Full wwPDB EM Validation Report

May 4, 2025 – 02:07 PM EDT

PDB ID	:	7SU3 / pdb_00007su3
EMDB ID	:	EMD-25439
Title	:	CryoEM structure of DNA-PK complex VII
Authors	:	Chen, X.; Liu, L.; Gellert, M.; Yang, W.
Deposited on	:	2021-11-16
Resolution	:	3.30 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:

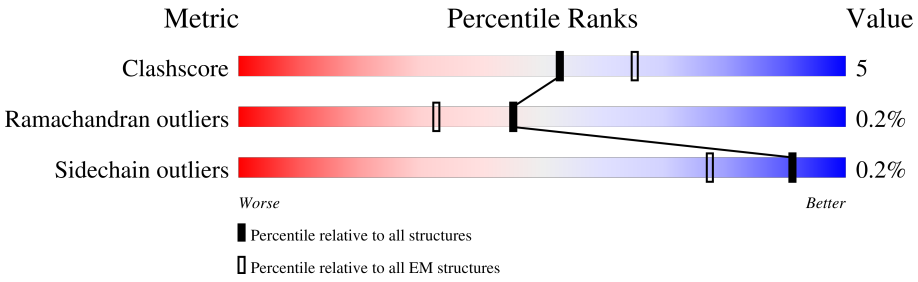
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	4128	80% 12% 8%
2	B	609	68% 13% 19%
3	C	732	27% 77% 14% 9%
4	D	24	79% 21%
4	F	24	17% 58% 21% 21%
5	E	16	31% 44% 25% 31%
5	G	16	62% 38%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 41242 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3802	30378	19481	5159	5541	197	7	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	496	4017	2573	682	744	18	1	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	669	5354	3420	899	1009	26	0	0

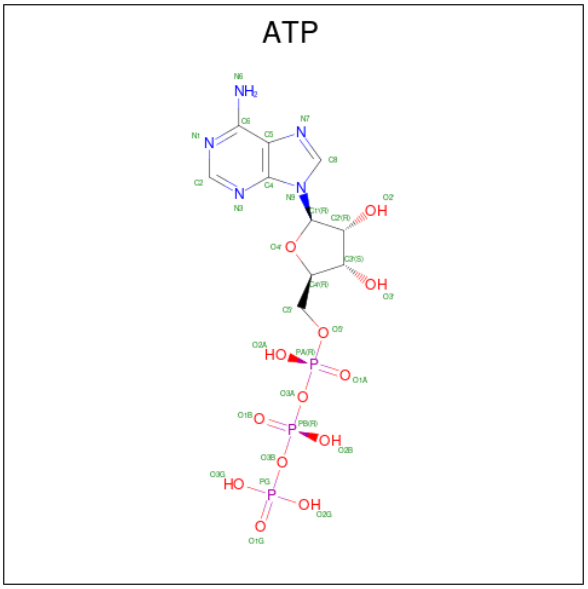
- Molecule 4 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	24	484	233	82	146	23	0	0
4	F	19	Total	C	N	O	P	0	0
			383	184	62	118	19		

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*G)-3').

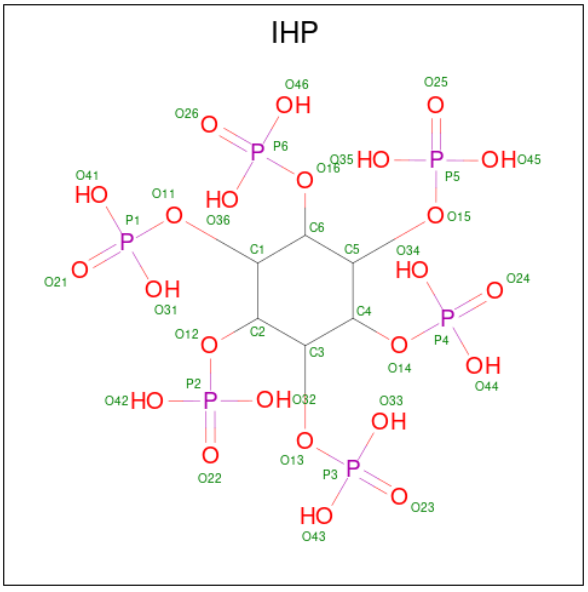
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	11	229	109	50	60	10	0	0
5	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



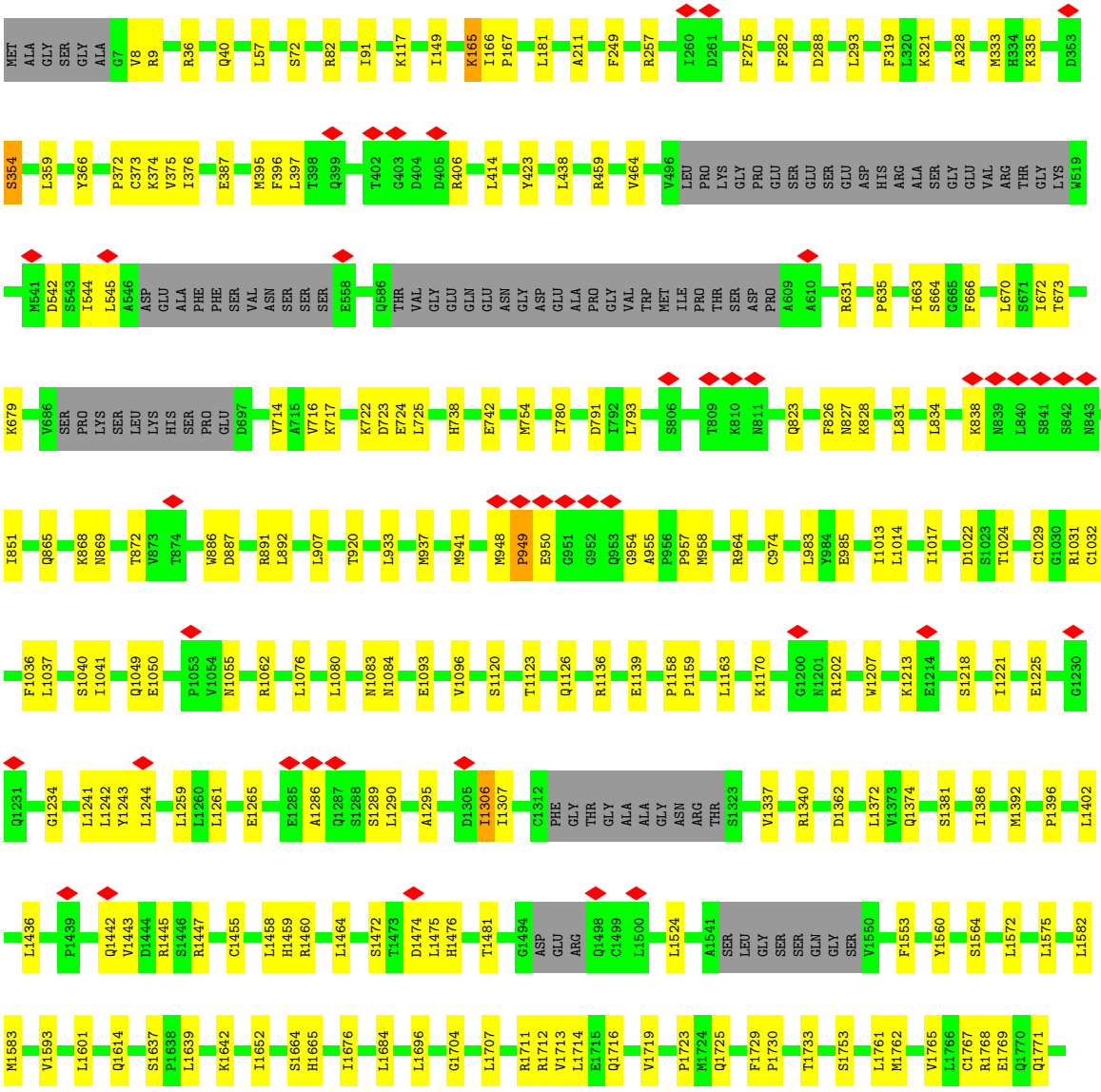
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	O	P	0
			36	6	24	6	

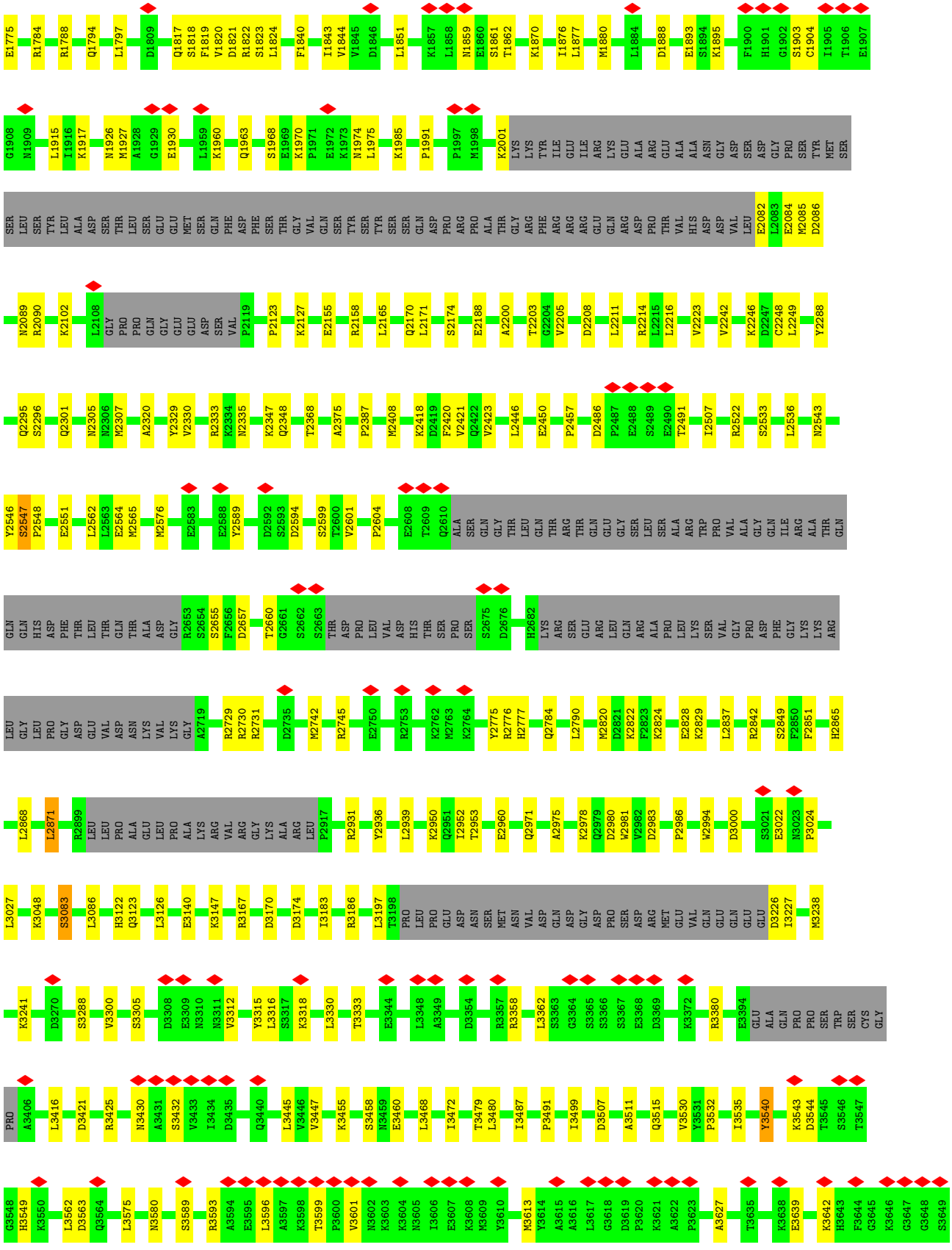
3 Residue-property plots (i)

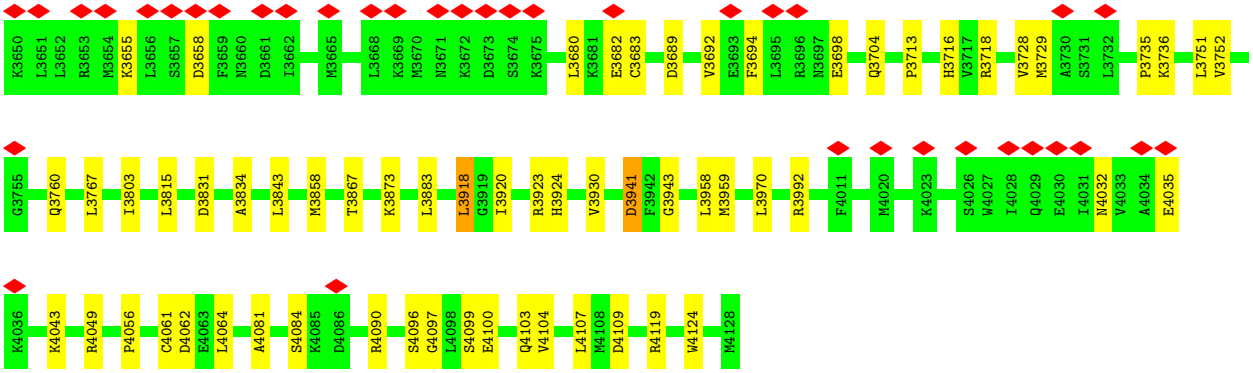
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

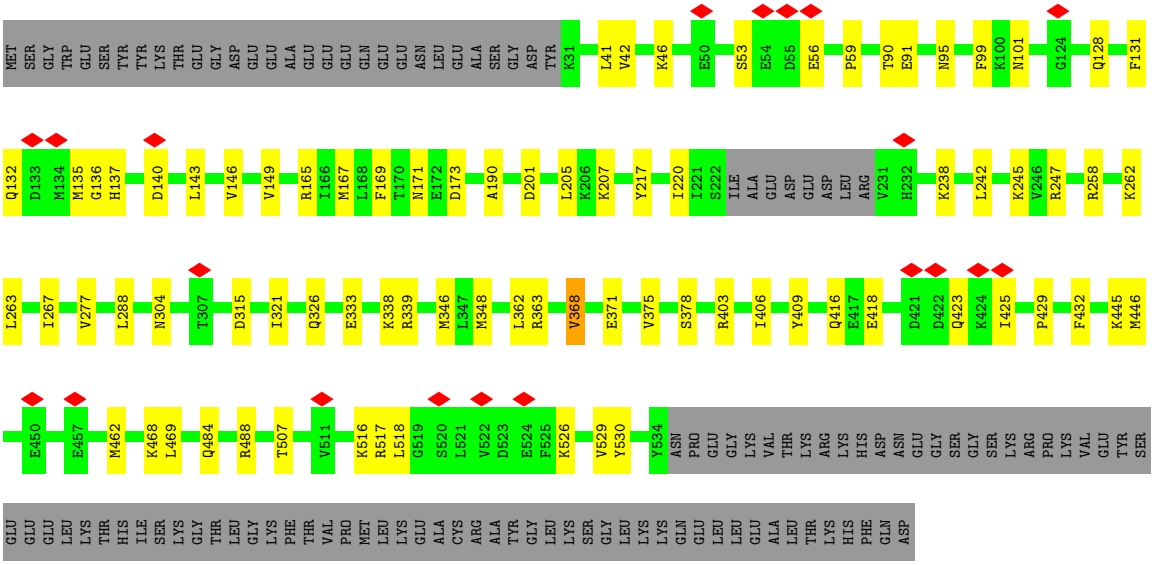






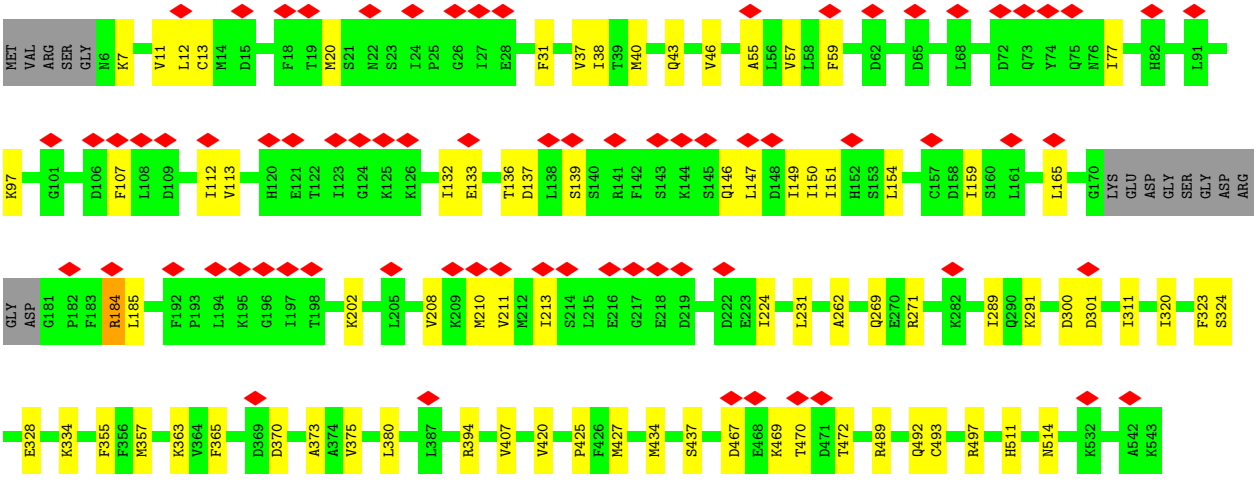
• Molecule 2: X-ray repair cross-complementing protein 6

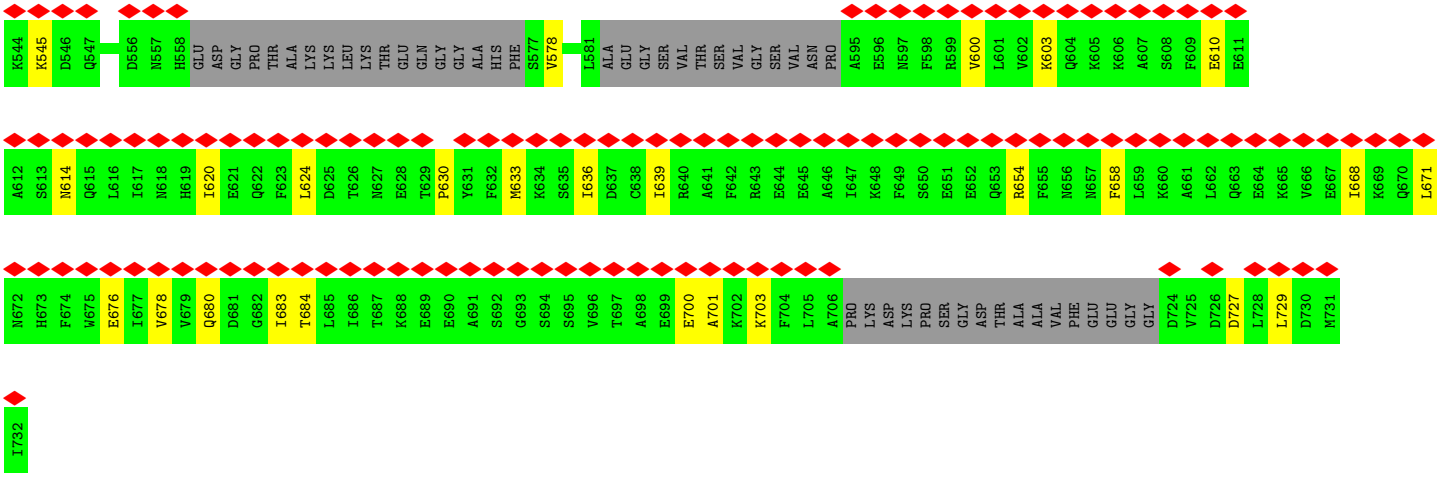
Chain B:



• Molecule 3: X-ray repair cross-complementing protein 5

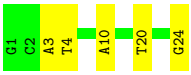
Chain C:





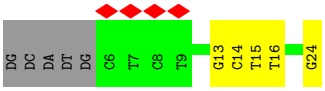
• Molecule 4: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP *CP*GP*AP*TP*AP*TP*CP*G)-3')

Chain D:



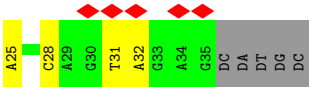
• Molecule 4: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP *CP*GP*AP*TP*AP*TP*CP*G)-3')

Chain F:



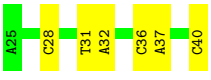
• Molecule 5: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*G)-3')

Chain E:



• Molecule 5: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*G)-3')

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0117	Depositor
Map size (Å)	399.84, 399.84, 399.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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: IHP, ATP

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	0.43	0/31017	0.65	11/41920 (0.0%)
2	B	0.41	0/4099	0.64	0/5520
3	C	0.34	0/5455	0.64	0/7352
4	D	0.54	0/540	0.57	0/831
4	F	0.41	0/426	0.57	0/654
5	E	0.24	0/259	0.44	0/399
5	G	0.57	0/372	0.51	0/573
All	All	0.42	0/42168	0.64	11/57249 (0.0%)

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	7
3	C	0	1
All	All	0	8

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	VAL	CA-C-N	6.07	133.13	121.54
1	A	8	VAL	C-N-CA	6.07	133.13	121.54
1	A	3599	THR	CA-C-N	5.78	140.88	127.00
1	A	3599	THR	C-N-CA	5.78	140.88	127.00
1	A	3122[A]	HIS	CA-C-N	5.37	131.79	121.54
1	A	3122[A]	HIS	C-N-CA	5.37	131.79	121.54
1	A	3122[B]	HIS	CA-C-N	5.37	131.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3122[B]	HIS	C-N-CA	5.37	131.79	121.54
1	A	354	SER	CA-C-N	5.14	129.64	122.08
1	A	354	SER	C-N-CA	5.14	129.64	122.08
1	A	948	MET	N-CA-C	5.04	120.96	109.81

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Peptide
1	A	166	ILE	Peptide
1	A	2223	VAL	Peptide
1	A	3479	THR	Peptide
1	A	3563	ASP	Peptide
1	A	3694	PHE	Peptide
1	A	3918	LEU	Peptide
3	C	184	ARG	Peptide

5.2 Too-close contacts (i)

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	30378	0	30738	298	0
2	B	4017	0	4104	58	0
3	C	5354	0	5369	70	0
4	D	484	0	274	5	0
4	F	383	0	217	4	0
5	E	229	0	124	3	0
5	G	330	0	180	4	0
6	A	31	0	12	1	0
7	B	36	0	6	1	0
All	All	41242	0	41024	419	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 5.

All (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:LYS:O	2:B:530:TYR:HB3	1.78	0.83
1:A:2170:GLN:O	1:A:2174:SER:HB2	1.83	0.78
1:A:1970:LYS:HB2	1:A:1975:LEU:HB3	1.72	0.70
1:A:1859:ASN:HD22	1:A:1862:THR:HG22	1.54	0.70
1:A:2242:VAL:O	1:A:2246:LYS:HB2	1.90	0.70
3:C:11:VAL:HG12	3:C:55:ALA:HB3	1.76	0.67
3:C:610:GLU:O	3:C:614:ASN:HB2	1.92	0.67
1:A:3312:VAL:HA	1:A:3316:LEU:HB2	1.76	0.66
1:A:865:GLN:HB3	1:A:3170:ASP:HB3	1.79	0.65
1:A:2216:LEU:HD22	1:A:2249:LEU:HD23	1.77	0.64
1:A:3123:GLN:HA	1:A:3126:LEU:HB2	1.79	0.64
1:A:72:SER:O	1:A:82:ARG:NH1	2.30	0.64
5:E:28:DC:H42	4:F:13:DG:H1	1.46	0.64
3:C:700:GLU:HG2	3:C:703:LYS:HE2	1.79	0.63
3:C:489:ARG:NH2	3:C:493:CYS:SG	2.71	0.63
1:A:868:LYS:NZ	1:A:3174:ASP:OD1	2.32	0.62
3:C:112:ILE:HD13	3:C:150:ILE:HG22	1.81	0.62
2:B:446:MET:HE3	3:C:363:LYS:HD2	1.82	0.61
1:A:2085:MET:HA	1:A:2089:ASN:HB3	1.81	0.61
1:A:1851:LEU:HA	1:A:1870:LYS:HE2	1.81	0.61
1:A:742:GLU:HG3	1:A:780:ILE:HG23	1.83	0.60
1:A:828:LYS:HA	1:A:831:LEU:HD12	1.82	0.60
6:A:4201:ATP:O5'	6:A:4201:ATP:H8	1.85	0.60
1:A:1888:ASP:HA	1:A:1893:GLU:HG3	1.83	0.60
1:A:2657:ASP:OD1	1:A:2657:ASP:N	2.35	0.60
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.83	0.60
1:A:2203:THR:HG22	1:A:2248:CYS:HB3	1.84	0.59
4:D:24:DG:HO3'	5:E:25:DA:HO5'	1.50	0.59
1:A:328:ALA:HB2	1:A:372:PRO:HD3	1.85	0.59
1:A:2931:ARG:NH1	1:A:2960:GLU:OE2	2.36	0.59
1:A:2086:ASP:OD2	1:A:2731:ARG:NH1	2.35	0.59
2:B:416:GLN:NE2	2:B:429:PRO:O	2.36	0.59
1:A:635:PRO:O	1:A:679:LYS:NZ	2.36	0.59
1:A:3815:LEU:HD22	1:A:3930:VAL:HG11	1.84	0.59
1:A:1664:SER:O	1:A:1665:HIS:ND1	2.36	0.58
1:A:2522:ARG:NH1	1:A:2564:GLU:OE2	2.36	0.58
2:B:321:ILE:HG13	2:B:326:GLN:HG3	1.86	0.58
1:A:2730:ARG:NH1	5:G:40:DC:O3'	2.37	0.58
3:C:154:LEU:HB2	3:C:159:ILE:HB	1.84	0.58
1:A:887:ASP:OD2	1:A:891:ARG:NH1	2.36	0.58
1:A:2953:THR:HB	1:A:2994:TRP:HE1	1.69	0.58
1:A:333:MET:SD	1:A:333:MET:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2952:ILE:HD11	1:A:2971:GLN:HB2	1.85	0.57
1:A:3867:THR:OG1	1:A:4119:ARG:NH2	2.37	0.57
2:B:462:MET:HE3	3:C:380:LEU:HB2	1.86	0.57
1:A:459:ARG:HH12	1:A:544:ILE:HD11	1.68	0.57
1:A:1396:PRO:HB3	1:A:1460:ARG:HH12	1.69	0.57
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.35	0.57
1:A:4061:CYS:HA	1:A:4064:LEU:HD12	1.86	0.57
3:C:185:LEU:HD23	3:C:511:HIS:HB3	1.87	0.56
1:A:1926:ASN:ND2	1:A:1974:ASN:O	2.39	0.56
1:A:2952:ILE:HG12	1:A:2975:ALA:HB2	1.88	0.56
2:B:165:ARG:NH1	2:B:201:ASP:OD2	2.38	0.56
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.38	0.56
2:B:165:ARG:HH22	2:B:167:MET:HE3	1.71	0.56
2:B:238:LYS:O	2:B:242:LEU:HB2	2.06	0.56
2:B:262:LYS:HD2	2:B:346:MET:HG2	1.88	0.56
1:A:3589:SER:OG	1:A:3593:ARG:NH2	2.39	0.55
1:A:1820:VAL:HG23	1:A:1824:LEU:HD23	1.89	0.55
2:B:507:THR:HG23	3:C:394:ARG:HE	1.70	0.55
1:A:1767:CYS:HB3	1:A:1818:SER:HB3	1.89	0.55
2:B:91:GLU:H	2:B:136:GLY:HA3	1.72	0.55
1:A:2820:MET:HE3	1:A:2829:LYS:HG2	1.88	0.55
1:A:3655:LYS:HB2	1:A:3658:ASP:HB3	1.89	0.55
1:A:117:LYS:HD2	3:C:300:ASP:HA	1.87	0.55
1:A:366:TYR:OH	1:A:387:GLU:OE2	2.25	0.55
3:C:492:GLN:NE2	3:C:493:CYS:SG	2.80	0.55
1:A:3751:LEU:HB3	1:A:3803:ILE:HB	1.89	0.55
1:A:3421:ASP:OD2	1:A:3425:ARG:NH2	2.39	0.55
1:A:1093:GLU:HA	1:A:1096:VAL:HG12	1.90	0.54
1:A:3698:GLU:OE2	1:A:3718:ARG:NH1	2.40	0.54
2:B:143:LEU:HA	2:B:146:VAL:HG12	1.88	0.54
1:A:1820:VAL:HA	1:A:1824:LEU:HB3	1.88	0.54
1:A:1991:PRO:O	1:A:2731:ARG:NH2	2.41	0.54
1:A:985:GLU:OE1	1:A:1031:ARG:NH1	2.39	0.54
1:A:2307:MET:HE2	1:A:2320:ALA:HA	1.89	0.54
1:A:3315:TYR:HA	1:A:3318:LYS:HG2	1.88	0.54
1:A:3843:LEU:HD22	1:A:3858:MET:HG2	1.89	0.54
2:B:173:ASP:OD1	2:B:207:LYS:NZ	2.41	0.54
1:A:1295:ALA:HB2	1:A:1362:ASP:HB3	1.89	0.54
2:B:315:ASP:OD1	2:B:315:ASP:N	2.40	0.53
1:A:2543:ASN:O	1:A:2842:ARG:NH2	2.40	0.53
1:A:1601:LEU:HD21	1:A:1652:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ASN:HD21	2:B:99:PHE:HB2	1.72	0.53
1:A:2978:LYS:O	1:A:2981:TRP:NE1	2.42	0.53
1:A:1637:SER:HB3	1:A:1642:LYS:HE3	1.90	0.53
1:A:3530:VAL:HG22	1:A:3562:LEU:HD22	1.89	0.53
2:B:217:TYR:HA	2:B:220:ILE:HG22	1.89	0.53
1:A:1443:VAL:O	1:A:1447:ARG:NH2	2.42	0.53
3:C:40:MET:HA	3:C:43:GLN:HE21	1.74	0.53
1:A:211:ALA:O	2:B:339:ARG:NH1	2.42	0.53
1:A:834:LEU:O	1:A:838:LYS:HB2	2.08	0.53
1:A:2776:ARG:NH2	1:A:2784:GLN:OE1	2.42	0.53
3:C:136:THR:OG1	3:C:137:ASP:N	2.40	0.53
3:C:624:LEU:HD12	3:C:671:LEU:HD13	1.91	0.53
1:A:2084:GLU:O	1:A:2089:ASN:ND2	2.40	0.53
1:A:2931:ARG:NH2	1:A:3000:ASP:OD2	2.41	0.53
2:B:59:PRO:HB3	2:B:205:LEU:HG	1.91	0.53
1:A:2421:VAL:HG13	1:A:2457:PRO:HG3	1.90	0.52
1:A:1036:PHE:O	1:A:1040:SER:HB3	2.09	0.52
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.43	0.52
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.91	0.52
2:B:484:GLN:OE1	2:B:488:ARG:NH1	2.42	0.52
3:C:678:VAL:HG13	3:C:683:ILE:HB	1.90	0.52
1:A:791:ASP:OD1	1:A:791:ASP:N	2.40	0.52
1:A:2155:GLU:OE2	1:A:2158:ARG:NH1	2.42	0.52
1:A:3689:ASP:OD1	1:A:3689:ASP:N	2.41	0.52
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.90	0.52
1:A:3511:ALA:O	1:A:3515:GLN:NE2	2.43	0.52
1:A:716:VAL:HB	1:A:1120:SER:HA	1.92	0.52
1:A:1794:GLN:HA	1:A:1797:LEU:HD12	1.91	0.52
1:A:2165:LEU:HD13	1:A:2200:ALA:HB3	1.91	0.52
2:B:468:LYS:HG3	2:B:517:ARG:HG3	1.92	0.52
1:A:40:GLN:HE22	1:A:823:GLN:HG3	1.73	0.51
1:A:869:ASN:O	1:A:872:THR:OG1	2.28	0.51
1:A:1784:ARG:HB3	1:A:1788:ARG:HH11	1.75	0.51
1:A:3458:SER:OG	1:A:3460:GLU:OE2	2.29	0.51
3:C:271:ARG:HH22	4:D:20:DT:H2'	1.75	0.51
1:A:3170:ASP:OD1	1:A:3170:ASP:N	2.43	0.51
1:A:1481:THR:HG22	1:A:1524:LEU:HD21	1.93	0.51
2:B:409:TYR:OH	3:C:269:GLN:NE2	2.42	0.51
1:A:3430:ASN:ND2	1:A:3432:SER:OG	2.44	0.51
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.39	0.51
1:A:723:ASP:OD2	1:A:723:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:ARG:NH1	1:A:957:PRO:O	2.45	0.50
1:A:1917:LYS:HB2	3:C:729:LEU:HD21	1.92	0.50
2:B:526:LYS:O	2:B:530:TYR:CB	2.57	0.50
1:A:1859:ASN:ND2	1:A:1861:SER:OG	2.43	0.50
1:A:1014:LEU:HD22	1:A:1062:ARG:HD2	1.93	0.50
1:A:1080:LEU:O	1:A:1084:ASN:ND2	2.39	0.50
1:A:4096:SER:OG	1:A:4097:GLY:N	2.38	0.50
2:B:368:VAL:HG22	2:B:432:PHE:HB2	1.93	0.50
1:A:4099:SER:OG	1:A:4100:GLU:N	2.44	0.50
3:C:684:THR:HG21	3:C:701:ALA:HB2	1.93	0.50
1:A:3728:VAL:HG22	1:A:3736:LYS:HG3	1.93	0.50
1:A:663:ILE:HG21	1:A:666:PHE:HD2	1.76	0.50
1:A:1017:ILE:HG12	1:A:1029:CYS:HB2	1.92	0.50
1:A:2824:LYS:HD2	1:A:2828:GLU:HG3	1.94	0.50
1:A:3197:LEU:HD23	1:A:3227:ILE:HG21	1.92	0.50
1:A:1442:GLN:OE1	1:A:1445:ARG:NH2	2.45	0.49
1:A:1877:LEU:HD13	1:A:1915:LEU:HD21	1.94	0.49
1:A:631:ARG:HG2	1:A:672:ILE:HD11	1.92	0.49
1:A:288:ASP:OD1	1:A:288:ASP:N	2.42	0.49
2:B:171:ASN:HB3	2:B:205:LEU:HB2	1.93	0.49
3:C:434:MET:SD	3:C:434:MET:N	2.86	0.49
2:B:304:ASN:HA	3:C:289:ILE:HA	1.95	0.49
3:C:77:ILE:HD13	3:C:113:VAL:HG11	1.95	0.49
1:A:1221:ILE:HD12	1:A:1286:ALA:HB3	1.94	0.49
1:A:3226:ASP:OD1	1:A:3226:ASP:N	2.46	0.49
1:A:3288:SER:O	1:A:3288:SER:OG	2.31	0.49
1:A:4084:SER:O	1:A:4084:SER:OG	2.30	0.49
3:C:13:CYS:HB3	3:C:59:PHE:HE2	1.77	0.49
1:A:3472:ILE:HG21	1:A:3480:LEU:HD13	1.94	0.49
1:A:2837:LEU:HD11	1:A:2871:LEU:HA	1.95	0.49
1:A:3362:LEU:O	1:A:3380:ARG:NH1	2.45	0.49
1:A:1696:LEU:HD21	1:A:1714:LEU:HD11	1.95	0.49
1:A:1474:ASP:OD1	1:A:1475:LEU:N	2.46	0.49
1:A:1676:ILE:HG23	1:A:1713:VAL:HG11	1.95	0.49
1:A:2546:TYR:OH	1:A:2551:GLU:OE2	2.20	0.49
2:B:469:LEU:HD11	2:B:518:LEU:HD11	1.94	0.49
1:A:2301:GLN:O	1:A:2305:ASN:HB2	2.13	0.48
1:A:2865:HIS:HB2	1:A:2868:LEU:HD12	1.93	0.48
1:A:3305:SER:HA	1:A:3358:ARG:HH12	1.79	0.48
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	1.96	0.48
3:C:301:ASP:OD1	3:C:301:ASP:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.79	0.48
1:A:3713:PRO:HA	1:A:3716:HIS:ND1	2.29	0.48
1:A:1753:SER:O	1:A:1753:SER:OG	2.26	0.48
3:C:43:GLN:HA	3:C:46:VAL:HG12	1.94	0.48
3:C:146:GLN:HA	3:C:149:ILE:HD13	1.95	0.48
1:A:1771:GLN:HE21	1:A:1775:GLU:HG3	1.78	0.48
1:A:1265:GLU:OE1	1:A:1340:ARG:NH1	2.40	0.48
1:A:2188:GLU:OE2	1:A:2729:ARG:NE	2.47	0.48
1:A:920:THR:O	1:A:920:THR:OG1	2.29	0.48
1:A:3455:LYS:HG2	1:A:3491:PRO:HD3	1.96	0.48
1:A:4104:VAL:HA	1:A:4107:LEU:HB3	1.95	0.48
2:B:53:SER:HB3	2:B:56:GLU:HB2	1.95	0.48
3:C:12:LEU:HD13	3:C:38:ILE:HD11	1.95	0.48
1:A:3416:LEU:HD21	1:A:3445:LEU:HG	1.96	0.47
1:A:3729:MET:HG3	1:A:3735:PRO:HD2	1.95	0.47
2:B:263:LEU:HB2	2:B:267:ILE:HB	1.96	0.47
1:A:373:CYS:HA	1:A:376:ILE:HG22	1.96	0.47
3:C:12:LEU:HD23	3:C:133:GLU:HB2	1.96	0.47
1:A:933:LEU:HG	1:A:937:MET:HE2	1.96	0.47
1:A:2742:MET:SD	1:A:2745:ARG:NH1	2.88	0.47
2:B:338:LYS:NZ	4:D:20:DT:OP1	2.47	0.47
1:A:714:VAL:HA	1:A:717:LYS:HG2	1.97	0.47
1:A:1076:LEU:HB2	1:A:1123:THR:HG22	1.97	0.47
1:A:1927:MET:SD	1:A:1927:MET:N	2.86	0.47
1:A:2849:SER:O	1:A:2849:SER:OG	2.33	0.47
3:C:97:LYS:HA	3:C:97:LYS:HD3	1.76	0.47
4:D:3:DA:H1'	4:D:4:DT:H5'	1.97	0.47
1:A:249:PHE:HZ	1:A:293:LEU:HD11	1.79	0.47
1:A:354:SER:HB2	1:A:359:LEU:HB2	1.97	0.47
1:A:1963:GLN:NE2	1:A:1968:SER:OG	2.47	0.47
1:A:3883:LEU:HB3	1:A:3970:LEU:HD13	1.95	0.47
1:A:4056:PRO:HG2	1:A:4107:LEU:HB2	1.96	0.47
1:A:754:MET:HE1	1:A:1022:ASP:HA	1.97	0.47
2:B:258:ARG:NH1	5:G:28:DC:OP2	2.45	0.47
1:A:2001:LYS:HB3	1:A:2082:GLU:HB3	1.97	0.47
1:A:2822:LYS:HE2	1:A:2822:LYS:HB3	1.68	0.47
1:A:36:ARG:NH2	1:A:823:GLN:O	2.48	0.47
1:A:3923:ARG:NH1	1:A:3941:ASP:O	2.47	0.47
1:A:2288:TYR:OH	1:A:2295:GLN:N	2.48	0.47
1:A:1639:LEU:HD22	1:A:1684:LEU:HD12	1.96	0.46
2:B:362:LEU:HD12	3:C:269:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:610:GLU:O	3:C:614:ASN:CB	2.60	0.46
1:A:1374:GLN:NE2	1:A:1381:SER:OG	2.47	0.46
3:C:208:VAL:HA	3:C:211:VAL:HG12	1.96	0.46
3:C:363:LYS:HG2	3:C:420:VAL:HG22	1.97	0.46
1:A:1817:GLN:O	1:A:1821:ASP:HB2	2.15	0.46
1:A:2533:SER:HA	1:A:2565:MET:HE3	1.97	0.46
1:A:827:ASN:N	1:A:827:ASN:OD1	2.45	0.46
2:B:445:LYS:NZ	7:B:701:IHP:O41	2.48	0.46
1:A:2330:VAL:HG13	1:A:2335:ASN:HB2	1.97	0.46
1:A:1241:LEU:O	1:A:1243:TYR:N	2.48	0.46
1:A:1840:PHE:HE2	1:A:1895:LYS:HB3	1.80	0.46
2:B:258:ARG:HH21	2:B:371:GLU:HG3	1.80	0.46
1:A:907:LEU:HD11	1:A:2790:LEU:HD21	1.97	0.46
1:A:1436:LEU:HD12	1:A:1445:ARG:HG3	1.97	0.46
1:A:1730:PRO:HG2	1:A:1733:THR:HG21	1.98	0.46
1:A:664:SER:HB2	1:A:725:LEU:HD22	1.98	0.46
1:A:2211:LEU:HD23	1:A:2214:ARG:HH21	1.80	0.46
3:C:600:VAL:HA	3:C:603:LYS:HG2	1.98	0.46
1:A:1572:LEU:HD13	1:A:1575:LEU:HD21	1.97	0.46
2:B:46:LYS:HD3	2:B:137:HIS:CE1	2.51	0.46
2:B:423:GLN:HG2	2:B:425:ILE:HG22	1.98	0.46
1:A:395:MET:HE3	1:A:395:MET:HB2	1.88	0.46
1:A:2368:THR:HG21	1:A:2375:ALA:HB2	1.98	0.46
1:A:3873:LYS:HB2	1:A:3873:LYS:HE3	1.74	0.46
3:C:467:ASP:N	3:C:467:ASP:OD1	2.49	0.46
1:A:892:LEU:HD21	1:A:941:MET:HG3	1.97	0.45
1:A:1170:LYS:HB3	1:A:1170:LYS:HE3	1.81	0.45
1:A:2408:MET:HE2	1:A:2408:MET:HB3	1.81	0.45
2:B:403:ARG:HH22	4:F:24:DG:H21	1.62	0.45
1:A:2205:VAL:HG23	1:A:2208:ASP:H	1.80	0.45
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.99	0.45
1:A:1719:VAL:HG21	3:C:630:PRO:HB2	1.99	0.45
3:C:151:ILE:HD11	3:C:211:VAL:HG22	1.97	0.45
1:A:3300:VAL:HG22	1:A:3333:THR:HG23	1.99	0.45
2:B:245:LYS:HB2	2:B:247:ARG:HH21	1.81	0.45
1:A:1582:LEU:HG	1:A:1593:VAL:HG23	1.98	0.45
2:B:403:ARG:HB2	2:B:406:ILE:HG13	1.98	0.45
1:A:165:LYS:HD2	1:A:165:LYS:HA	1.76	0.45
1:A:950:GLU:O	1:A:955:ALA:N	2.49	0.45
1:A:3544:ASP:OD1	1:A:3549:HIS:NE2	2.37	0.45
2:B:95:ASN:HD22	2:B:149:VAL:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASN:ND2	2:B:140:ASP:O	2.34	0.45
2:B:333:GLU:OE1	3:C:497:ARG:NH1	2.49	0.45
1:A:3596:LEU:HD23	1:A:3601:VAL:HG21	1.99	0.45
1:A:1843:ILE:HD11	1:A:1880:MET:HE1	1.99	0.45
1:A:3760:GLN:NE2	1:A:3943:GLY:O	2.50	0.45
1:A:1163:LEU:HD12	1:A:1163:LEU:HA	1.82	0.45
1:A:1306:ILE:HG13	1:A:1307:ILE:H	1.82	0.45
1:A:4090:ARG:NH1	1:A:4109:ASP:OD2	2.49	0.45
3:C:334:LYS:HA	3:C:334:LYS:HD3	1.66	0.45
3:C:427:MET:HE3	3:C:427:MET:HB3	1.93	0.45
3:C:467:ASP:OD1	3:C:472:THR:OG1	2.34	0.45
1:A:1960:LYS:HD3	1:A:1960:LYS:HA	1.83	0.45
1:A:3167:ARG:O	1:A:3186:ARG:NH2	2.41	0.45
1:A:1241:LEU:HD22	1:A:1244:LEU:HD11	1.98	0.44
1:A:1927:MET:HB2	1:A:1930:GLU:HB2	1.99	0.44
1:A:2507:ILE:HG21	1:A:2547:SER:HB3	1.99	0.44
1:A:949:PRO:HB2	1:A:954:GLY:HA3	1.97	0.44
1:A:1524:LEU:HD23	1:A:1524:LEU:HA	1.82	0.44
1:A:1876:ILE:HG22	1:A:1880:MET:HE2	1.99	0.44
1:A:2387:PRO:HD3	1:A:2418:LYS:HG3	2.00	0.44
1:A:2657:ASP:OD2	1:A:2660:THR:OG1	2.35	0.44
1:A:2849:SER:O	1:A:2851:PHE:N	2.49	0.44
3:C:676:GLU:O	3:C:680:GLN:HB2	2.17	0.44
1:A:738:HIS:O	1:A:742:GLU:N	2.50	0.44
1:A:1218:SER:HB2	1:A:1286:ALA:HB1	2.00	0.44
1:A:3613:MET:HE3	1:A:3613:MET:HB3	1.78	0.44
3:C:20:MET:HG3	3:C:31:PHE:HB2	2.00	0.44
3:C:355:PHE:O	3:C:425:PRO:HD3	2.18	0.44
1:A:1225:GLU:OE2	1:A:1290:LEU:N	2.51	0.44
3:C:323:PHE:HE2	3:C:328:GLU:HA	1.82	0.44
3:C:633:MET:HA	3:C:636:ILE:HG22	1.99	0.44
1:A:1136:ARG:HA	1:A:1139:GLU:HG2	2.00	0.44
1:A:2086:ASP:O	1:A:2090:ARG:NH1	2.50	0.44
1:A:2655:SER:O	1:A:2655:SER:OG	2.31	0.44
1:A:3958:LEU:HD22	1:A:4081:ALA:HB2	2.00	0.44
2:B:418:GLU:OE2	3:C:437:SER:OG	2.36	0.44
1:A:372:PRO:HA	1:A:375:VAL:HG12	2.00	0.43
1:A:958:MET:HB3	1:A:958:MET:HE2	1.75	0.43
2:B:445:LYS:HD2	2:B:445:LYS:HA	1.89	0.43
1:A:374:LYS:HD2	1:A:423:TYR:HB3	2.00	0.43
1:A:1472:SER:OG	1:A:1476:HIS:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2950:LYS:HE3	1:A:2986:PRO:HG3	2.00	0.43
1:A:2242:VAL:O	1:A:2246:LYS:CB	2.61	0.43
1:A:1037:LEU:HD23	1:A:1037:LEU:HA	1.87	0.43
1:A:670:LEU:HA	1:A:673:THR:HG22	2.00	0.43
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	2.01	0.43
1:A:4032:ASN:HB3	1:A:4035:GLU:HB2	2.01	0.43
3:C:165:LEU:HD11	3:C:224:ILE:HD11	2.01	0.43
1:A:542:ASP:HA	1:A:545:LEU:HB2	1.99	0.43
1:A:1762:MET:HA	1:A:1765:VAL:HG22	2.01	0.43
3:C:202:LYS:HB3	3:C:202:LYS:HE2	1.86	0.43
3:C:262:ALA:O	3:C:365:PHE:N	2.52	0.43
1:A:2347:LYS:HB2	1:A:2347:LYS:HE3	1.80	0.43
1:A:9:ARG:HB2	1:A:57:LEU:HD13	2.00	0.43
1:A:2936:TYR:HA	1:A:2939:LEU:HB2	2.00	0.43
1:A:3022:GLU:HG3	1:A:3024:PRO:HG2	2.01	0.43
1:A:851:ILE:HD13	1:A:851:ILE:HA	1.90	0.43
2:B:42:VAL:HA	2:B:169:PHE:HB2	2.01	0.43
1:A:1917:LYS:HG3	3:C:729:LEU:HD11	2.01	0.42
1:A:2420:PHE:HA	1:A:2423:VAL:HG12	2.00	0.42
1:A:3858:MET:HE1	1:A:4119:ARG:HB3	2.01	0.42
1:A:2589:TYR:HB2	1:A:2777:HIS:HD2	1.85	0.42
1:A:983:LEU:HD11	1:A:2775:TYR:CE1	2.54	0.42
2:B:375:VAL:HG13	2:B:378:SER:HB2	2.01	0.42
3:C:107:PHE:HE2	3:C:139:SER:H	1.66	0.42
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	2.01	0.42
1:A:1963:GLN:O	1:A:1968:SER:OG	2.37	0.42
3:C:184:ARG:HH11	3:C:514:ASN:HA	1.83	0.42
3:C:545:LYS:NZ	4:D:10:DA:OP2	2.51	0.42
1:A:414:LEU:HG	1:A:464:VAL:HG21	2.00	0.42
1:A:1202:ARG:HH21	1:A:1207:TRP:CD1	2.38	0.42
1:A:2536:LEU:HD23	1:A:2824:LYS:HE3	2.01	0.42
1:A:1213:LYS:HD3	1:A:1213:LYS:HA	1.80	0.42
1:A:2576:MET:HE3	1:A:2576:MET:HB2	1.86	0.42
1:A:3680:LEU:HD12	1:A:3683:CYS:HB3	2.01	0.42
2:B:46:LYS:HD3	2:B:137:HIS:HE1	1.84	0.42
2:B:90:THR:HB	2:B:135:MET:HG3	2.02	0.42
2:B:516:LYS:HA	2:B:516:LYS:HD3	1.88	0.42
3:C:7:LYS:HE3	3:C:7:LYS:HB2	1.79	0.42
3:C:37:VAL:HG22	3:C:231:LEU:HD13	2.00	0.42
3:C:291:LYS:HE2	3:C:291:LYS:HB2	1.87	0.42
5:E:31:DT:H2"	5:E:32:DA:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:15:DT:H1'	4:F:16:DT:H5'	2.01	0.42
1:A:396:PHE:HE2	1:A:438:LEU:HD11	1.85	0.42
1:A:722:LYS:HB3	1:A:722:LYS:HE2	1.87	0.42
1:A:1225:GLU:OE1	1:A:1289:SER:OG	2.37	0.42
1:A:1711:ARG:HH22	1:A:1761:LEU:HD13	1.85	0.42
1:A:3183:ILE:HD12	1:A:3238:MET:HB3	2.02	0.42
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.54	0.42
1:A:3575:LEU:HD22	1:A:3752:VAL:HG21	2.02	0.42
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.44	0.42
2:B:190:ALA:HB2	2:B:220:ILE:HG13	2.00	0.42
2:B:277:VAL:HB	3:C:357:MET:HE1	2.01	0.42
3:C:668:ILE:HD12	3:C:668:ILE:HA	1.93	0.42
1:A:2562:LEU:HD23	1:A:2562:LEU:HA	1.91	0.42
2:B:288:LEU:HD21	3:C:320:ILE:HG21	2.01	0.42
1:A:335:LYS:HG3	1:A:376:ILE:HD11	2.02	0.42
1:A:868:LYS:H	1:A:868:LYS:HG2	1.61	0.42
1:A:886:TRP:O	1:A:964[B]:ARG:NH1	2.51	0.42
1:A:724:GLU:HG2	1:A:2604:PRO:HA	2.02	0.42
1:A:1386:ILE:HG22	1:A:1392:MET:HE2	2.02	0.42
1:A:1840:PHE:O	1:A:1844:VAL:HG23	2.20	0.42
1:A:3704:GLN:HB3	1:A:3716:HIS:HD2	1.85	0.42
3:C:311:ILE:HD11	3:C:324:SER:HB3	2.01	0.42
1:A:2329:TYR:CZ	1:A:2333:ARG:HD2	2.55	0.41
1:A:2486:ASP:OD1	1:A:2491:THR:OG1	2.37	0.41
1:A:3140:GLU:OE1	1:A:3167:ARG:NH2	2.49	0.41
2:B:41:LEU:HD12	2:B:41:LEU:HA	1.85	0.41
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	2.01	0.41
1:A:2307:MET:HB2	1:A:2348:GLN:HG2	2.02	0.41
1:A:3330:LEU:HD12	1:A:3330:LEU:HA	1.88	0.41
1:A:3580:ASN:OD1	1:A:3736:LYS:NZ	2.53	0.41
3:C:11:VAL:HG23	3:C:132:ILE:HG23	2.02	0.41
1:A:1050:GLU:HA	1:A:1055:ASN:HD22	1.85	0.41
1:A:2983:ASP:OD1	1:A:2983:ASP:N	2.52	0.41
1:A:3639:GLU:HA	1:A:3642:LYS:HZ2	1.84	0.41
1:A:3959:MET:HE3	1:A:3959:MET:HB3	1.91	0.41
2:B:46:LYS:HA	2:B:137:HIS:CE1	2.55	0.41
1:A:793:LEU:HD12	1:A:869:ASN:HB2	2.03	0.41
1:A:1158:PRO:HA	1:A:1159:PRO:HD3	1.94	0.41
1:A:1560:TYR:O	1:A:1564:SER:OG	2.26	0.41
1:A:1761:LEU:HD12	1:A:1761:LEU:HA	1.84	0.41
1:A:1819:PHE:O	1:A:1823:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2599:SER:OG	1:A:2601:VAL:HG12	2.21	0.41
1:A:3918:LEU:O	1:A:3920:ILE:HG13	2.21	0.41
2:B:529:VAL:HG22	3:C:375:VAL:HG13	2.03	0.41
1:A:3083:SER:HA	1:A:3086:LEU:HB2	2.02	0.41
1:A:3499:ILE:HD12	1:A:3499:ILE:HA	1.89	0.41
3:C:620:ILE:HD13	3:C:639:ILE:HG12	2.02	0.41
1:A:1903:SER:OG	1:A:1904:CYS:N	2.52	0.41
1:A:3147:LYS:HE3	1:A:3147:LYS:HB2	1.85	0.41
2:B:128:GLN:O	2:B:132:GLN:HG2	2.20	0.41
2:B:131:PHE:CZ	2:B:135:MET:HG2	2.56	0.41
5:G:31:DT:H2"	5:G:32:DA:C8	2.55	0.41
1:A:321:LYS:HB2	1:A:321:LYS:HE3	1.85	0.41
1:A:974:CYS:HB2	1:A:1024:THR:HG22	2.03	0.41
1:A:1013:ILE:HD13	1:A:1032:CYS:HB3	2.02	0.41
1:A:1055:ASN:OD1	1:A:1055:ASN:N	2.54	0.41
1:A:1725:GLN:HA	1:A:1768:ARG:HH21	1.85	0.41
2:B:201:ASP:N	2:B:201:ASP:OD1	2.54	0.41
3:C:210:MET:HA	3:C:213:ILE:HG22	2.03	0.41
1:A:149:ILE:HG23	1:A:181:LEU:HD22	2.03	0.41
1:A:1041:ILE:HA	1:A:1049:GLN:HE22	1.86	0.41
1:A:1307:ILE:HD13	1:A:1307:ILE:HA	1.96	0.41
1:A:2594:ASP:OD1	1:A:2594:ASP:N	2.53	0.41
1:A:3532:PRO:HA	1:A:3535:ILE:HG22	2.03	0.41
1:A:3543:LYS:HB3	1:A:3543:LYS:HE2	1.91	0.41
3:C:370:ASP:HB3	3:C:373:ALA:HB3	2.03	0.41
4:F:14:DC:H4'	4:F:15:DT:H5'	2.03	0.41
1:A:395:MET:O	1:A:406:ARG:NH2	2.47	0.41
1:A:1712:ARG:HH22	1:A:1716:GLN:HB2	1.86	0.41
1:A:1985:LYS:HD3	1:A:1985:LYS:HA	1.87	0.41
1:A:2102:LYS:HB2	1:A:2102:LYS:HE2	1.96	0.41
1:A:2446:LEU:HD22	1:A:2450:GLU:HG3	2.03	0.41
5:G:36:DC:H2"	5:G:37:DA:C8	2.56	0.41
1:A:1723:PRO:HG3	1:A:1729:PHE:CD2	2.56	0.40
1:A:2171:LEU:HD12	1:A:2171:LEU:HA	1.95	0.40
1:A:3027:LEU:HD11	1:A:3048:LYS:HE3	2.02	0.40
3:C:654:ARG:HH12	3:C:658:PHE:HB2	1.85	0.40
1:A:1572:LEU:O	1:A:1614:GLN:NE2	2.54	0.40
1:A:3241:LYS:HE2	1:A:3241:LYS:HB2	1.88	0.40
3:C:147:LEU:HD12	3:C:147:LEU:HA	1.95	0.40
3:C:469:LYS:HA	3:C:469:LYS:HD3	1.81	0.40
1:A:397:LEU:HD13	1:A:438:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2123:PRO:O	1:A:2127:LYS:N	2.52	0.40
1:A:3924:HIS:HB3	1:A:4124:TRP:HA	2.02	0.40
1:A:4043:LYS:HA	1:A:4043:LYS:HD3	1.93	0.40
1:A:91:ILE:HD12	1:A:826:PHE:HB3	2.03	0.40
1:A:1583:MET:HE2	1:A:1583:MET:HB3	1.97	0.40
1:A:1704:GLY:HA2	1:A:1707:LEU:HB3	2.02	0.40
1:A:3627:ALA:HB3	1:A:3682:GLU:HB2	2.04	0.40
2:B:348:MET:HE3	2:B:348:MET:HB2	1.73	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	3777/4128 (92%)	3424 (91%)	341 (9%)	12 (0%)	37	66
2	B	493/609 (81%)	440 (89%)	53 (11%)	0	100	100
3	C	659/732 (90%)	588 (89%)	71 (11%)	0	100	100
All	All	4929/5469 (90%)	4452 (90%)	465 (9%)	12 (0%)	45	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1242	LEU
1	A	167	PRO
1	A	2296	SER
1	A	1553	PHE
1	A	3083	SER
1	A	949	PRO
1	A	2548	PRO
1	A	2871	LEU
1	A	3941	ASP

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Mol	Chain	Res	Type
1	A	2547	SER
1	A	1306	ILE
1	A	3692	VAL

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	3367/3671 (92%)	3362 (100%)	5 (0%)	92 96
2	B	452/548 (82%)	449 (99%)	3 (1%)	81 88
3	C	598/649 (92%)	593 (99%)	5 (1%)	79 87
All	All	4417/4868 (91%)	4404 (100%)	13 (0%)	91 94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257[A]	ARG
1	A	257[B]	ARG
1	A	282	PHE
1	A	3487	ILE
1	A	3540	TYR
2	B	363[A]	ARG
2	B	363[B]	ARG
2	B	368	VAL
3	C	57	VAL
3	C	407	VAL
3	C	470	THR
3	C	578	VAL
3	C	727	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	278	HIS
1	A	289	ASN
1	A	305	ASN
1	A	562	HIS
1	A	720	GLN
1	A	1048	GLN
1	A	1175	HIS
1	A	1201	ASN
1	A	1374	GLN
1	A	1466	ASN
1	A	1584	GLN
1	A	1613	HIS
1	A	1737	ASN
1	A	1771	GLN
1	A	1859	ASN
1	A	1946	ASN
1	A	1963	GLN
1	A	1974	ASN
1	A	2183	HIS
1	A	2306	ASN
1	A	2353	GLN
1	A	2426	HIS
1	A	2472	GLN
1	A	2475	ASN
1	A	2483	ASN
1	A	2514	ASN
1	A	2777	HIS
1	A	2807	GLN
1	A	3105	ASN
1	A	3108	GLN
1	A	3113	ASN
1	A	3148	GLN
1	A	3327	ASN
1	A	3379	GLN
1	A	3384	HIS
1	A	3430	ASN
1	A	3457	ASN
1	A	3697	ASN
1	A	3748	HIS
1	A	3808	ASN
1	A	4015	ASN

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Mol	Chain	Res	Type
1	A	4037	ASN
2	B	68	GLN
2	B	95	ASN
2	B	137	HIS
2	B	152	ASN
2	B	178	ASN
2	B	515	ASN
3	C	43	GLN
3	C	45	GLN
3	C	104	GLN
3	C	146	GLN
3	C	547	GLN
3	C	551	GLN
3	C	663	GLN
3	C	680	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
7	IHP	B	701	-	36,36,36	1.55	6 (16%)	60,60,60	1.11	4 (6%)
6	ATP	A	4201	-	28,33,33	0.99	0	34,52,52	1.21	3 (8%)

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
7	IHP	B	701	-	-	7/30/54/54	0/1/1/1
6	ATP	A	4201	-	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	701	IHP	P2-O12	3.44	1.65	1.59
7	B	701	IHP	P4-O14	3.38	1.65	1.59
7	B	701	IHP	P5-O15	3.12	1.65	1.59
7	B	701	IHP	P3-O13	3.10	1.65	1.59
7	B	701	IHP	P6-O16	3.09	1.64	1.59
7	B	701	IHP	P1-O11	3.03	1.64	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4201	ATP	N3-C2-N1	-3.66	123.70	128.67
7	B	701	IHP	C4-C3-C2	2.89	116.76	110.43
7	B	701	IHP	C6-C5-C4	2.75	116.47	110.43
6	A	4201	ATP	C4-C5-N7	-2.55	106.64	109.34
7	B	701	IHP	C3-C2-C1	2.26	115.37	110.43
7	B	701	IHP	P3-O13-C3	-2.25	117.42	123.43
6	A	4201	ATP	C4'-O4'-C1'	2.06	111.82	109.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4201	ATP	O4'-C4'-C5'-O5'
6	A	4201	ATP	PB-O3A-PA-O2A
6	A	4201	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
7	B	701	IHP	C4-O14-P4-O34
7	B	701	IHP	C6-C5-O15-P5
7	B	701	IHP	C1-C6-O16-P6
7	B	701	IHP	C5-O15-P5-O25
7	B	701	IHP	C6-O16-P6-O26
6	A	4201	ATP	PB-O3A-PA-O1A
7	B	701	IHP	C4-O14-P4-O44
7	B	701	IHP	C6-O16-P6-O46

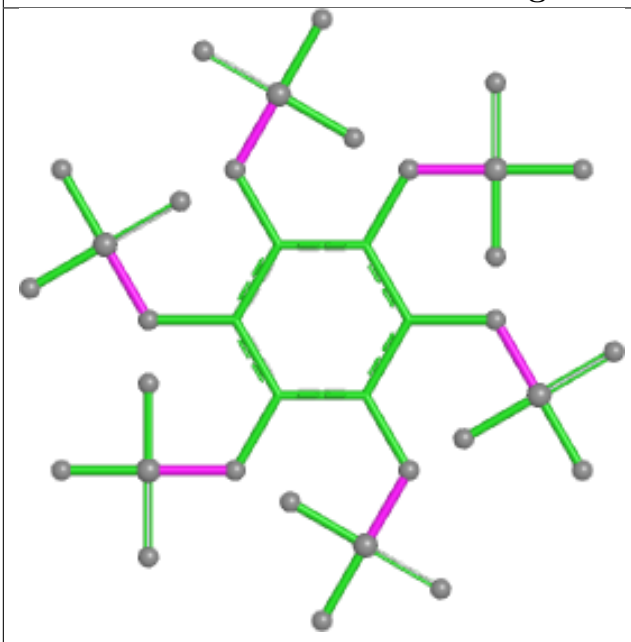
There are no ring outliers.

2 monomers are involved in 2 short contacts:

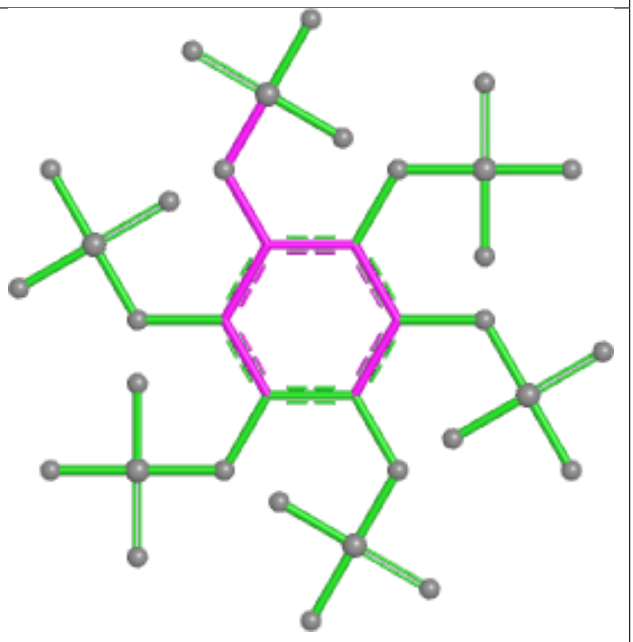
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	701	IHP	1	0
6	A	4201	ATP	1	0

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 then 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.

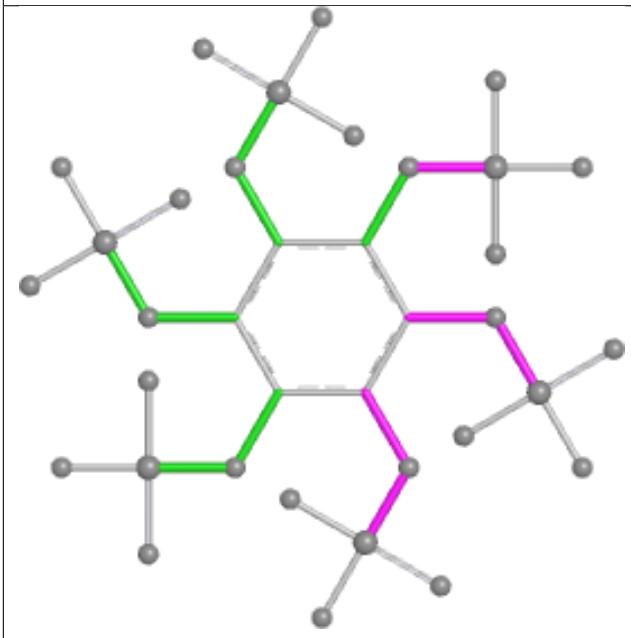
Ligand IHP B 701



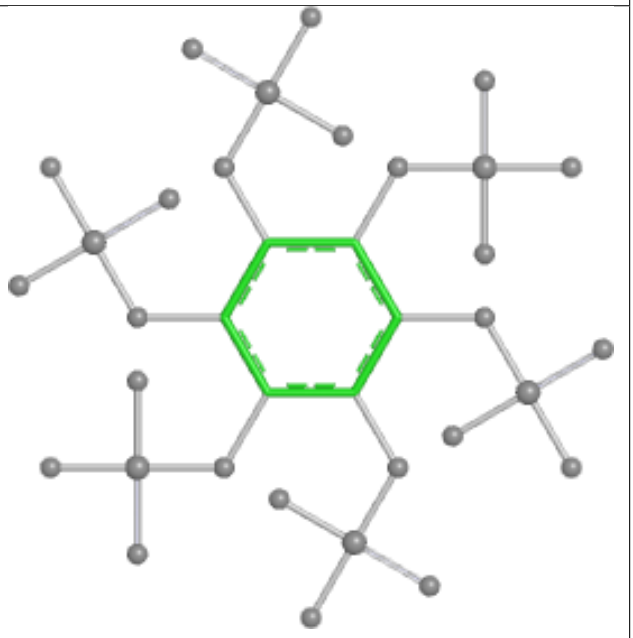
Bond lengths



Bond angles

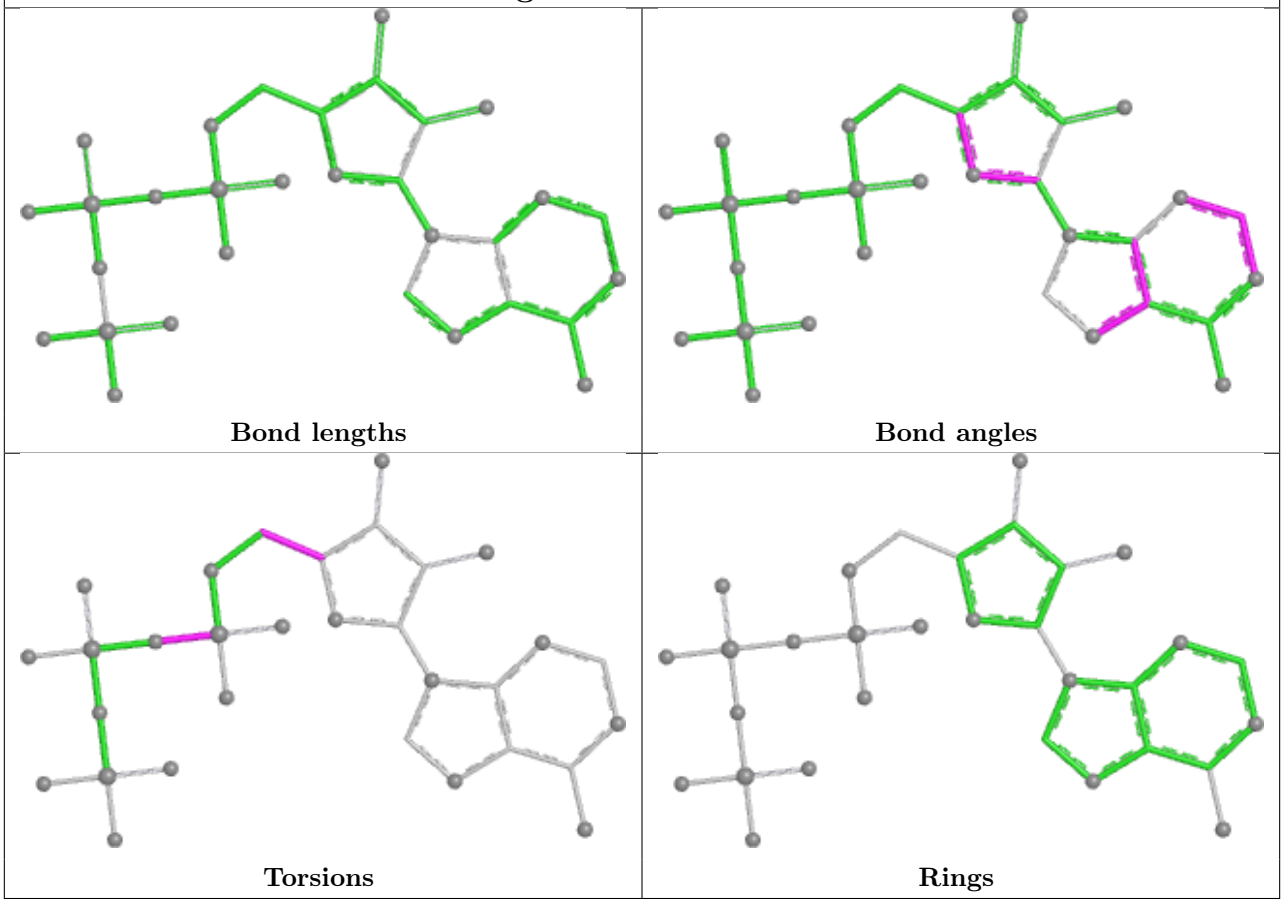


Torsions



Rings

Ligand ATP A 4201



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.

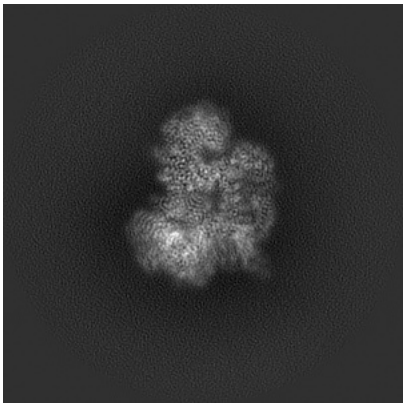
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25439. These allow visual inspection of the internal detail of the map and identification of artifacts.

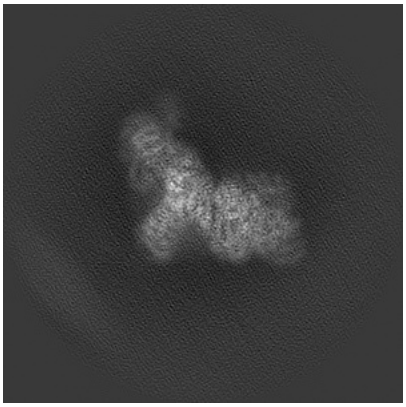
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

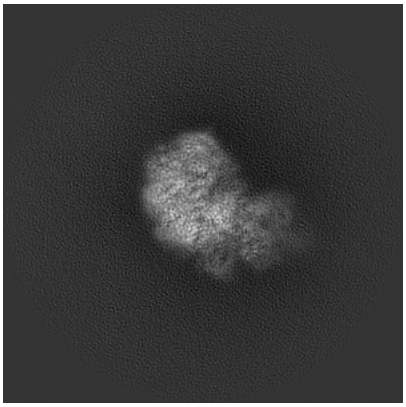
6.1.1 Primary map



X



Y

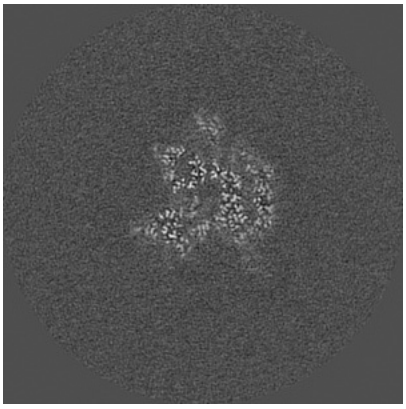


Z

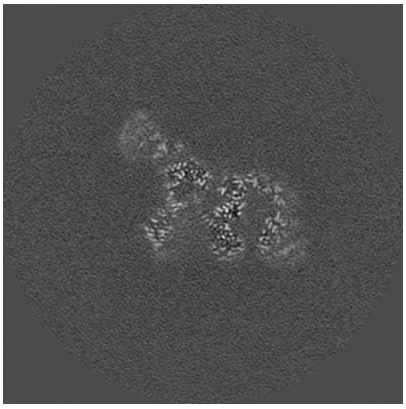
The images above show the map projected in three orthogonal directions.

6.2 Central slices

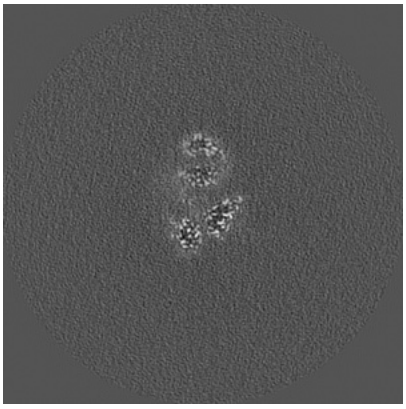
6.2.1 Primary map



X Index: 240



Y Index: 240

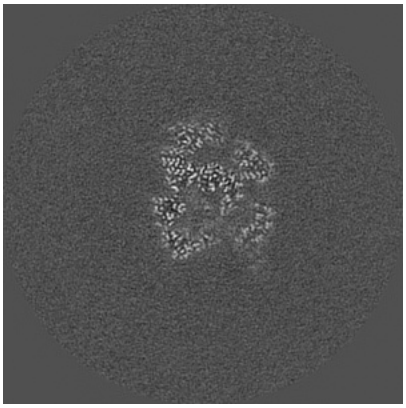


Z Index: 240

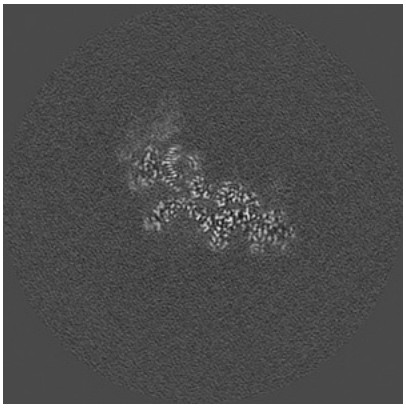
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

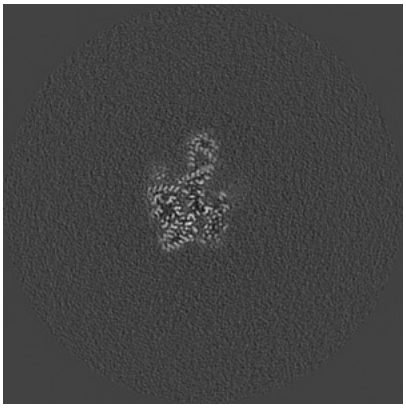
6.3.1 Primary map



X Index: 227



Y Index: 210

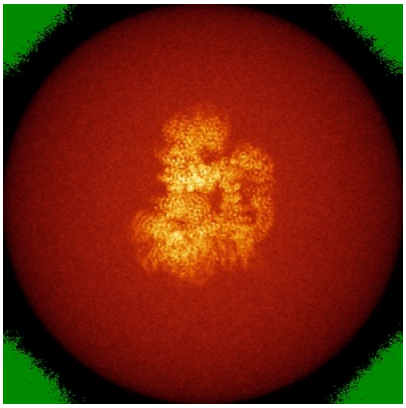


Z Index: 271

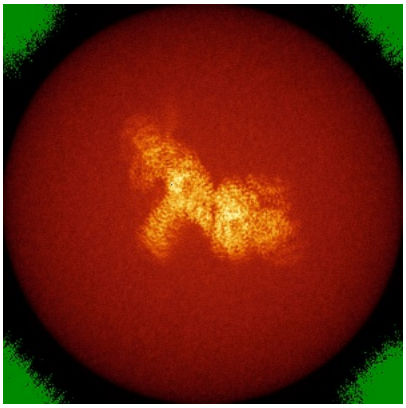
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

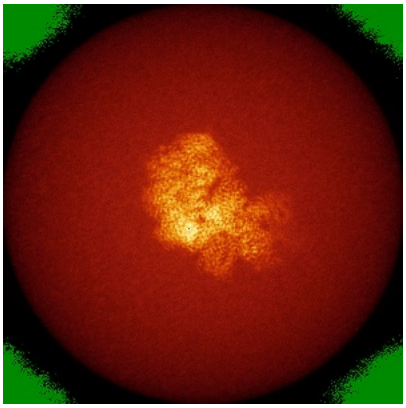
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

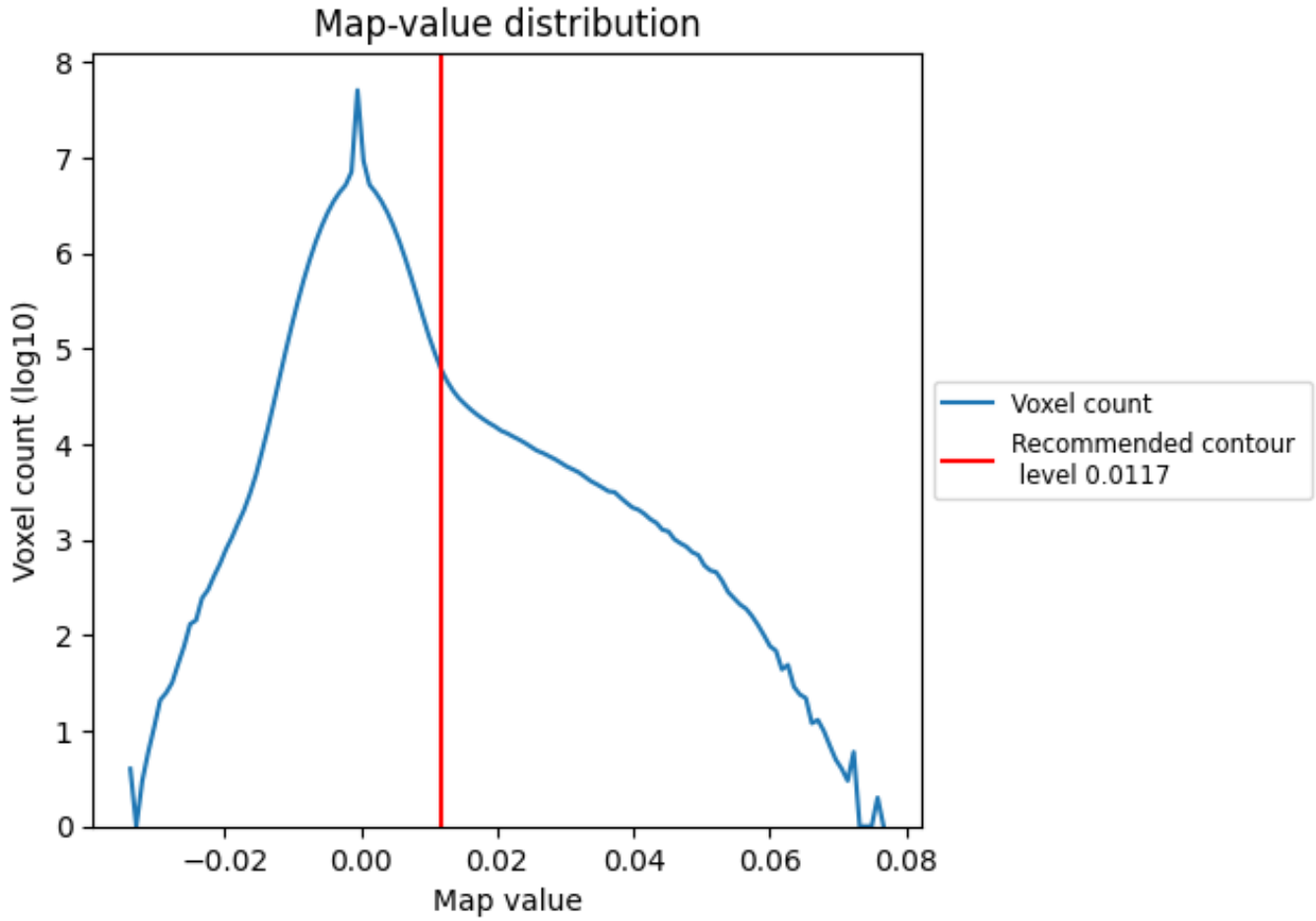
6.6 Mask visualisation (i)

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

7 Map analysis

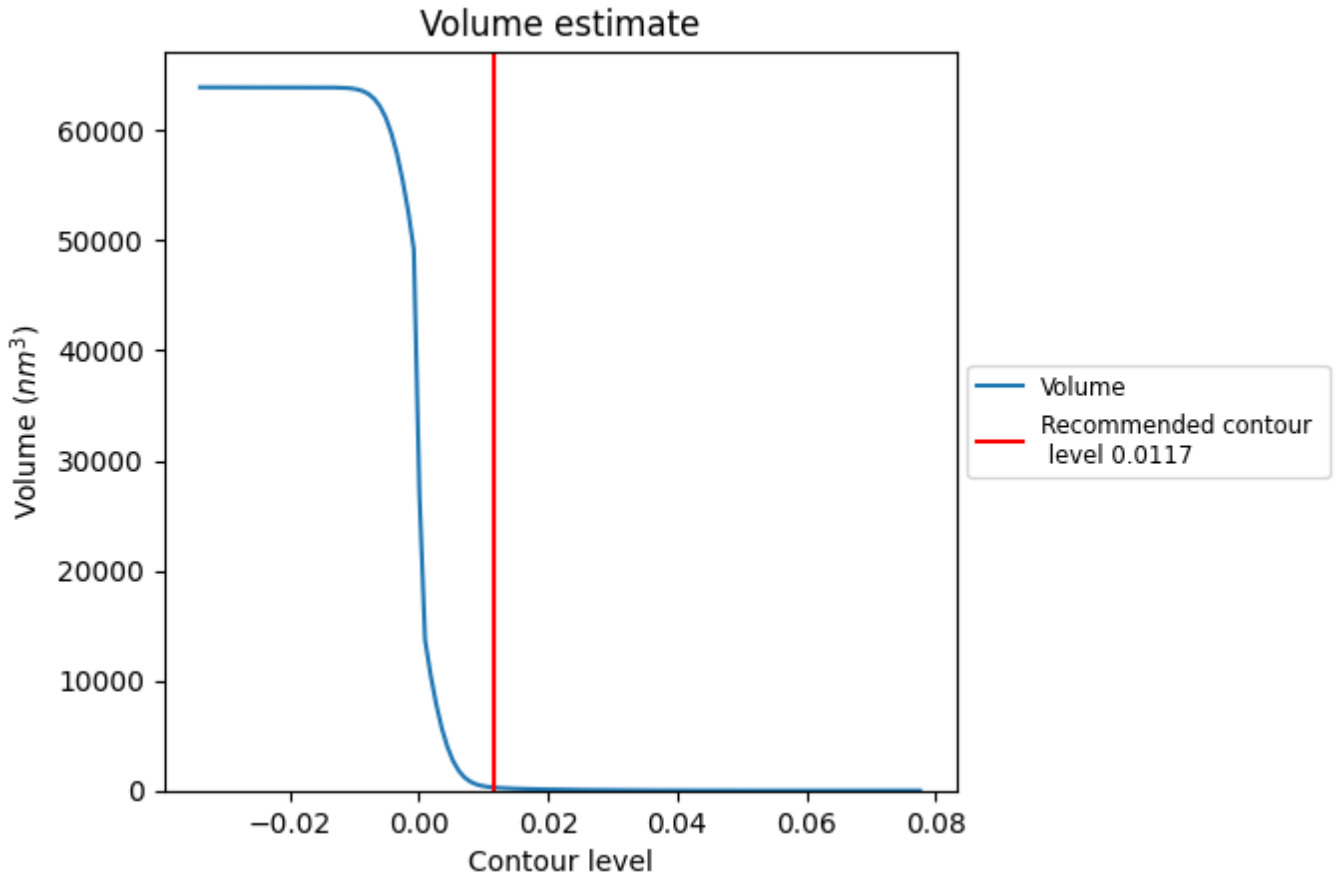
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

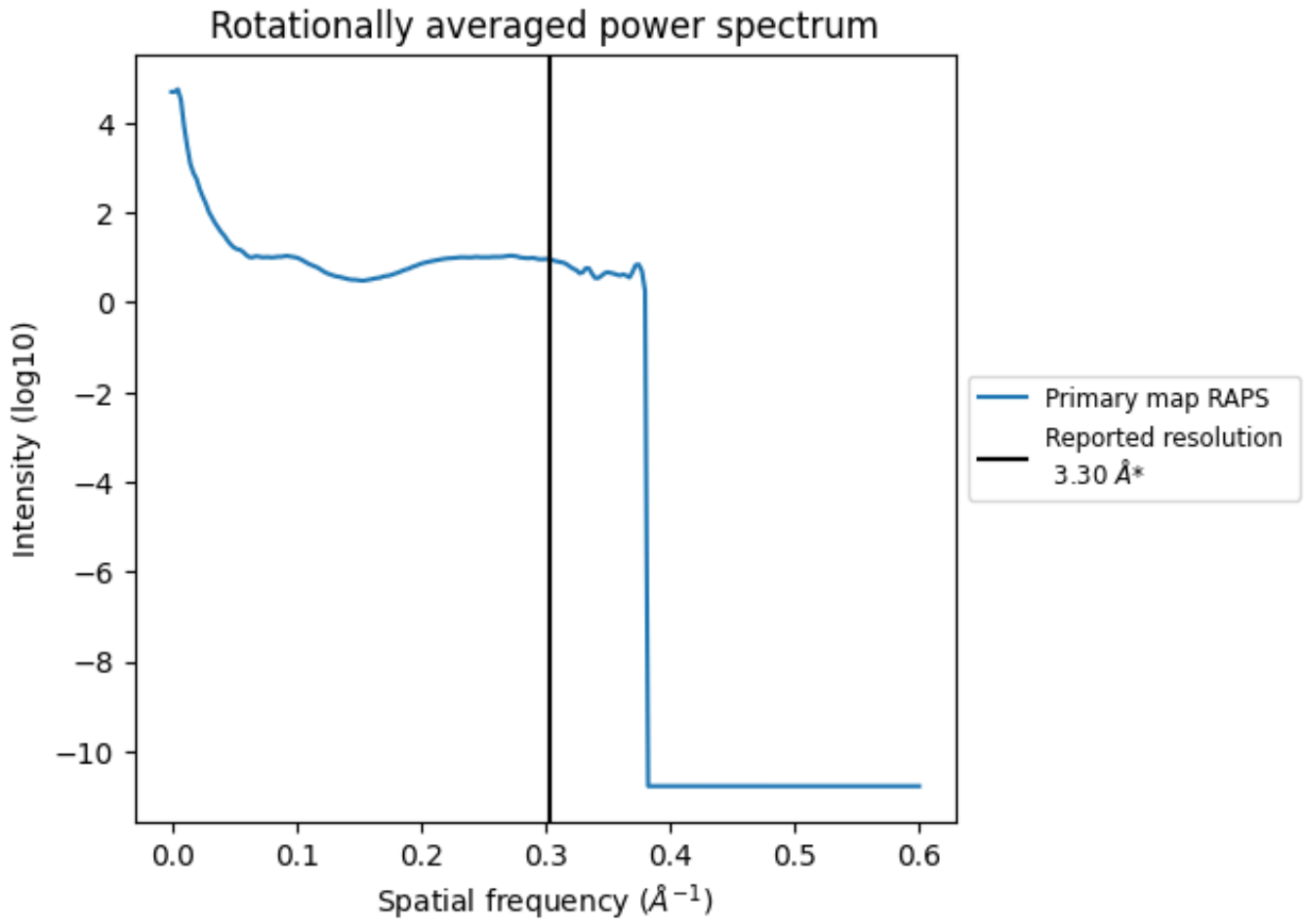
7.2 Volume estimate



The volume at the recommended contour level is 274 nm^3; this corresponds to an approximate mass of 247 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)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

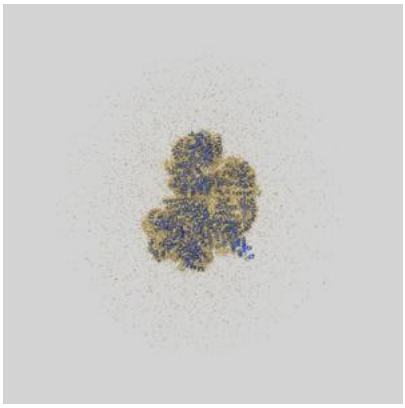
8 Fourier-Shell correlation (i)

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

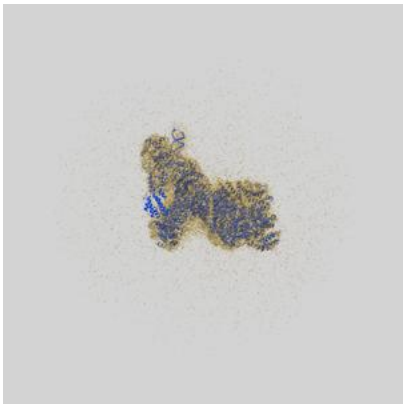
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25439 and PDB model 7SU3. Per-residue inclusion information can be found in section 3 on page 5.

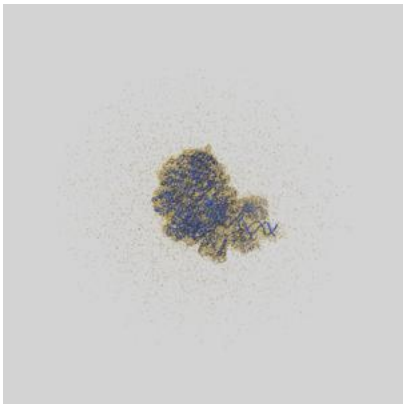
9.1 Map-model overlay



X



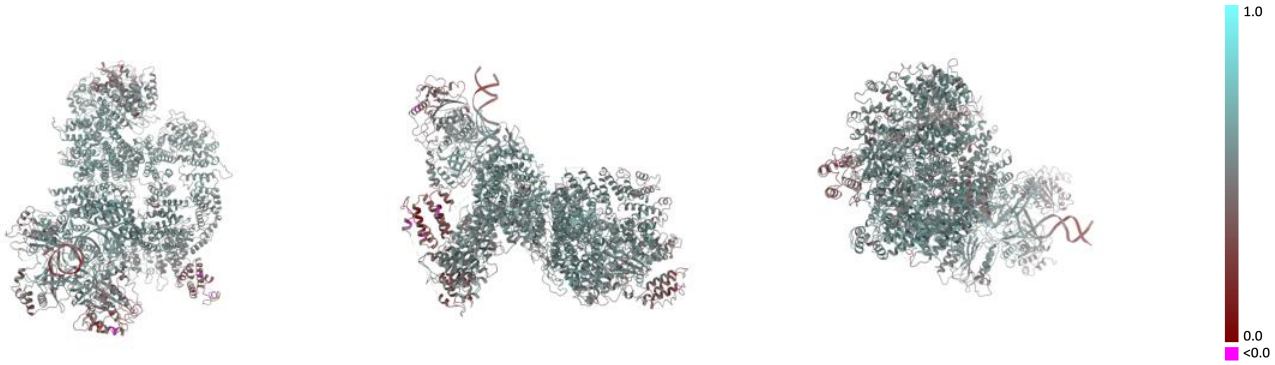
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117 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.

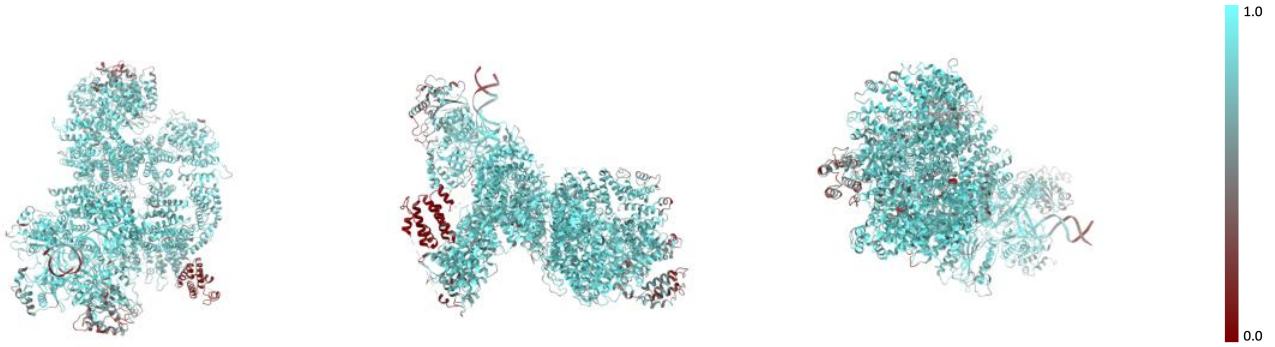
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

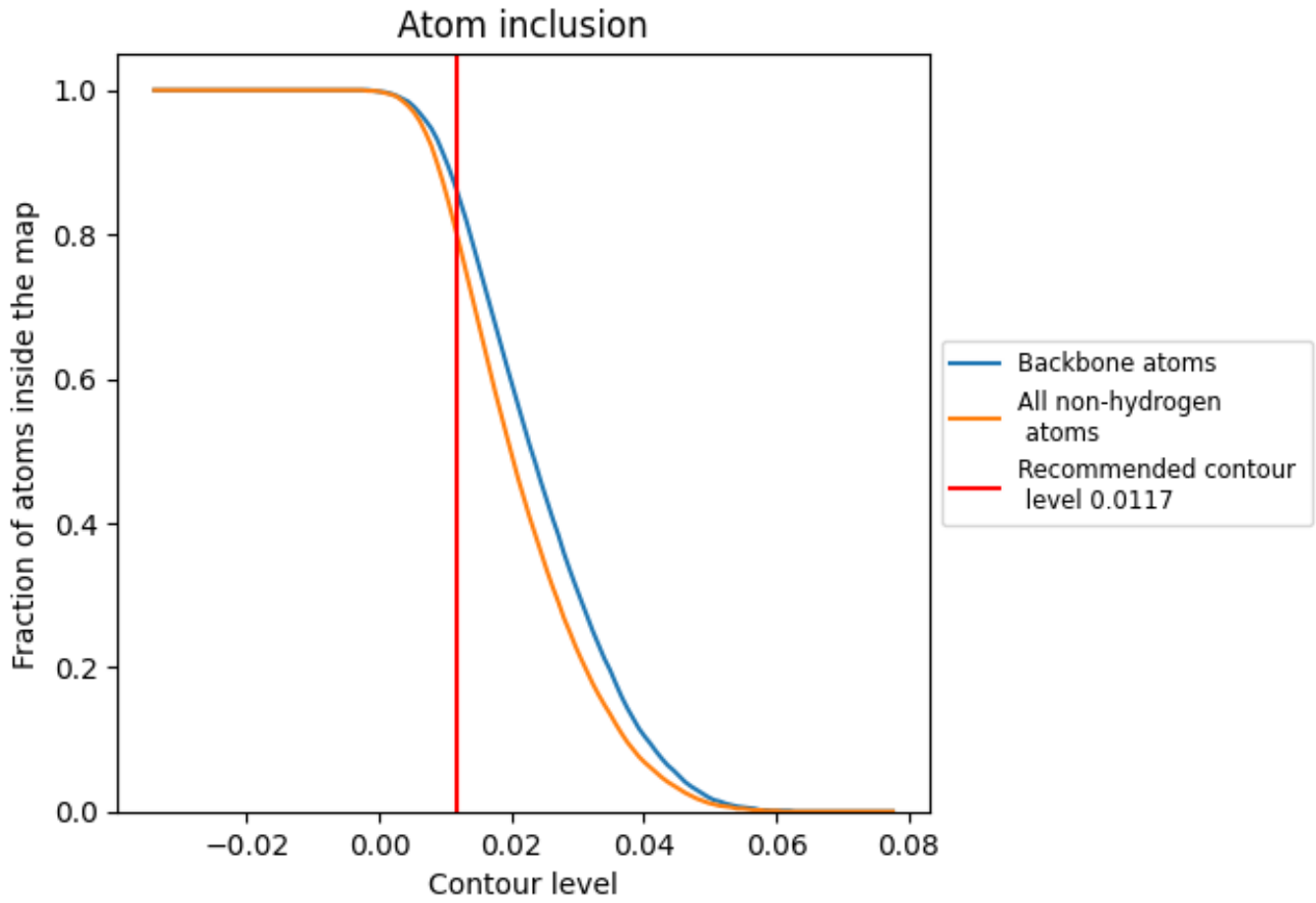
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0117).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0117) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.5280
A	0.8380	0.5440
B	0.8210	0.5270
C	0.5920	0.4420
D	0.9750	0.5970
E	0.4590	0.2740
F	0.6790	0.4270
G	0.9880	0.6160