA:CA	2.63	0.62
3:E:80:GLU:HB3	3:E:83:ARG:HH21	1.65	0.62
2:C:534:GLN:O	2:C:538:THR:HG23	2.00	0.62
1:A:571:LEU:HA	1:A:574:ILE:HD11	1.80	0.61
1:B:585:LYS:HG2	1:B:586:VAL:N	2.15	0.61
1:A:535:GLU:OE1	1:A:536:PHE:N	2.32	0.61
1:B:204:LYS:NZ	1:B:288:GLU:OE1	2.28	0.61
1:A:297:TRP:O	1:A:338:ARG:NH2	2.30	0.60
2:C:441:ALA:HB1	2:C:451:ASN:HD21	1.65	0.60
2:C:494:ALA:HA	2:C:497:ARG:HB2	1.82	0.60
3:E:235:ARG:H	3:E:235:ARG:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLU:OE1	1:B:536:PHE:N	2.32	0.60
1:A:76:LEU:HA	1:A:94:THR:OG1	2.01	0.60
1:A:330:SER:HB2	1:A:338:ARG:HG2	1.84	0.60
1:A:80:LEU:CD2	1:A:91:ILE:HG12	2.32	0.59
3:E:95:GLU:HA	3:E:98:TRP:HD1	1.66	0.59
1:A:281:LYS:O	1:A:282:GLU:HG3	2.01	0.59
2:C:524:LEU:HD22	2:C:530:TRP:HE1	1.66	0.59
1:B:391:SER:OG	1:B:392:GLU:N	2.34	0.59
1:B:414:LYS:HD3	3:E:116:VAL:HG21	1.82	0.59
1:A:527:GLU:OE2	1:A:527:GLU:N	2.29	0.59
1:A:391:SER:OG	1:A:392:GLU:N	2.35	0.59
1:A:123:GLN:NE2	1:A:126:ALA:HA	2.17	0.59
1:B:485:LYS:H	1:B:488:GLN:HG3	1.67	0.59
2:C:579:ALA:HB1	2:C:581:LEU:HG	1.84	0.59
3:E:168:TRP:O	3:E:172:GLN:CB	2.50	0.58
1:A:304:ILE:HG23	1:A:308:GLU:HG3	1.84	0.58
1:A:693:LYS:HG2	1:A:698:ILE:HD12	1.85	0.58
1:B:526:ASP:O	1:B:529:CYS:N	2.35	0.58
1:B:561:GLN:NE2	1:B:589:SER:O	2.37	0.58
1:A:572:CYS:HB3	1:A:586:VAL:HG23	1.84	0.58
1:B:589:SER:OG	1:B:590:ASN:N	2.36	0.58
1:B:480:TYR:CE2	1:B:517:GLU:HB3	2.38	0.58
1:B:572:CYS:HB3	1:B:586:VAL:HG23	1.84	0.58
2:C:518:ALA:HA	2:C:523:LYS:HB2	1.85	0.58
1:A:589:SER:OG	1:A:590:ASN:N	2.36	0.58
2:C:487:ARG:HB3	2:C:487:ARG:NH1	2.17	0.58
1:A:561:GLN:NE2	1:A:589:SER:O	2.37	0.58
3:E:57:CYS:HB2	3:E:95:GLU:HG2	1.86	0.58
3:E:46:GLU:HG3	3:E:105:MET:HE1	1.85	0.58
1:A:620:ARG:HE	1:A:625:MET:HB2	1.70	0.57
1:A:87:ARG:HA	1:A:198:LEU:HD11	1.85	0.57
1:B:629:ALA:H	2:C:375:ASP:HB2	1.69	0.57
1:B:39:SER:OG	1:B:40:ASN:N	2.36	0.57
3:E:207:GLU:HB2	3:E:256:LEU:CD1	2.34	0.57
1:A:204:LYS:HG3	1:A:290:LEU:HD23	1.87	0.57
2:C:565:GLU:HG2	2:C:566:THR:H	1.68	0.57
1:A:123:GLN:HE22	1:A:126:ALA:CA	2.18	0.57
1:B:527:GLU:OE2	1:B:527:GLU:N	2.29	0.57
1:B:540:THR:OG1	1:B:541:LEU:N	2.37	0.57
2:C:565:GLU:OE1	2:C:565:GLU:N	2.30	0.57
1:A:80:LEU:CD2	1:A:91:ILE:HG23	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:433:LYS:HD2	2:C:494:ALA:HB1	1.88	0.56
1:B:327:LYS:NZ	3:E:127:SER:HB3	2.21	0.56
1:B:75:GLU:H	1:B:75:GLU:CD	2.13	0.56
1:B:224:LYS:NZ	1:B:283:LYS:HD3	2.21	0.56
3:E:170:ASP:O	3:E:174:TYR:HB2	2.06	0.56
1:A:526:ASP:O	1:A:529:CYS:N	2.35	0.56
1:B:327:LYS:HZ2	3:E:127:SER:HB3	1.71	0.56
2:C:461:LEU:O	2:C:464:ARG:HB2	2.05	0.56
3:E:193:TRP:O	3:E:197:LEU:HB2	2.06	0.56
1:B:204:LYS:HG3	1:B:290:LEU:HD23	1.87	0.56
1:A:118:PHE:HD2	1:A:130:MET:HE1	1.69	0.56
1:B:153:LYS:HD2	1:B:159:GLN:OE1	2.06	0.55
2:C:441:ALA:HB1	2:C:451:ASN:ND2	2.20	0.55
1:B:589:SER:HB2	1:B:635:GLU:HB3	1.87	0.55
3:E:213:THR:O	3:E:216:MET:HB2	2.05	0.55
3:E:43:PHE:HZ	3:E:109:GLU:HG3	1.71	0.55
1:A:99:THR:HG22	1:A:157:ASP:HB2	1.88	0.55
1:A:589:SER:HB2	1:A:635:GLU:HB3	1.87	0.55
1:B:43:ILE:O	1:B:46:ARG:N	2.39	0.55
2:C:338:LEU:HD11	2:C:377:CYS:SG	2.46	0.55
1:A:283:LYS:HE3	2:C:526:LYS:HZ1	1.71	0.55
1:B:174:THR:HG23	1:B:174:THR:O	2.05	0.55
3:E:164:MET:SD	3:E:205:LEU:HD21	2.47	0.55
1:A:195:THR:HG22	1:A:195:THR:O	2.06	0.55
1:A:80:LEU:HD22	1:A:91:ILE:HG12	1.89	0.54
1:B:585:LYS:HG2	1:B:586:VAL:H	1.72	0.54
3:E:84:LEU:HD12	3:E:87:GLU:HB2	1.89	0.54
3:E:207:GLU:HA	3:E:210:ALA:HB3	1.88	0.54
1:B:40:ASN:OD1	1:B:41:LYS:N	2.41	0.54
3:E:224:LYS:C	3:E:227:LYS:H	2.15	0.54
1:A:607:THR:HG23	1:A:610:MET:HE2	1.89	0.54
1:B:651:GLU:HA	1:B:654:LYS:HZ3	1.72	0.54
3:E:47:LYS:HA	3:E:105:MET:HE3	1.88	0.54
1:B:408:ILE:HD11	3:E:7:TRP:HE3	1.72	0.54
1:A:651:GLU:HA	1:A:654:LYS:HZ3	1.72	0.54
1:A:323:HIS:CD2	1:A:326:VAL:HG13	2.43	0.54
1:B:323:HIS:CD2	1:B:326:VAL:HG13	2.43	0.54
2:C:458:LYS:HB3	2:C:464:ARG:O	2.07	0.54
1:A:351:LEU:HD11	1:A:383:ASN:HB2	1.90	0.53
2:C:377:CYS:SG	2:C:550:VAL:HG21	2.49	0.53
1:A:43:ILE:O	1:A:46:ARG:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:436:ALA:O	2:C:439:VAL:HG12	2.08	0.53
1:A:540:THR:OG1	1:A:541:LEU:N	2.37	0.53
3:E:165:LEU:HD13	3:E:170:ASP:HB3	1.91	0.53
1:A:679:GLU:H	1:A:679:GLU:CD	2.17	0.53
1:B:147:LYS:HZ1	1:B:189:HIS:CE1	2.27	0.53
3:E:231:ARG:HA	3:E:234:PHE:CE2	2.44	0.53
1:B:220:LEU:HB2	1:B:290:LEU:HD11	1.91	0.53
1:B:666:LEU:HA	1:B:669:THR:HG22	1.91	0.53
1:B:679:GLU:CD	1:B:679:GLU:H	2.17	0.53
2:C:517:LEU:HB3	2:C:523:LYS:HZ2	1.74	0.53
2:C:542:ASN:HD22	2:C:555:LYS:HE2	1.72	0.53
1:B:58:LYS:HD2	1:B:96:ILE:HD11	1.90	0.52
1:B:395:PRO:HA	3:E:4:TYR:CZ	2.44	0.52
1:A:113:SER:OG	1:A:116:LYS:HB3	2.08	0.52
1:A:524:PRO:HG2	1:B:620:ARG:HE	1.75	0.52
1:A:17:VAL:HG23	1:A:17:VAL:O	2.10	0.52
1:A:313:TYR:HB2	1:A:342:PHE:CE2	2.44	0.52
3:E:207:GLU:HB2	3:E:256:LEU:HD13	1.91	0.52
3:E:155:TYR:HB2	3:E:158:GLN:HG2	1.91	0.52
1:A:283:LYS:HE3	2:C:526:LYS:HZ2	1.75	0.52
1:A:113:SER:OG	1:A:116:LYS:CB	2.57	0.52
1:A:220:LEU:HB2	1:A:290:LEU:HD11	1.91	0.52
1:A:505:SER:OG	1:A:506:ALA:N	2.42	0.52
1:B:56:LEU:HD22	1:B:76:LEU:HB3	1.91	0.52
2:C:325:LEU:O	2:C:326:ARG:C	2.48	0.52
1:A:666:LEU:HA	1:A:669:THR:HG22	1.91	0.51
2:C:520:LYS:NZ	2:C:578:ARG:HB3	2.25	0.51
1:A:123:GLN:NE2	1:A:126:ALA:N	2.57	0.51
1:B:601:THR:HG21	1:B:607:THR:HA	1.92	0.51
1:A:557:GLU:HA	1:A:560:LYS:HE3	1.93	0.51
1:B:75:GLU:OE2	1:B:75:GLU:N	2.35	0.51
3:E:181:LEU:HD21	3:E:235:ARG:HH22	1.75	0.51
1:B:56:LEU:HD23	1:B:95:GLY:HA2	1.93	0.51
3:E:198:GLU:HB2	3:E:206:MET:HG3	1.93	0.51
1:A:544:VAL:HA	1:A:549:LEU:HD12	1.93	0.51
1:B:505:SER:OG	1:B:506:ALA:N	2.43	0.51
1:A:397:ASN:OD1	1:A:398:ILE:N	2.44	0.51
2:C:467:GLN:HB3	2:C:470:GLN:HG3	1.93	0.51
3:E:40:MET:HG3	3:E:41:GLU:N	2.24	0.51
3:E:198:GLU:HB3	3:E:267:ALA:CB	2.41	0.51
1:A:80:LEU:CD2	1:A:91:ILE:CG1	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HB2	1:A:160:TYR:CE2	2.45	0.51
2:C:516:ILE:HG22	2:C:517:LEU:H	1.76	0.51
1:B:397:ASN:OD1	1:B:398:ILE:N	2.44	0.50
1:B:49:ILE:HD11	1:B:80:LEU:HD11	1.93	0.50
1:B:557:GLU:HA	1:B:560:LYS:HE3	1.93	0.50
3:E:259:PHE:O	3:E:263:VAL:HG23	2.11	0.50
2:C:516:ILE:O	2:C:519:LEU:HB3	2.12	0.50
1:A:80:LEU:HD21	1:A:91:ILE:HG23	1.93	0.50
1:B:58:LYS:HB2	1:B:96:ILE:HG12	1.93	0.50
1:A:531:GLN:OE1	2:C:310:HIS:HB3	2.12	0.50
1:A:59:ILE:HD13	1:A:96:ILE:HG13	1.93	0.49
2:C:443:ALA:O	2:C:444:TYR:C	2.53	0.49
1:A:681:PRO:HB2	1:B:673:SER:HA	1.94	0.49
1:B:480:TYR:HE2	1:B:517:GLU:HB3	1.77	0.49
2:C:480:PRO:HA	2:C:483:ARG:HH11	1.78	0.49
3:E:193:TRP:CZ3	3:E:209:VAL:HG21	2.47	0.49
3:E:257:GLU:HA	3:E:260:LYS:HB3	1.94	0.49
3:E:51:ASP:O	3:E:55:ARG:HG3	2.12	0.49
3:E:202:LYS:HE2	3:E:205:LEU:HD12	1.93	0.49
2:C:451:ASN:OD1	2:C:454:TYR:N	2.37	0.49
1:A:480:TYR:CE1	1:A:491:ILE:HG23	2.47	0.49
1:B:467:THR:HB	1:B:518:VAL:O	2.13	0.49
2:C:565:GLU:H	2:C:565:GLU:CD	2.15	0.49
1:A:73:GLY:H	1:A:182:ARG:HH12	1.61	0.49
1:A:574:ILE:O	1:A:578:ILE:HG22	2.13	0.49
1:B:408:ILE:HD11	3:E:10:ILE:CD1	2.42	0.49
1:B:480:TYR:CE1	1:B:491:ILE:HG23	2.47	0.49
3:E:166:ARG:HA	3:E:211:HIS:NE2	2.27	0.49
1:B:408:ILE:CD1	3:E:10:ILE:CD1	2.91	0.49
1:A:171:THR:CG2	1:B:19:THR:HG22	2.41	0.48
1:A:226:ARG:O	1:A:280:ILE:CG2	2.59	0.48
1:A:223:GLU:HG3	1:A:284:TYR:O	2.13	0.48
2:C:526:LYS:HB2	2:C:564:CYS:SG	2.53	0.48
1:A:99:THR:HG23	1:A:154:HIS:CD2	2.37	0.48
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.63	0.48
1:A:123:GLN:HE22	1:A:126:ALA:N	2.11	0.48
1:B:365:VAL:O	1:B:366:ARG:C	2.56	0.48
1:B:604:TYR:O	2:C:320:ASN:ND2	2.45	0.48
3:E:189:TYR:CE2	3:E:193:TRP:HB2	2.49	0.48
1:B:320:TRP:CB	3:E:182:VAL:HG21	2.42	0.48
1:B:574:ILE:O	1:B:578:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:LYS:CG	3:E:95:GLU:CD	2.85	0.48
3:E:80:GLU:OE1	3:E:83:ARG:NH2	2.46	0.48
1:B:489:LYS:HA	1:B:489:LYS:HD3	1.66	0.48
1:B:549:LEU:HD12	1:B:549:LEU:HA	1.76	0.48
2:C:481:ASP:N	2:C:481:ASP:OD1	2.46	0.48
3:E:114:TRP:HB3	3:E:119:LEU:HG	1.95	0.48
1:B:293:THR:HG21	1:B:315:SER:OG	2.14	0.48
1:B:610:MET:HG2	2:C:318:MET:SD	2.54	0.48
3:E:156:GLU:O	3:E:160:LYS:HG3	2.14	0.48
1:A:609:ASN:OD1	1:A:610:MET:N	2.47	0.48
1:B:100:LYS:HB2	1:B:160:TYR:CE2	2.49	0.48
3:E:273:LYS:HB2	3:E:273:LYS:HE2	1.51	0.48
1:B:555:GLU:HA	1:B:558:LYS:HD2	1.96	0.47
3:E:102:LEU:O	3:E:105:MET:HB2	2.14	0.47
1:A:80:LEU:CD2	1:A:91:ILE:HD13	2.41	0.47
1:B:365:VAL:C	1:B:367:ARG:N	2.67	0.47
1:B:579:LEU:HD21	1:B:667:TYR:CD1	2.49	0.47
2:C:519:LEU:HA	2:C:524:LEU:HG	1.95	0.47
3:E:211:HIS:O	3:E:215:VAL:HB	2.13	0.47
1:A:555:GLU:HA	1:A:558:LYS:HD2	1.95	0.47
1:A:570:ASN:O	1:A:574:ILE:HG13	2.14	0.47
1:A:637:ASN:OD1	1:A:640:HIS:HB2	2.15	0.47
1:B:355:ARG:HA	1:B:355:ARG:HD2	1.59	0.47
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.63	0.47
1:A:80:LEU:HD23	1:A:91:ILE:HG23	1.96	0.47
1:A:281:LYS:O	1:A:282:GLU:CG	2.63	0.47
1:B:424:PHE:O	1:B:427:LEU:N	2.47	0.47
3:E:60:LYS:HB3	3:E:60:LYS:HE3	1.72	0.47
1:B:547:GLU:HA	1:B:600:VAL:HG21	1.97	0.47
2:C:538:THR:HG21	2:C:559:LEU:HD21	1.96	0.47
1:B:585:LYS:CG	1:B:586:VAL:N	2.77	0.47
1:B:637:ASN:OD1	1:B:640:HIS:HB2	2.15	0.47
2:C:341:MET:HE1	2:C:550:VAL:HG23	1.97	0.47
3:E:69:LYS:O	3:E:73:VAL:HG23	2.15	0.47
3:E:78:LYS:O	3:E:81:LEU:HB3	2.15	0.47
1:B:175:ASP:OD1	1:B:176:THR:N	2.48	0.47
2:C:555:LYS:O	2:C:559:LEU:HB2	2.14	0.47
3:E:8:ASP:OD1	3:E:9:HIS:N	2.48	0.47
2:C:329:LEU:HD23	2:C:329:LEU:HA	1.68	0.47
2:C:372:LEU:HA	2:C:372:LEU:HD23	1.68	0.47
3:E:223:ALA:O	3:E:227:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:235:ARG:HD2	3:E:235:ARG:N	2.30	0.47
1:A:498:THR:O	1:A:502:VAL:HG22	2.15	0.46
2:C:476:GLU:HA	2:C:483:ARG:NH2	2.29	0.46
1:B:195:THR:HG23	1:B:198:LEU:HD12	1.96	0.46
1:B:313:TYR:HB2	1:B:342:PHE:CE2	2.51	0.46
1:B:498:THR:O	1:B:502:VAL:HG22	2.15	0.46
2:C:492:ARG:O	2:C:497:ARG:NH1	2.31	0.46
3:E:160:LYS:HA	3:E:193:TRP:CZ3	2.50	0.46
3:E:240:LYS:O	3:E:241:ILE:HD13	2.15	0.46
1:A:152:THR:HG23	1:A:152:THR:O	2.14	0.46
3:E:217:GLN:HA	3:E:220:LEU:HB2	1.98	0.46
1:B:573:LYS:HE2	1:B:573:LYS:HB3	1.63	0.46
2:C:344:LEU:HD21	2:C:508:HIS:CE1	2.51	0.46
1:A:281:LYS:C	1:A:282:GLU:HG3	2.39	0.46
1:B:585:LYS:CG	1:B:586:VAL:H	2.29	0.46
1:A:131:ILE:H	1:A:131:ILE:HG12	1.61	0.46
2:C:501:ARG:HD2	2:C:501:ARG:HA	1.69	0.46
3:E:38:GLU:O	3:E:41:GLU:HG3	2.15	0.46
3:E:211:HIS:CD2	3:E:212:GLN:HG2	2.50	0.46
1:A:416:LEU:HA	1:A:416:LEU:HD23	1.63	0.46
3:E:209:VAL:O	3:E:212:GLN:N	2.48	0.46
1:B:628:MET:CG	2:C:374:PRO:HB2	2.35	0.45
1:A:371:MET:HE2	1:A:371:MET:HB3	1.77	0.45
2:C:445:GLU:O	2:C:446:ILE:C	2.59	0.45
2:C:554:MET:HE2	2:C:554:MET:HB3	1.74	0.45
3:E:160:LYS:HG2	3:E:193:TRP:CE2	2.51	0.45
3:E:206:MET:SD	3:E:263:VAL:HG11	2.55	0.45
1:A:283:LYS:CE	2:C:526:LYS:HZ2	2.30	0.45
1:B:393:ASP:OD1	1:B:393:ASP:N	2.49	0.45
1:B:30:MET:HE2	1:B:110:ILE:HD11	1.99	0.45
1:B:180:MET:HE3	1:B:180:MET:HB2	1.62	0.45
3:E:108:LYS:O	3:E:112:MET:N	2.50	0.45
1:A:227:ASP:C	1:A:280:ILE:CG2	2.90	0.45
1:A:281:LYS:HB2	1:A:284:TYR:CE1	2.51	0.45
2:C:384:ASP:HB2	3:E:31:TRP:CZ2	2.52	0.45
3:E:211:HIS:NE2	3:E:212:GLN:HG2	2.32	0.45
3:E:198:GLU:CB	3:E:206:MET:HG3	2.46	0.45
3:E:263:VAL:HG22	3:E:266:ARG:NH2	2.32	0.45
1:A:573:LYS:HB3	1:A:573:LYS:HE2	1.63	0.45
1:A:393:ASP:N	1:A:393:ASP:OD1	2.49	0.45
1:A:474:MET:HE3	1:A:474:MET:HB2	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:514:GLU:O	2:C:519:LEU:HG	2.17	0.45
1:B:287:GLN:N	1:B:287:GLN:OE1	2.49	0.44
2:C:562:LEU:HD23	2:C:562:LEU:HA	1.78	0.44
1:A:84:LYS:HA	1:A:198:LEU:HD13	1.97	0.44
3:E:80:GLU:HA	3:E:83:ARG:HG3	1.99	0.44
3:E:93:LYS:HD2	3:E:93:LYS:HA	1.62	0.44
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.59	0.44
1:A:489:LYS:HA	1:A:489:LYS:HD3	1.66	0.44
1:B:414:LYS:HD3	3:E:116:VAL:CG2	2.47	0.44
2:C:569:GLN:O	2:C:572:LEU:HG	2.17	0.44
3:E:103:GLU:HG3	3:E:107:LYS:NZ	2.32	0.44
3:E:229:ASP:HB3	3:E:231:ARG:CG	2.40	0.44
1:A:615:LYS:HB2	1:A:615:LYS:HE2	1.82	0.44
1:A:476:SER:OG	1:A:478:LYS:N	2.50	0.44
1:A:560:LYS:HE3	1:A:560:LYS:HB3	1.84	0.44
3:E:190:LEU:HD23	3:E:216:MET:SD	2.58	0.44
3:E:263:VAL:HG13	3:E:266:ARG:HH21	1.82	0.44
1:A:290:LEU:HD12	1:A:290:LEU:H	1.83	0.44
1:B:562:GLU:O	1:B:566:THR:HG23	2.18	0.44
2:C:443:ALA:HA	2:C:446:ILE:HG13	1.99	0.44
1:A:294:LYS:HD3	1:A:294:LYS:HA	1.64	0.44
1:B:220:LEU:HD23	1:B:221:PHE:N	2.33	0.44
3:E:190:LEU:HD12	3:E:190:LEU:HA	1.58	0.44
1:A:574:ILE:HA	1:A:577:ASP:OD2	2.18	0.43
1:B:568:PHE:CE1	1:B:647:ARG:HD2	2.53	0.43
3:E:85:GLN:HE21	3:E:92:ARG:HH12	1.65	0.43
3:E:181:LEU:CD2	3:E:235:ARG:HH22	2.31	0.43
1:B:644:GLU:O	1:B:648:GLN:HG2	2.18	0.43
3:E:69:LYS:HA	3:E:69:LYS:HD3	1.49	0.43
1:A:644:GLU:O	1:A:648:GLN:HG2	2.18	0.43
1:B:571:LEU:O	1:B:575:MET:HG3	2.18	0.43
1:B:574:ILE:HA	1:B:577:ASP:OD2	2.18	0.43
1:A:569:GLU:H	1:A:569:GLU:HG2	1.63	0.43
1:B:604:TYR:CD1	2:C:322:PRO:HB2	2.53	0.43
3:E:157:LYS:HE2	3:E:157:LYS:H	1.82	0.43
1:A:562:GLU:O	1:A:566:THR:HG23	2.18	0.43
1:A:564:LYS:HA	1:A:564:LYS:HD3	1.79	0.43
1:B:419:LYS:HD3	1:B:419:LYS:HA	1.79	0.43
2:C:462:GLU:CD	2:C:462:GLU:H	2.27	0.43
1:B:371:MET:HB3	1:B:371:MET:HE2	1.78	0.43
1:B:569:GLU:H	1:B:569:GLU:HG2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:LYS:HZ1	2:C:578:ARG:HB3	1.83	0.43
3:E:159:ILE:O	3:E:162:PHE:HD1	2.01	0.43
1:A:220:LEU:HD23	1:A:221:PHE:N	2.33	0.43
1:A:568:PHE:CE1	1:A:647:ARG:HD2	2.53	0.43
2:C:322:PRO:HG2	2:C:323:CYS:SG	2.59	0.43
2:C:496:LYS:HB2	2:C:496:LYS:HE2	1.76	0.43
3:E:84:LEU:O	3:E:84:LEU:HG	2.18	0.43
1:B:428:ALA:HA	1:B:434:TYR:CD2	2.54	0.43
2:C:565:GLU:HG2	2:C:566:THR:N	2.34	0.43
3:E:50:LEU:HG	3:E:98:TRP:HE3	1.84	0.43
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.61	0.43
1:B:290:LEU:HD12	1:B:290:LEU:H	1.83	0.43
1:B:678:LEU:H	1:B:678:LEU:HG	1.52	0.43
2:C:467:GLN:HB3	2:C:470:GLN:CG	2.48	0.43
3:E:214:ILE:HD12	3:E:214:ILE:HA	1.71	0.43
1:A:226:ARG:HB2	1:A:282:GLU:N	2.34	0.42
1:A:556:GLU:OE1	1:A:556:GLU:N	2.28	0.42
1:A:571:LEU:O	1:A:575:MET:HG3	2.18	0.42
1:B:38:TYR:CG	1:B:43:ILE:HD11	2.54	0.42
3:E:68:LEU:HG	3:E:84:LEU:HD23	2.01	0.42
1:A:80:LEU:CD2	1:A:91:ILE:CD1	2.98	0.42
1:A:566:THR:HA	1:A:569:GLU:OE2	2.19	0.42
1:B:317:THR:O	1:B:318:ASN:C	2.61	0.42
2:C:324:THR:O	2:C:325:LEU:C	2.61	0.42
3:E:260:LYS:HZ3	3:E:264:ARG:NE	2.17	0.42
1:A:227:ASP:O	1:A:280:ILE:HG21	2.19	0.42
1:A:319:ASP:OD1	1:A:320:TRP:N	2.52	0.42
1:A:428:ALA:HA	1:A:434:TYR:CD2	2.54	0.42
1:A:556:GLU:H	1:A:556:GLU:CD	2.20	0.42
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.87	0.42
1:B:15:GLU:HB3	1:B:16:GLU:H	1.53	0.42
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.79	0.42
1:B:283:LYS:O	1:B:284:TYR:C	2.63	0.42
1:B:459:LEU:HA	1:B:459:LEU:HD23	1.82	0.42
2:C:363:LEU:HA	2:C:363:LEU:HD12	1.62	0.42
1:B:175:ASP:OD1	1:B:177:GLY:N	2.51	0.42
1:A:227:ASP:C	1:A:280:ILE:HG21	2.44	0.42
1:A:431:LYS:HA	1:A:431:LYS:HD3	1.57	0.42
1:A:662:LEU:HD21	1:B:696:LEU:HD11	2.02	0.42
1:B:226:ARG:HB3	1:B:281:LYS:HA	2.01	0.42
1:B:455:ASN:O	1:B:459:LEU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:381:VAL:HA	3:E:22:ASN:O	2.20	0.42
3:E:54:CYS:HB3	3:E:98:TRP:HB3	2.02	0.42
1:A:171:THR:HB	1:B:17:VAL:CG1	2.49	0.42
3:E:253:ASN:O	3:E:254:ASP:C	2.62	0.42
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.86	0.42
1:B:174:THR:O	1:B:174:THR:CG2	2.68	0.42
3:E:154:LYS:HA	3:E:154:LYS:HD2	1.87	0.42
1:A:162:TRP:CD1	1:A:162:TRP:C	2.98	0.42
1:A:464:ARG:HB3	1:A:474:MET:HB3	2.01	0.42
1:B:495:THR:HA	1:B:521:MET:O	2.20	0.42
3:E:161:HIS:HB2	3:E:174:TYR:HE2	1.84	0.42
1:A:430:ASP:O	1:A:431:LYS:C	2.63	0.42
3:E:210:ALA:HA	3:E:213:THR:OG1	2.19	0.42
1:A:180:MET:HE1	1:A:185:LYS:HB3	2.02	0.41
1:A:385:ILE:HD13	1:A:385:ILE:HA	1.84	0.41
1:B:488:GLN:C	1:B:490:HIS:H	2.27	0.41
2:C:458:LYS:HG3	2:C:465:SER:C	2.45	0.41
3:E:205:LEU:O	3:E:209:VAL:HG12	2.20	0.41
1:A:171:THR:HB	1:B:17:VAL:HG13	2.02	0.41
1:A:226:ARG:O	1:A:227:ASP:C	2.63	0.41
1:A:526:ASP:O	1:A:527:GLU:C	2.63	0.41
1:B:570:ASN:OD1	1:B:573:LYS:NZ	2.52	0.41
2:C:449:LEU:HD12	2:C:475:PRO:HD3	2.02	0.41
3:E:169:ASP:O	3:E:173:LYS:HE2	2.20	0.41
1:A:579:LEU:HD21	1:A:667:TYR:CD1	2.56	0.41
2:C:487:ARG:HB3	2:C:487:ARG:CZ	2.50	0.41
1:B:566:THR:HA	1:B:569:GLU:OE2	2.20	0.41
1:A:43:ILE:HG13	1:A:44:PHE:N	2.34	0.41
1:A:297:TRP:NE1	1:A:390:ASP:OD2	2.45	0.41
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.82	0.41
1:B:485:LYS:C	1:B:487:ASN:H	2.28	0.41
3:E:129:VAL:O	3:E:131:THR:HG23	2.20	0.41
3:E:222:LEU:HA	3:E:222:LEU:HD12	1.74	0.41
1:A:195:THR:O	1:A:195:THR:CG2	2.69	0.41
1:B:84:LYS:HE3	1:B:84:LYS:HB3	1.82	0.41
1:B:668:GLU:HB3	1:B:684:HIS:HD2	1.85	0.41
3:E:68:LEU:HD22	3:E:81:LEU:HA	2.03	0.41
3:E:219:ILE:HD12	3:E:219:ILE:HA	1.82	0.41
1:A:58:LYS:HG2	1:A:130:MET:HE1	2.03	0.41
1:A:113:SER:OG	1:A:116:LYS:HB2	2.21	0.41
1:A:554:ASP:OD1	1:A:557:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLU:HB3	1:A:684:HIS:HD2	1.85	0.41
1:A:690:ARG:CZ	1:A:690:ARG:HB2	2.51	0.41
1:B:43:ILE:HG13	1:B:44:PHE:N	2.34	0.41
1:B:100:LYS:HZ3	1:B:100:LYS:HG3	1.81	0.41
1:B:280:ILE:O	1:B:281:LYS:C	2.63	0.41
1:B:396:LEU:HA	1:B:396:LEU:HD23	1.59	0.41
1:B:436:LYS:O	1:B:439:GLU:HG3	2.21	0.41
1:B:628:MET:HB3	1:B:628:MET:HE3	1.76	0.41
2:C:569:GLN:HA	2:C:572:LEU:CD2	2.51	0.41
3:E:71:LEU:HD13	3:E:71:LEU:HA	1.94	0.41
3:E:193:TRP:NE1	3:E:197:LEU:HG	2.36	0.41
3:E:197:LEU:HA	3:E:197:LEU:HD23	1.78	0.41
1:A:436:LYS:O	1:A:439:GLU:HG3	2.21	0.41
1:A:495:THR:HA	1:A:521:MET:O	2.20	0.41
3:E:212:GLN:O	3:E:216:MET:HG3	2.20	0.41
3:E:254:ASP:O	3:E:257:GLU:HG2	2.21	0.41
1:A:506:ALA:HA	1:A:509:GLU:OE2	2.21	0.40
1:B:506:ALA:HA	1:B:509:GLU:OE2	2.21	0.40
2:C:337:ARG:NH2	2:C:551:GLU:OE1	2.54	0.40
2:C:559:LEU:HD23	2:C:559:LEU:HA	1.84	0.40
3:E:175:LEU:HB3	3:E:181:LEU:CD1	2.49	0.40
1:A:672:LEU:HD11	1:B:678:LEU:HD11	2.03	0.40
1:B:175:ASP:CG	1:B:177:GLY:H	2.28	0.40
2:C:480:PRO:HA	2:C:483:ARG:NH1	2.35	0.40
1:A:510:ARG:HA	1:A:510:ARG:HD2	1.86	0.40
1:A:611:GLU:O	1:A:615:LYS:HG3	2.21	0.40
2:C:461:LEU:HD23	2:C:461:LEU:HA	1.93	0.40
3:E:182:VAL:HG22	3:E:231:ARG:HB3	2.02	0.40
1:B:653:ASP:OD2	1:B:656:ASP:HB2	2.22	0.40
2:C:338:LEU:O	2:C:342:MET:HG2	2.22	0.40
3:E:161:HIS:O	3:E:165:LEU:HG	2.20	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	628/732 (86%)	598 (95%)	30 (5%)	0	100	100
1	B	629/732 (86%)	592 (94%)	37 (6%)	0	100	100
2	C	230/494 (47%)	209 (91%)	21 (9%)	0	100	100
3	E	248/378 (66%)	238 (96%)	10 (4%)	0	100	100
All	All	1735/2336 (74%)	1637 (94%)	98 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	573/666 (86%)	506 (88%)	67 (12%)	4	9
1	B	574/666 (86%)	494 (86%)	80 (14%)	3	5
2	C	195/406 (48%)	167 (86%)	28 (14%)	2	5
3	E	229/340 (67%)	202 (88%)	27 (12%)	4	8
All	All	1571/2078 (76%)	1369 (87%)	202 (13%)	6	6

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	23	GLN
1	A	26	ILE
1	A	32	LEU
1	A	75	GLU
1	A	81	ILE
1	A	90	THR
1	A	91	ILE
1	A	96	ILE
1	A	99	THR

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Mol	Chain	Res	Type
1	A	104	ILE
1	A	110	ILE
1	A	128	ILE
1	A	131	ILE
1	A	147	LYS
1	A	151	ILE
1	A	153	LYS
1	A	173	ARG
1	A	174	THR
1	A	176	THR
1	A	178	GLU
1	A	207	VAL
1	A	209	LYS
1	A	214	ILE
1	A	226	ARG
1	A	287	GLN
1	A	292	LYS
1	A	293	THR
1	A	294	LYS
1	A	315	SER
1	A	326	VAL
1	A	340	LEU
1	A	378	ILE
1	A	383	ASN
1	A	385	ILE
1	A	410	LYS
1	A	421	LEU
1	A	431	LYS
1	A	468	SER
1	A	474	MET
1	A	476	SER
1	A	486	GLU
1	A	494	ILE
1	A	495	THR
1	A	505	SER
1	A	508	VAL
1	A	514	HIS
1	A	529	CYS
1	A	530	VAL
1	A	540	THR
1	A	564	LYS
1	A	574	ILE

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Mol	Chain	Res	Type
1	A	580	GLU
1	A	581	LYS
1	A	583	VAL
1	A	585	LYS
1	A	589	SER
1	A	593	VAL
1	A	600	VAL
1	A	601	THR
1	A	603	THR
1	A	615	LYS
1	A	636	ILE
1	A	653	ASP
1	A	665	LEU
1	A	672	LEU
1	A	678	LEU
1	B	15	GLU
1	B	26	ILE
1	B	28	GLN
1	B	49	ILE
1	B	53	SER
1	B	63	SER
1	B	77	HIS
1	B	91	ILE
1	B	96	ILE
1	B	100	LYS
1	B	110	ILE
1	B	112	LYS
1	B	119	MET
1	B	122	LEU
1	B	128	ILE
1	B	136	VAL
1	B	152	THR
1	B	157	ASP
1	B	163	GLU
1	B	165	SER
1	B	180	MET
1	B	186	VAL
1	B	207	VAL
1	B	210	HIS
1	B	223	GLU
1	B	282	GLU
1	B	284	TYR

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Mol	Chain	Res	Type
1	B	293	THR
1	B	305	THR
1	B	317	THR
1	B	326	VAL
1	B	335	LEU
1	B	340	LEU
1	B	357	LYS
1	B	367	ARG
1	B	378	ILE
1	B	421	LEU
1	B	422	GLU
1	B	427	LEU
1	B	453	SER
1	B	468	SER
1	B	473	GLU
1	B	476	SER
1	B	477	LEU
1	B	485	LYS
1	B	494	ILE
1	B	495	THR
1	B	498	THR
1	B	499	LYS
1	B	508	VAL
1	B	514	HIS
1	B	529	CYS
1	B	530	VAL
1	B	540	THR
1	B	547	GLU
1	B	574	ILE
1	B	580	GLU
1	B	583	VAL
1	B	589	SER
1	B	593	VAL
1	B	600	VAL
1	B	601	THR
1	B	603	THR
1	B	607	THR
1	B	610	MET
1	B	612	ARG
1	B	615	LYS
1	B	624	THR
1	B	625	MET

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Mol	Chain	Res	Type
1	B	628	MET
1	B	632	LYS
1	B	636	ILE
1	B	653	ASP
1	B	656	ASP
1	B	658	SER
1	B	662	LEU
1	B	672	LEU
1	B	678	LEU
1	B	693	LYS
1	B	698	ILE
2	C	306	GLU
2	C	313	THR
2	C	333	THR
2	C	346	LEU
2	C	351	ASP
2	C	353	LEU
2	C	375	ASP
2	C	442	ILE
2	C	444	TYR
2	C	446	ILE
2	C	449	LEU
2	C	456	GLN
2	C	467	GLN
2	C	468	GLU
2	C	474	LEU
2	C	477	SER
2	C	481	ASP
2	C	510	SER
2	C	516	ILE
2	C	517	LEU
2	C	519	LEU
2	C	525	ASP
2	C	539	LEU
2	C	543	ARG
2	C	545	THR
2	C	547	LYS
2	C	549	CYS
2	C	576	SER
3	E	50	LEU
3	E	52	ARG
3	E	63	GLU

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Mol	Chain	Res	Type
3	E	69	LYS
3	E	93	LYS
3	E	102	LEU
3	E	103	GLU
3	E	118	THR
3	E	119	LEU
3	E	121	LYS
3	E	156	GLU
3	E	162	PHE
3	E	164	MET
3	E	169	ASP
3	E	179	VAL
3	E	180	HIS
3	E	181	LEU
3	E	185	GLU
3	E	186	THR
3	E	197	LEU
3	E	199	VAL
3	E	203	CYS
3	E	214	ILE
3	E	215	VAL
3	E	220	LEU
3	E	231	ARG
3	E	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	123	GLN
1	A	154	HIS
1	A	155	ASN
1	A	287	GLN
1	A	306	ASN
1	A	359	ASN
1	A	405	GLN
1	A	415	ASN
1	A	444	ASN
1	A	450	HIS
1	A	617	GLN
1	A	655	ASN
1	A	684	HIS

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Mol	Chain	Res	Type
1	A	686	ASN
1	B	35	ASN
1	B	77	HIS
1	B	79	ASN
1	B	133	GLN
1	B	155	ASN
1	B	189	HIS
1	B	212	GLN
1	B	300	ASN
1	B	354	ASN
1	B	415	ASN
1	B	444	ASN
1	B	450	HIS
1	B	488	GLN
1	B	514	HIS
1	B	531	GLN
1	B	617	GLN
1	B	684	HIS
1	B	686	ASN
2	C	332	ASN
2	C	352	HIS
2	C	456	GLN
2	C	467	GLN
2	C	542	ASN
3	E	44	GLN
3	E	85	GLN
3	E	172	GLN
3	E	178	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SEP	E	13	3	8,9,10	0.74	0	8,12,14	1.26	1 (12%)

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	SEP	E	13	3	-	4/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	E	13	SEP	O3P-P-OG	-2.37	100.44	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	13	SEP	CB-OG-P-O1P
3	E	13	SEP	CB-OG-P-O2P
3	E	13	SEP	CB-OG-P-O3P
3	E	13	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ADP	B	801	-	24,29,29	1.00	1 (4%)	29,45,45	1.47	4 (13%)
4	ADP	A	801	-	24,29,29	0.98	1 (4%)	29,45,45	1.51	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	801	-	-	2/12/32/32	0/3/3/3
4	ADP	A	801	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ADP	C5-C4	2.10	1.46	1.40
4	B	801	ADP	C5-C4	2.05	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	ADP	PA-O3A-PB	-3.86	119.56	132.83
4	A	801	ADP	PA-O3A-PB	-3.84	119.67	132.83
4	B	801	ADP	N3-C2-N1	-3.14	123.77	128.68
4	A	801	ADP	N3-C2-N1	-3.14	123.77	128.68
4	A	801	ADP	C3'-C2'-C1'	2.76	105.14	100.98
4	A	801	ADP	C4-C5-N7	-2.54	106.75	109.40
4	B	801	ADP	C4-C5-N7	-2.49	106.81	109.40
4	B	801	ADP	C3'-C2'-C1'	2.38	104.56	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

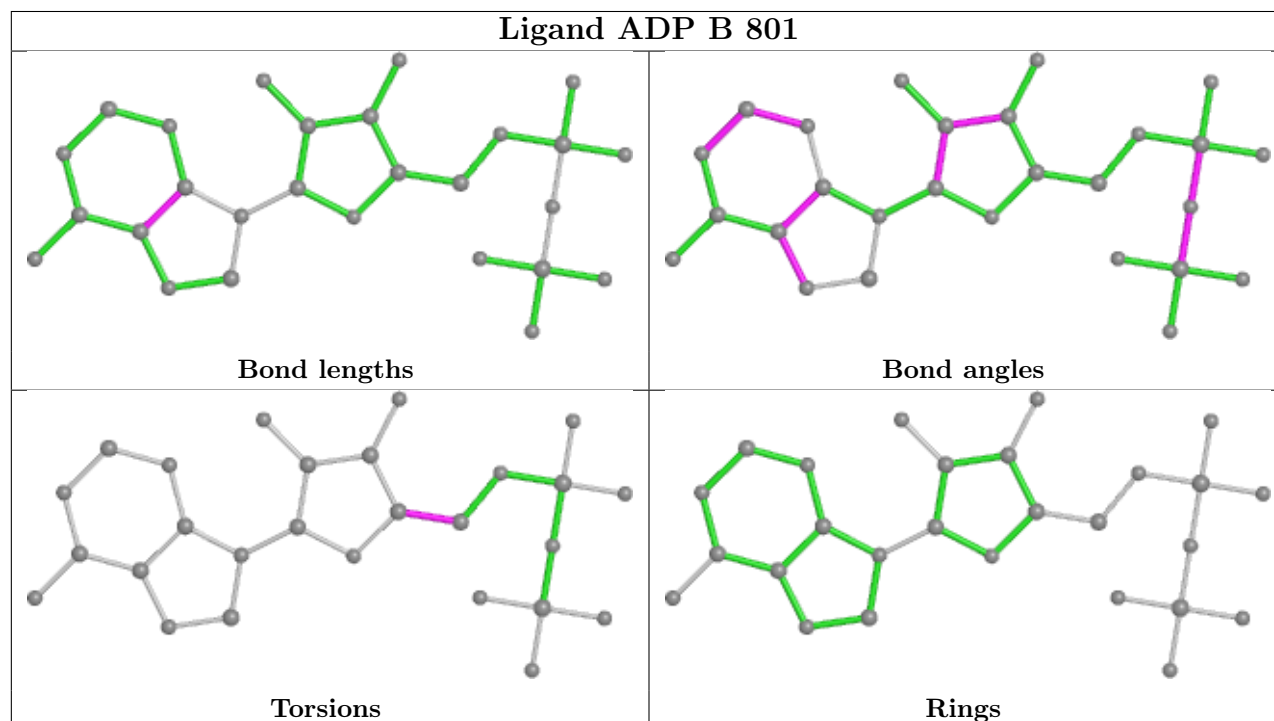


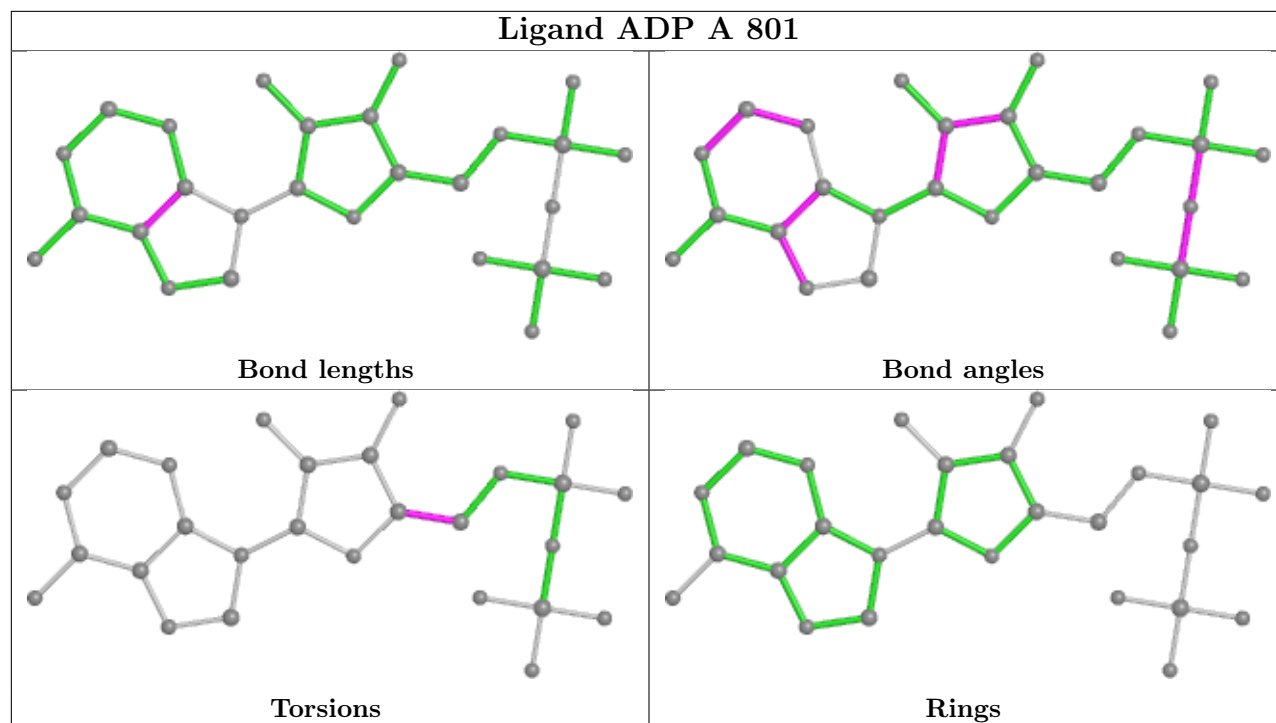
Mol	Chain	Res	Type	Atoms
4	A	801	ADP	O4'-C4'-C5'-O5'
4	B	801	ADP	O4'-C4'-C5'-O5'
4	A	801	ADP	C3'-C4'-C5'-O5'
4	B	801	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

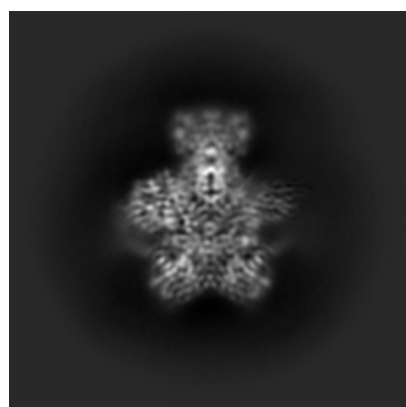
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62508. These allow visual inspection of the internal detail of the map and identification of artifacts.

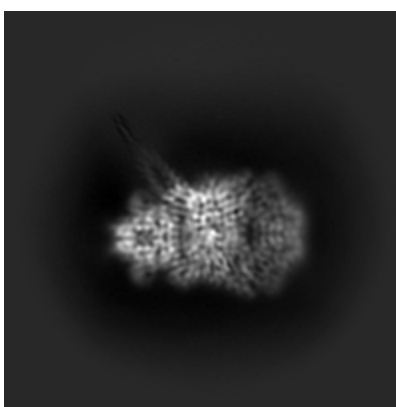
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

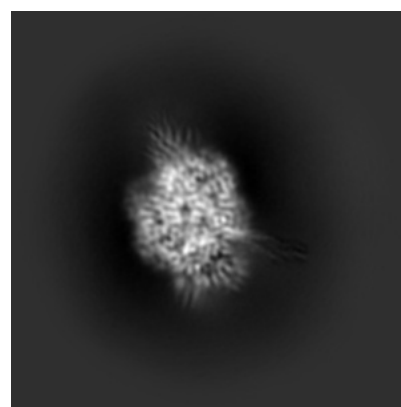
#### 6.1.1 Primary map



X



Y

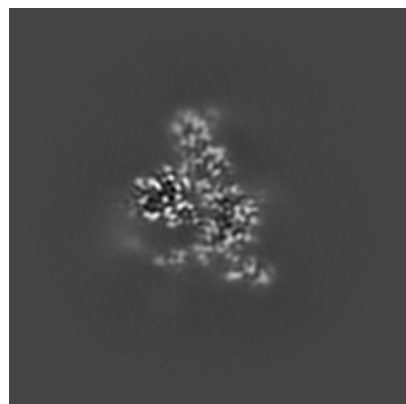


Z

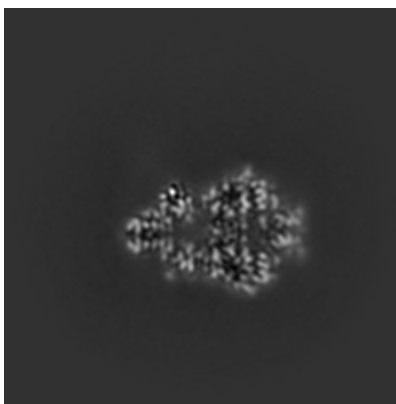
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 140



Y Index: 140

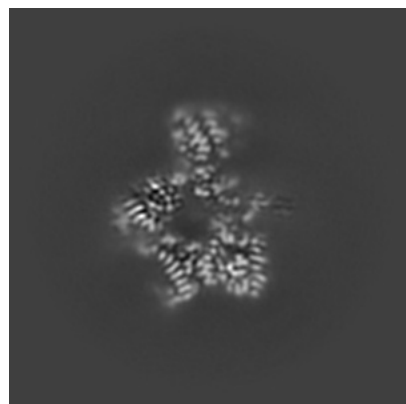


Z Index: 140

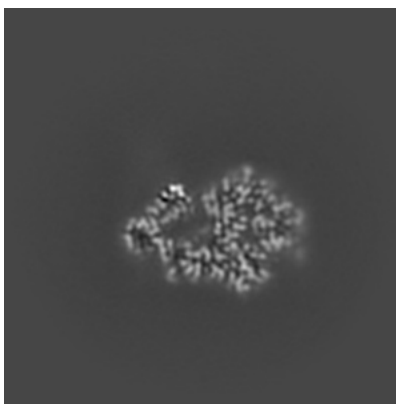
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 128



Y Index: 137

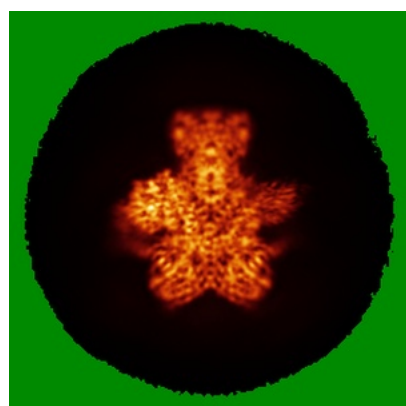


Z Index: 140

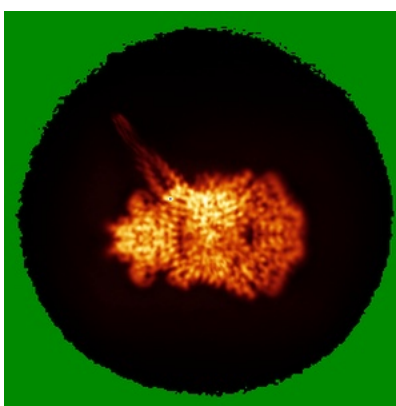
The images above show the largest variance slices of the map in three orthogonal directions.

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

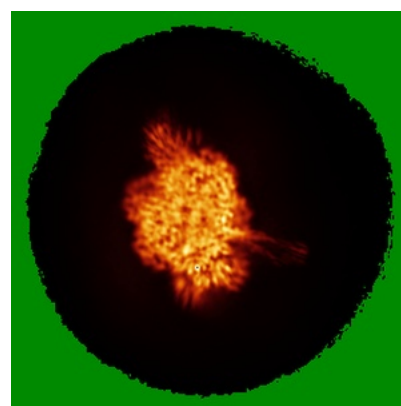
### 6.4.1 Primary map



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 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

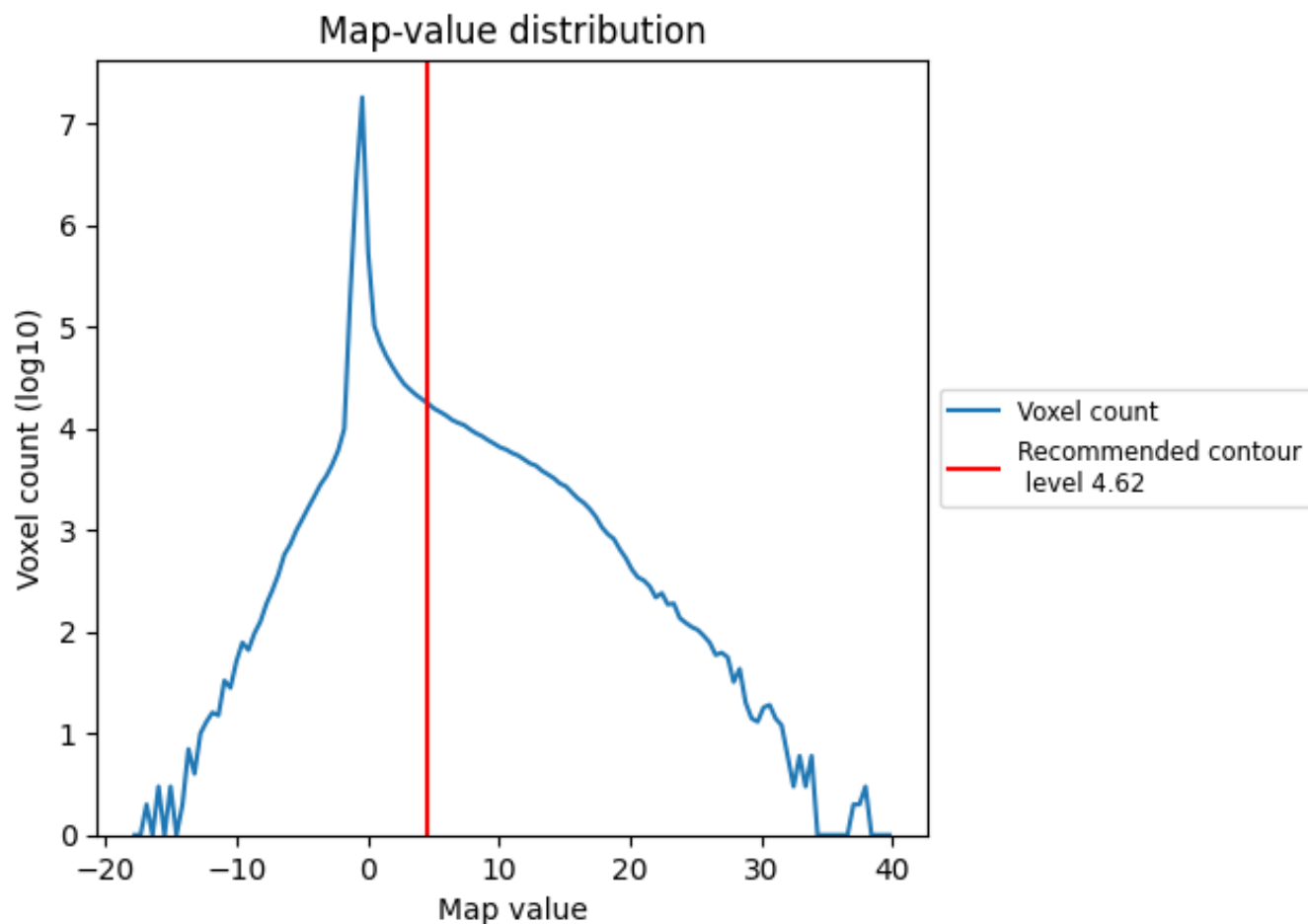
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

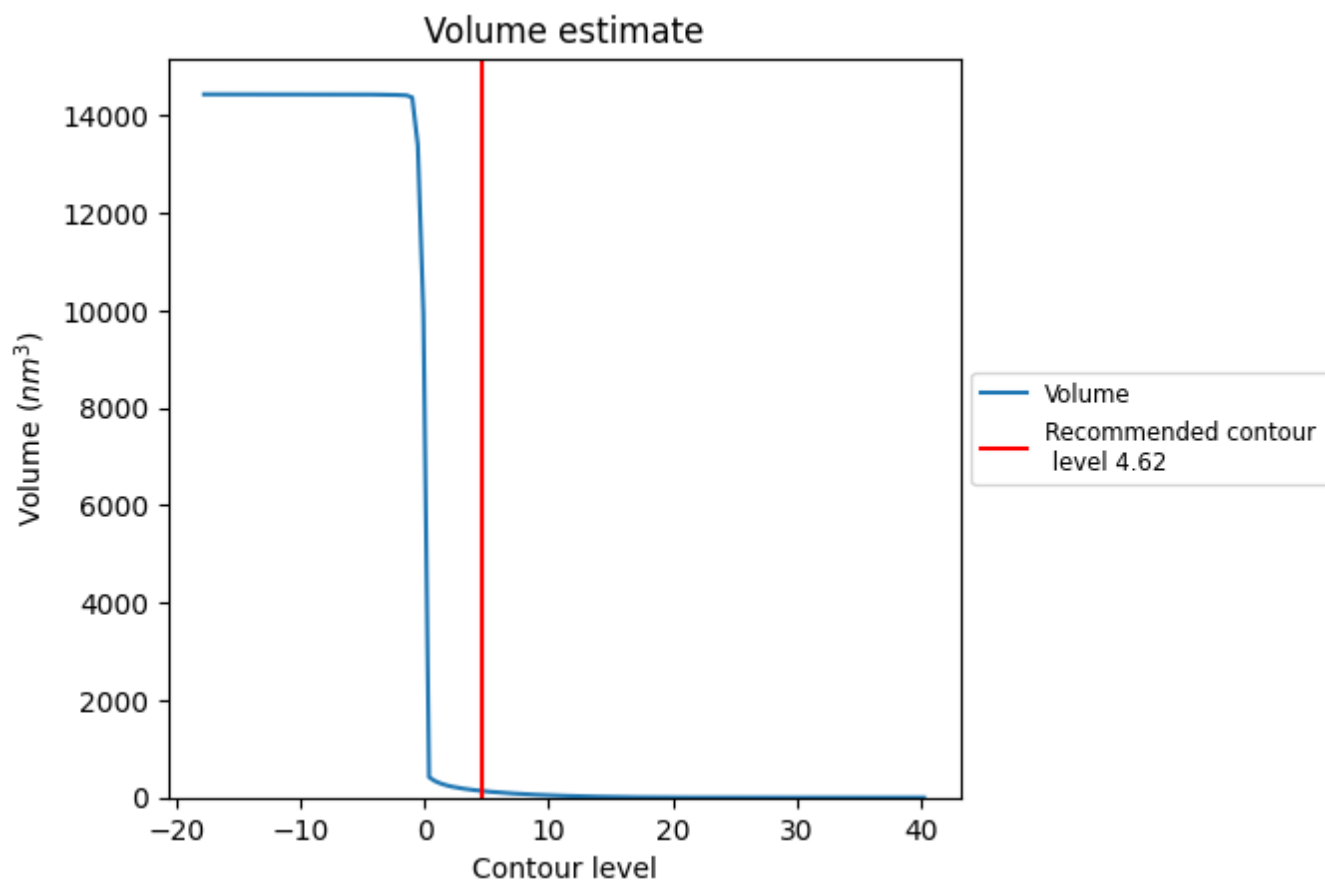
This section contains the results of statistical analysis of the map.

### 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.

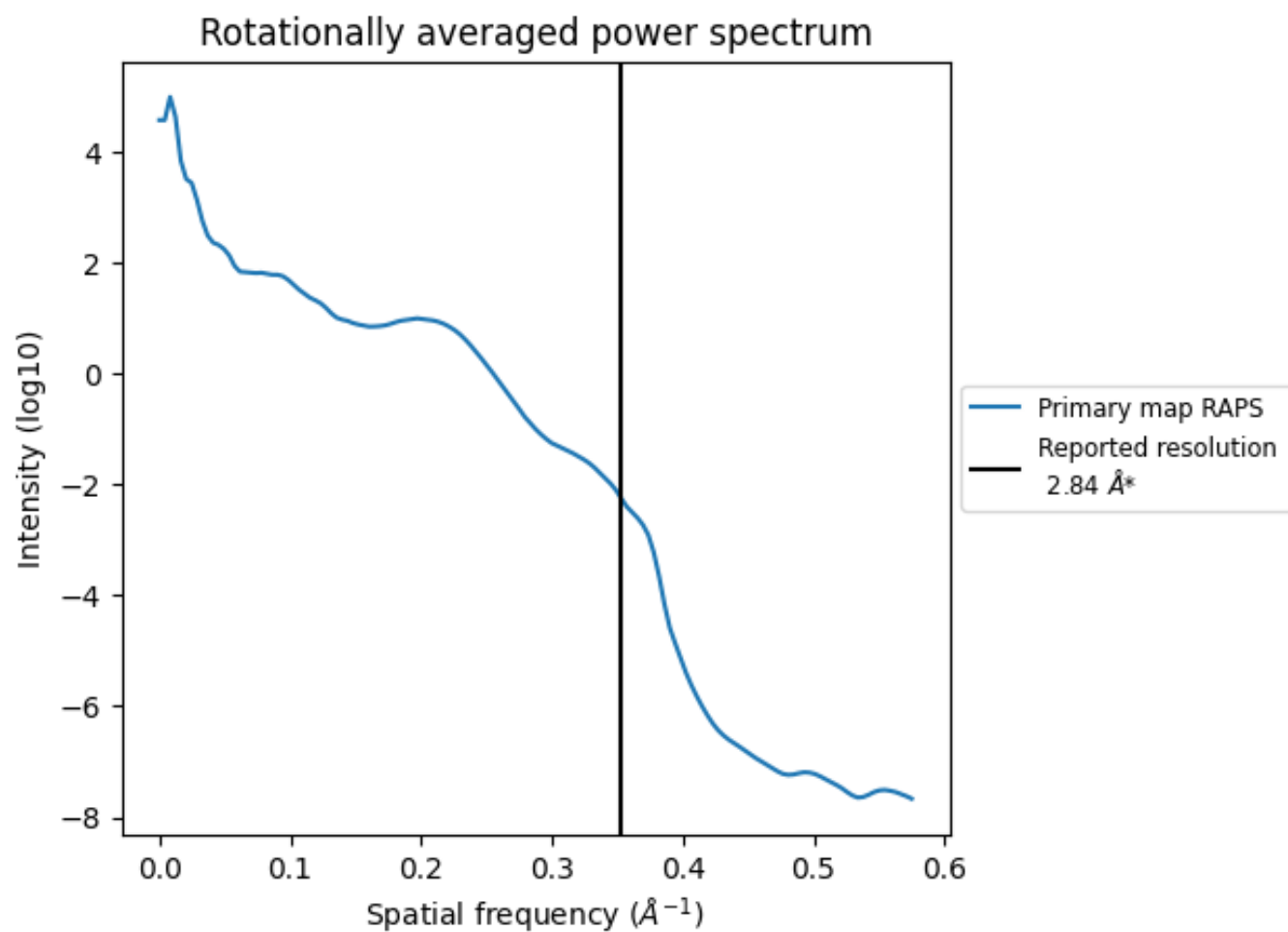
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136  $\text{nm}^3$ ; this corresponds to an approximate mass of 123 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 0.352  $\text{\AA}^{-1}$



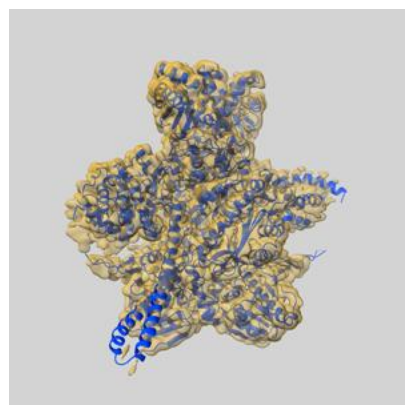
## 8 Fourier-Shell correlation ⓘ

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

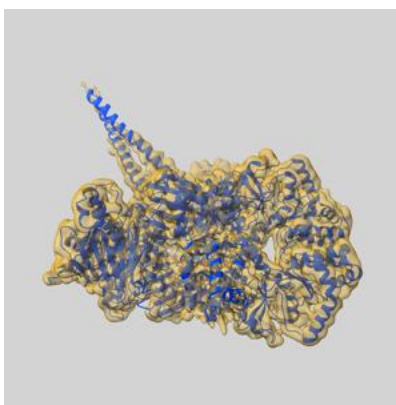
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62508 and PDB model 9KQN. Per-residue inclusion information can be found in section [3](#) on page [5](#).

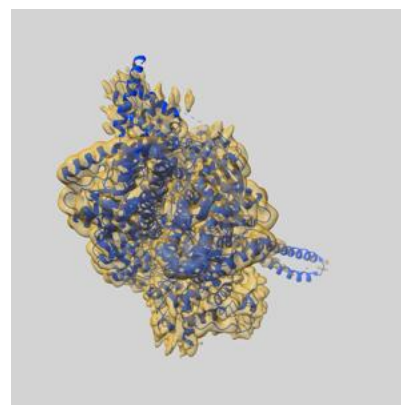
### 9.1 Map-model overlay [i](#)



X



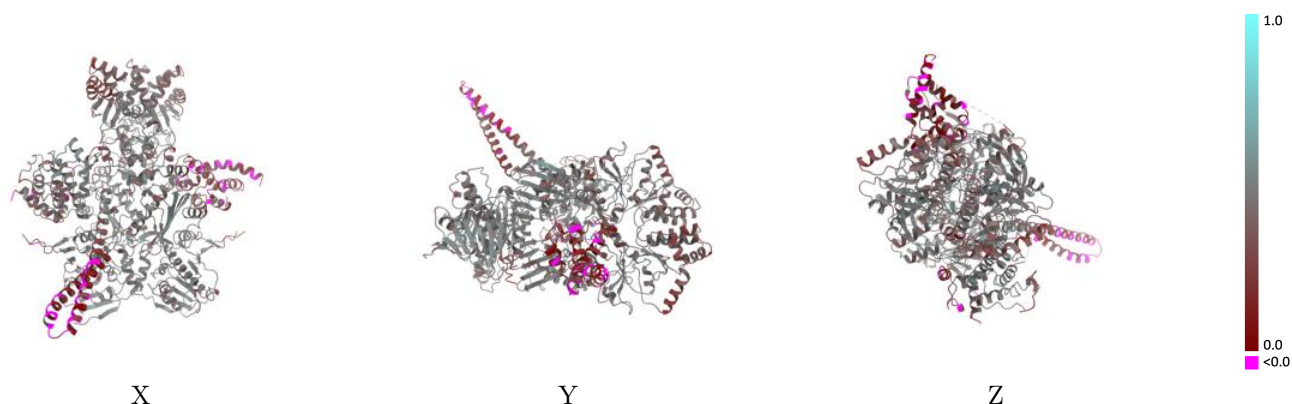
Y



Z

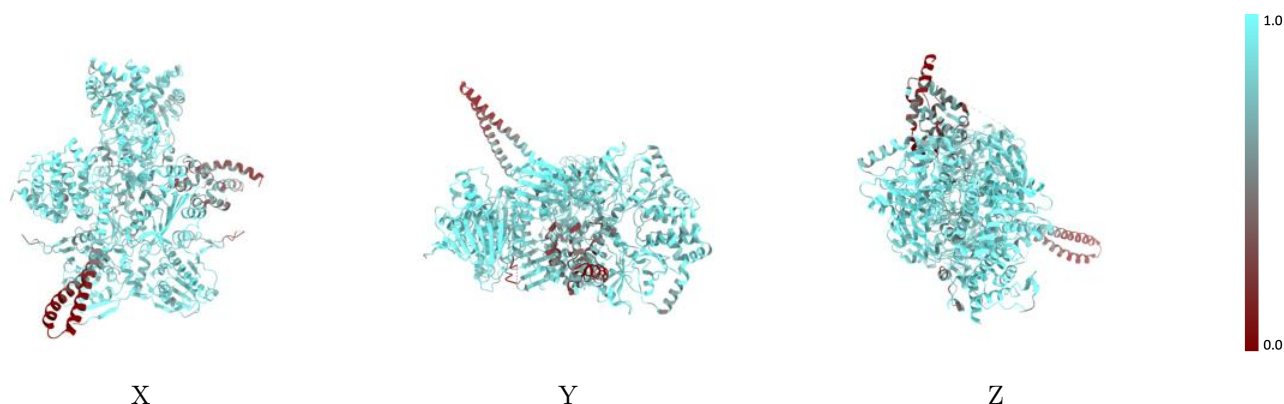
The images above show the 3D surface view of the map at the recommended contour level 4.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



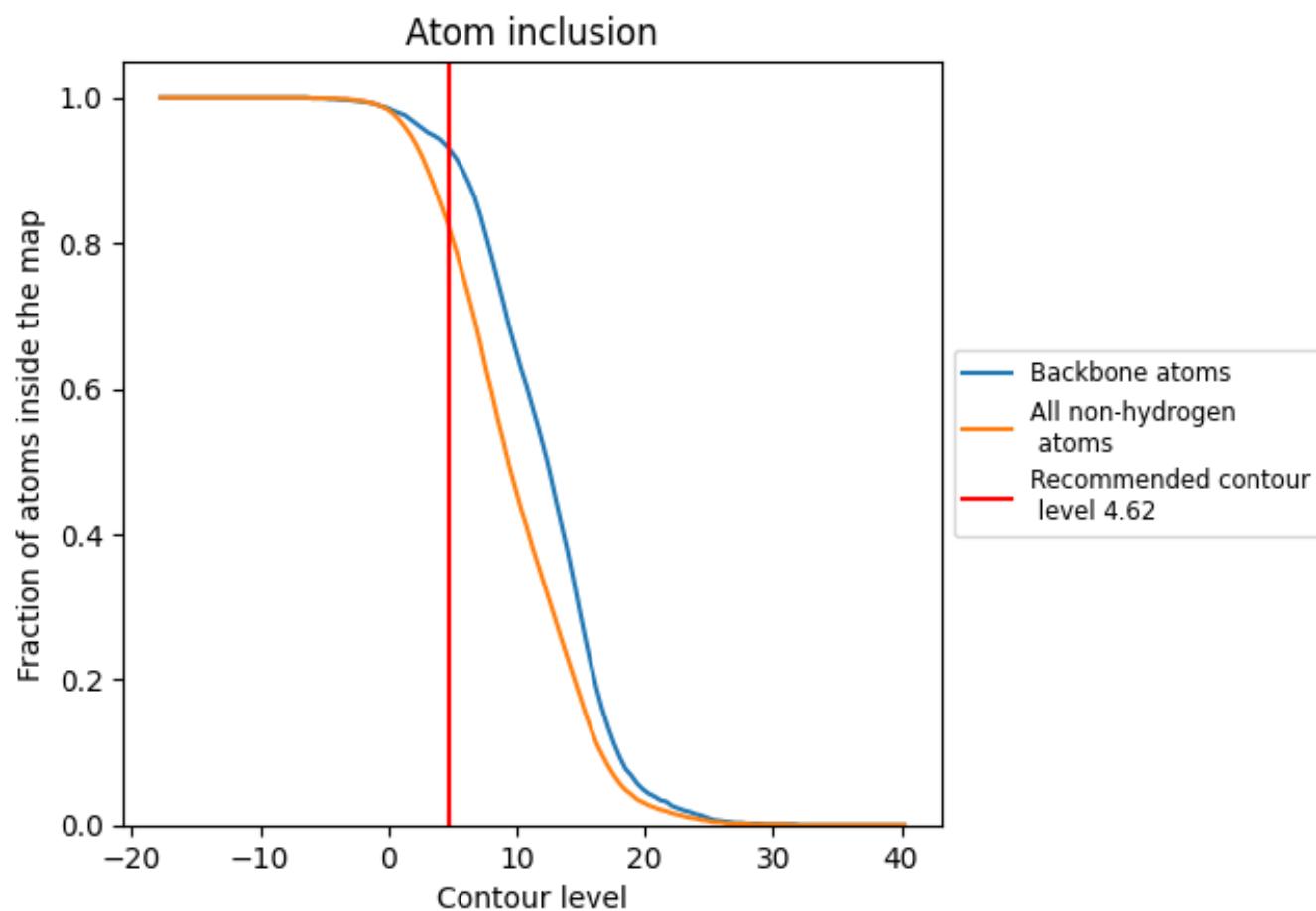
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.62).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8270	<div></div> 0.4010
A	<div></div> 0.8750	<div></div> 0.4440
B	<div></div> 0.8780	<div></div> 0.4390
C	<div></div> 0.8960	<div></div> 0.3990
E	<div></div> 0.5210	<div></div> 0.2080

