



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:59 PM UTC

PDB ID : 7V0K / pdb_00007v0k
EMDB ID : EMD-26943
Title : Consensus refinement of human erythrocyte ankyrin-1 complex (Composite map)
Authors : Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.
Deposited on : 2022-05-10
Resolution : 2.40 Å (reported)
Based on initial model : 4YZF

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

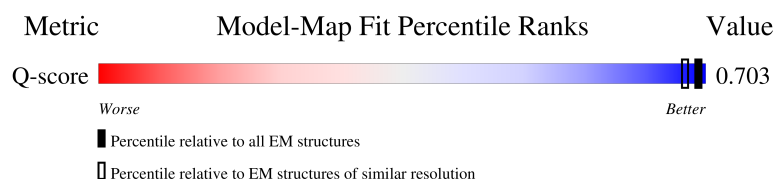
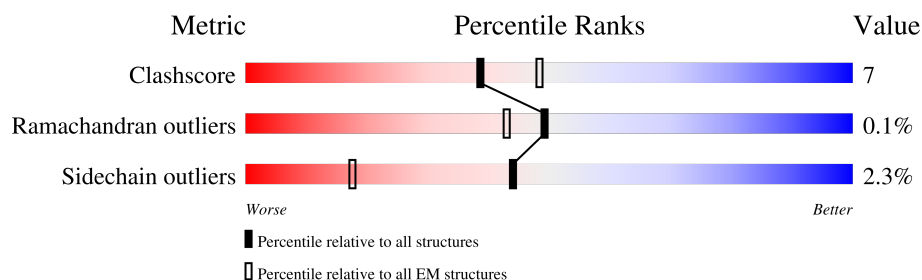
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	K	417	
2	L	409	
2	Q	409	

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Mol	Chain	Length	Quality of chain
3	H	1881	21%76%
4	O	911	70%18%12%
4	P	911	71%18%11%
4	W	911	96%
5	X	691	84%11%5%
6	D	150	18%8%73%
6	N	150	7%22%5%73%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 32037 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 Blood group Rh(CE) polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	380	Total	C	N	O	S	3	0
			2954	1968	477	491	18		

- Molecule 2 is a protein called Ammonium transporter Rh type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	388	Total	C	N	O	S	0	0
			2938	1928	473	513	24		
2	Q	390	Total	C	N	O	S	0	0
			2954	1940	475	515	24		

- Molecule 3 is a protein called Ankyrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	451	Total	C	N	O	S	0	0
			3431	2144	643	632	12		

- Molecule 4 is a protein called Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	32	Total	C	N	O	S	0	0
			233	142	34	54	3		
4	O	804	Total	C	N	O	S	0	0
			6339	4170	1047	1098	24		
4	P	814	Total	C	N	O	S	0	0
			6406	4207	1060	1115	24		

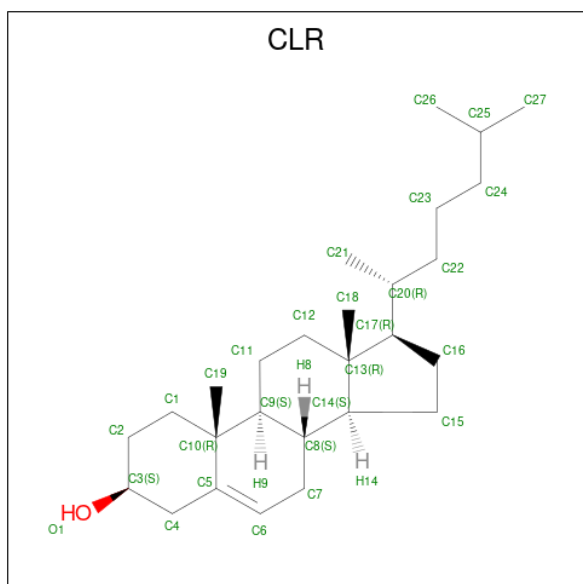
- Molecule 5 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	658	Total	C	N	O	S	0	0
			5174	3282	916	953	23		

- Molecule 6 is a protein called Glycophorin-A.

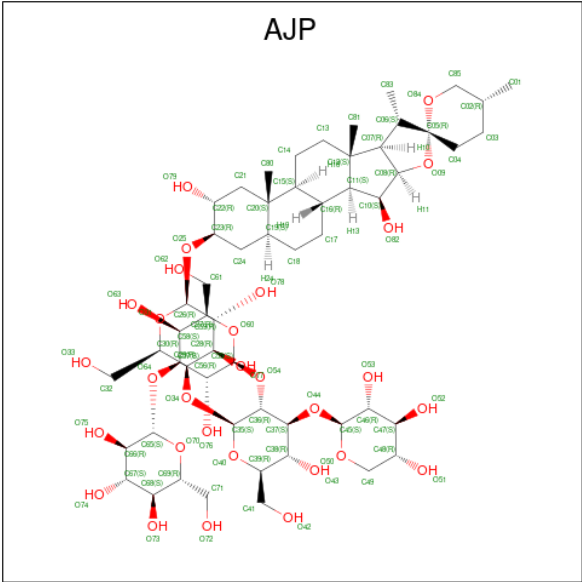
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	40	Total	C	N	O	S	0	0
			302	198	51	52	1		
6	D	40	Total	C	N	O	S	0	0
			302	198	51	52	1		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



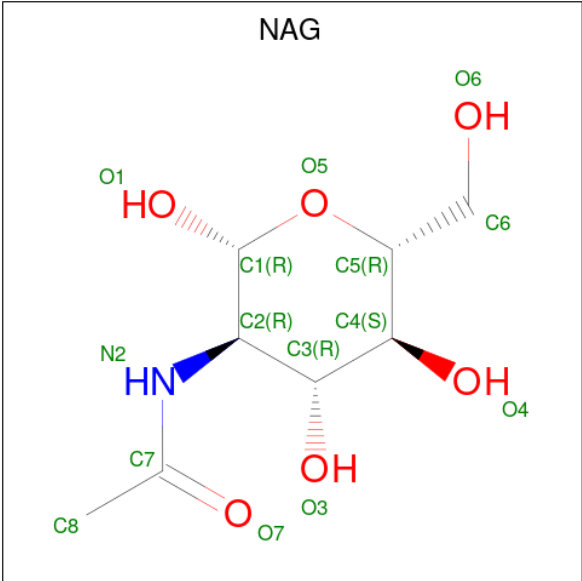
Mol	Chain	Residues	Atoms			AltConf
7	L	1	Total	C	O	0
			28	27	1	
7	L	1	Total	C	O	0
			28	27	1	
7	O	1	Total	C	O	0
			28	27	1	
7	O	1	Total	C	O	0
			28	27	1	
7	P	1	Total	C	O	0
			28	27	1	
7	P	1	Total	C	O	0
			28	27	1	

- Molecule 8 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



Mol	Chain	Residues	Atoms			AltConf
8	Q	1	Total	C	O	0
			32	27	5	
8	Q	1	Total	C	O	0
			43	33	10	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



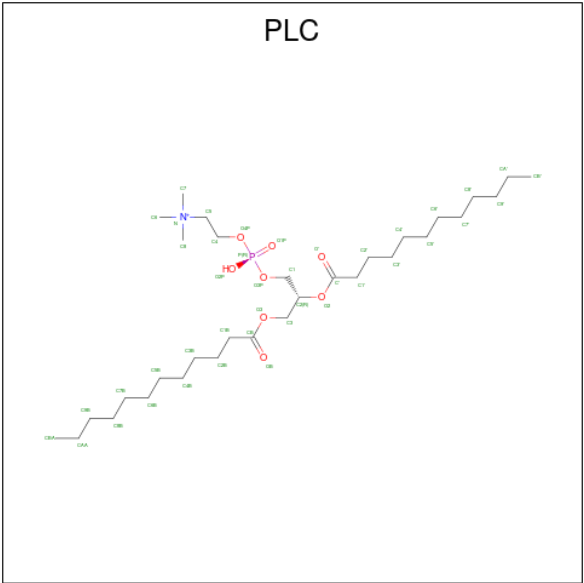
Mol	Chain	Residues	Atoms				AltConf
9	O	1	Total	C	N	O	0
			14	8	1	5	

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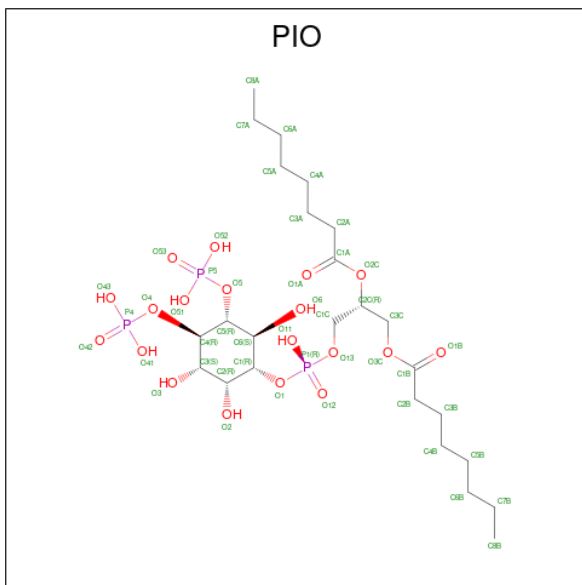
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	P	1	14	8	1	5	0

- Molecule 10 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	O	1	42	32	1	8	1	0
10	P	1	42	32	1	8	1	0

- Molecule 11 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	P	1	Total 47	C 25	O 19	P 3	0
11	P	1	Total 47	C 25	O 19	P 3	0

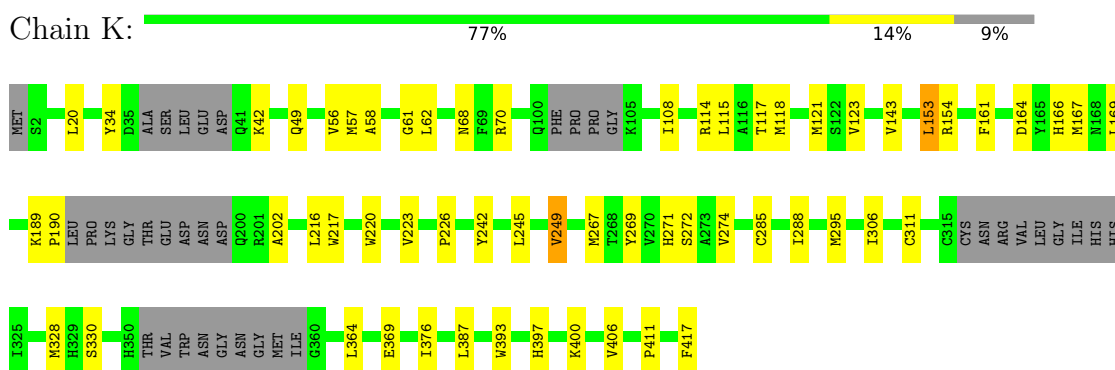
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	AltConf
12	K	54	Total O 54 54	0
12	L	89	Total O 89 89	0
12	Q	80	Total O 80 80	0
12	H	76	Total O 77 77	1
12	W	1	Total O 1 1	0
12	X	190	Total O 190 190	0
12	O	11	Total O 11 11	0
12	P	53	Total O 53 53	0

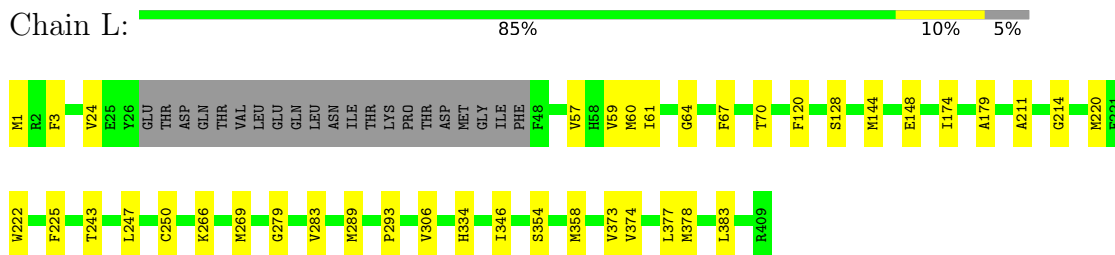
3 Residue-property plots

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

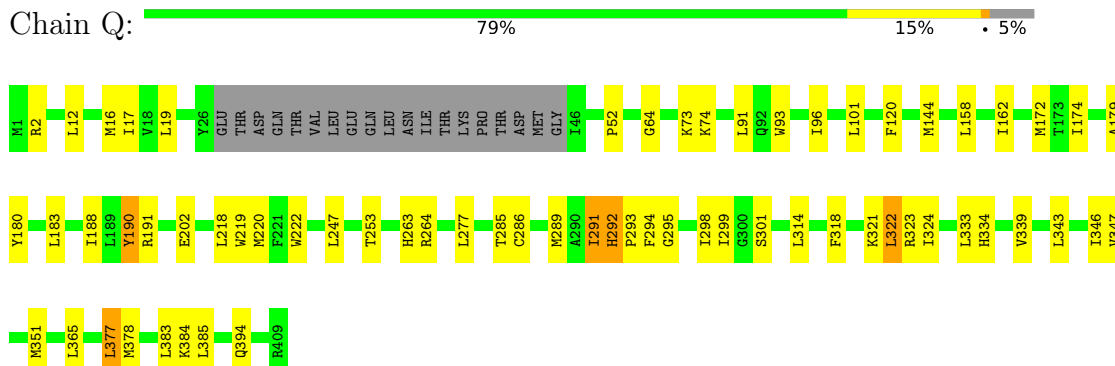
- Molecule 1: Blood group Rh(CE) polypeptide



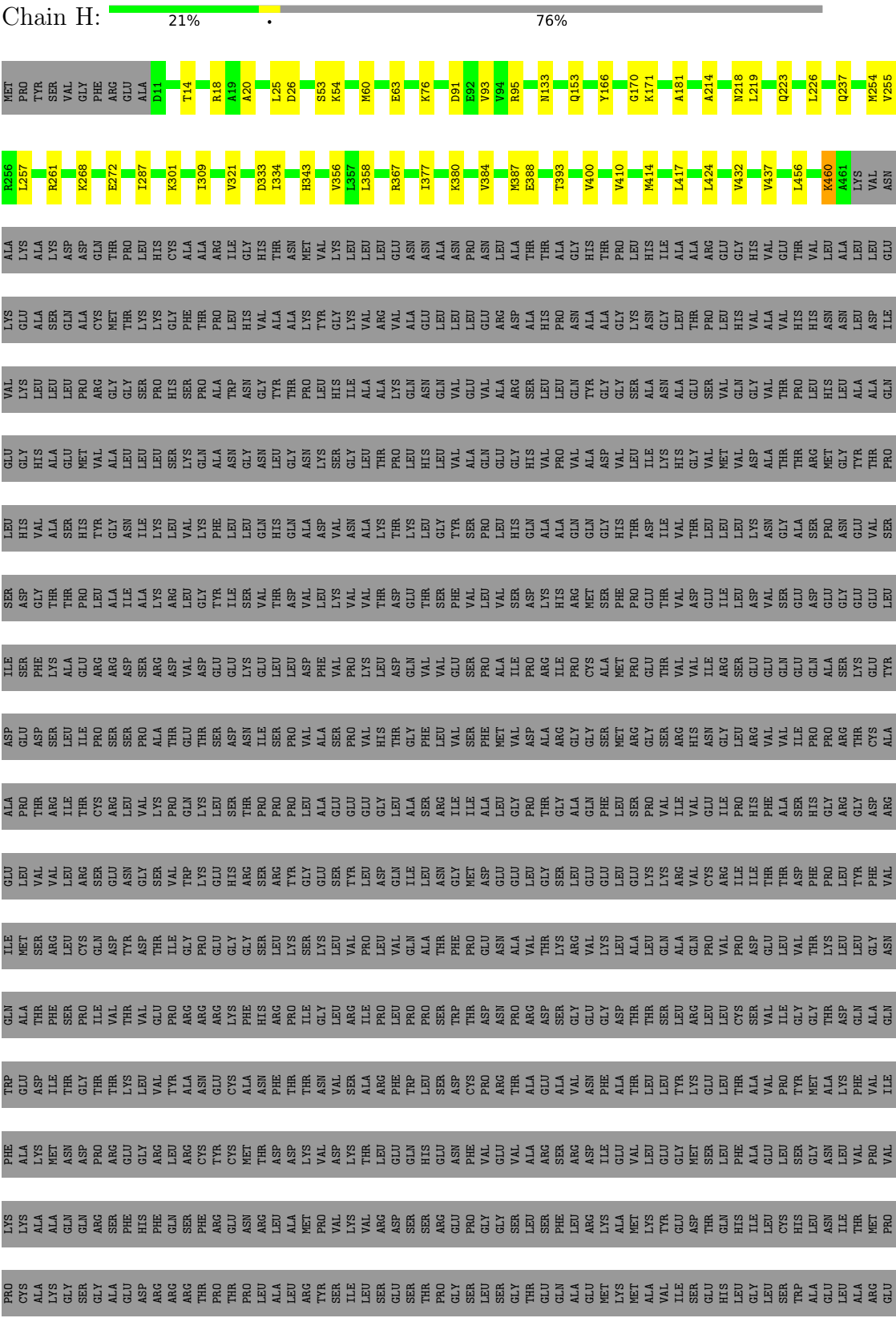
- Molecule 2: Ammonium transporter Rh type A



- Molecule 2: Ammonium transporter Rh type A

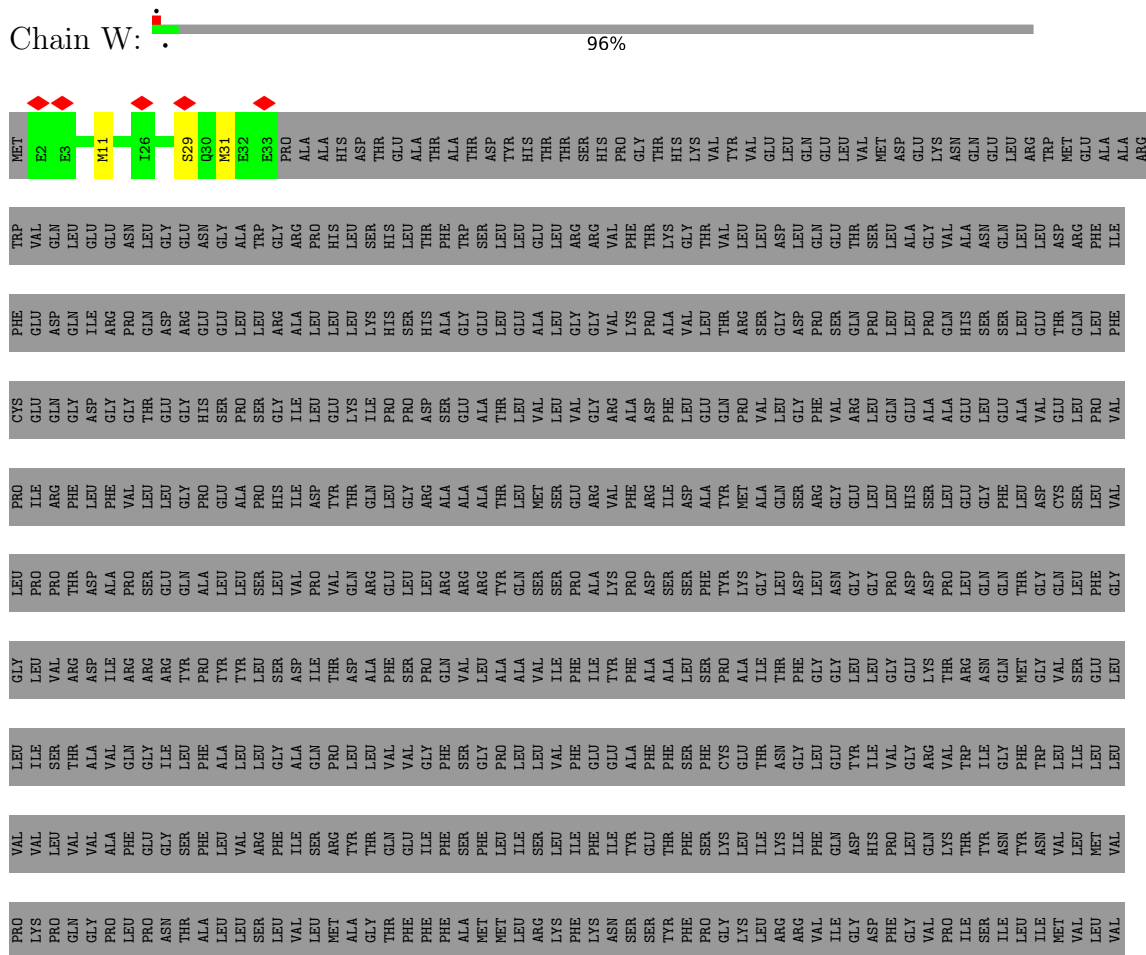


● Molecule 3: Ankyrin-1



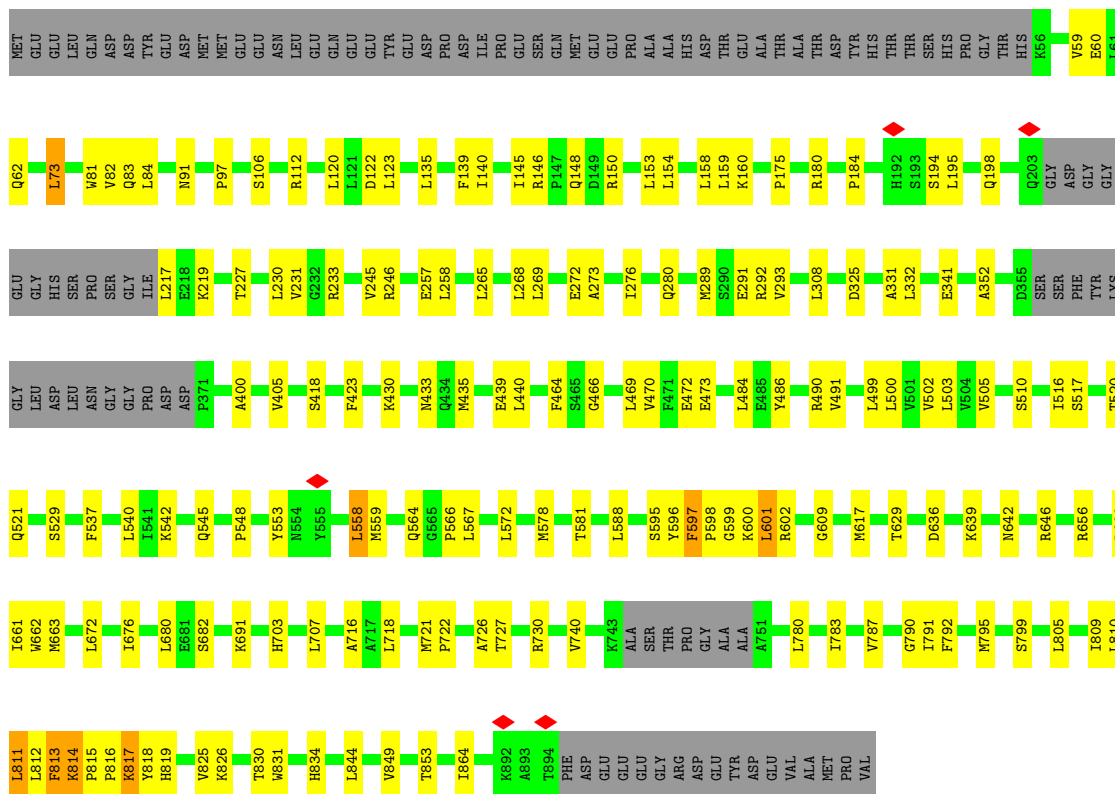
GLU	HIS	GLU	GLN	VAL	ASP	ALA	ALA	GLY	LEU
HIS	GLU	GLN	GLN	THR	SER	LEU	SER	VAL	GLN
GLU	GLU	GLU	GLY	GLY	GLU	GLU	GLU	ASP	PHE
VAL	VAL	ALA	PRO	PRO	GLU	PRO	ALA	ALA	VAL
THR	THR	LYS	HIS	SER	VAL	ARG	PRO	ILE	SER
VAL	ASP	ASN	THR	SER	SER	GLN	GLY	ARG	GLU
GLU	GLU	THR	PHE	GLY	LEU	GLY	LEU	ASN	ILE
GLY	GLY	PHE	GLN	GLN	VAL	GLN	ALA	LYS	ARG
PRO	PRO	THR	THR	THR	GLY	GLY	ALA	THR	ILE
GLU	LEU	VAL	VAL	SER	GLY	ALA	VAL	GLU	ARG
ASP	ASP	VAL	THR	GLN	ILE	ASP	HIS	ASP	VAL
PRO	PRO	GLN	MET	THR	GLY	LEU	ASP	ARG	GLU
SER	SER	GLY	MET	GLY	GLY	GLY	THR	THR	GLN
GLU	GLU	ASN	GLY	GLY	GLN	VAL	MET	THR	ASN
LEU	LEU	GLU	GLY	GLY	ALA	VAL	LEU	ASP	SER
GLU	GLU	PHE	LEU	GLU	ARG	GLU	GLU	ARG	SER
VAL	VAL	GLN	GLU	GLU	ILE	ASP	MET	ASP	LEU
ASN	ASN	ASN	PRO	THR	ASP	ASP	SER	TYR	LEU
ILE	ILE	ILE	GLY	GLY	HIS	THR	ASP	SER	GLU
ASP	ASP	PRO	GLY	GLY	VAL	VAL	MET	SER	GLN
TYR	TYR	GLY	SER	SER	PRO	SER	GLN	SER	SER
PHE	PHE	GLU	GLN	THR	THR	SER	SER	PRO	VAL
MET	MET	GLN	GLU	VAL	VAL	ASP	THR	VAL	ALA
LYS	HIS	VAL	THR	TYR	SER	ALA	ALA	SER	LEU
HIS	HIS	THR	GLY	GLY	GLN	THR	SER	GLN	LEU
THR	THR	ASP	SER	GLY	GLN	ALA	GLY	MET	ASN
SER	SER	GLU	VAL	VAL	VAL	ASN	GLY	ASN	ASN
PRO	PRO	GLN	GLY	GLY	THR	GLY	LEU	GLY	LEU
ASN	ASN	GLN	LEU	GLU	GLU	LEU	THR	TYR	TRP
PRO	HIS	PHE	VAL	VAL	ARG	ILE	PRO	SER	VAL
THR	THR	SER	SER	SER	ASP	ASP	ILE	SER	ASN
SER	SER	ASP	VAL	GLN	GLN	LEU	LEU	LEU	GLU
PRO	THR	GLU	GLY	SER	ASP	GLY	VAL	ASP	GLN
ASN	ASN	GLN	HIS	GLY	LEU	GLN	ALA	GLU	GLY
PRO	ASN	ASN	THR	THR	GLN	GLU	ALA	LEU	ASN
GLY	GLY	ILE	THR	THR	GLY	GLY	SER	ALA	GLY
ASN	ASN	LYS	GLN	GLN	ALA	ARG	LEU	GLY	GLY
GLY	GLY	LYS	PRO	PRO	ASP	SER	GLU	ASP	GLU
ASN	ASN	ILE	GLU	GLY	GLY	GLU	CYS	LEU	LEU
LEU	LEU	ARG	ALA	ALA	ILE	GLU	TYR	THR	THR
ASN	ASN	VAL	VAL	VAL	THR	GLY	LYS	GLY	GLY
GLY	GLY	VAL	SER	SER	THR	GLY	ALA	LEU	GLN
ASN	ASN	VAL	GLN	GLN	TYR	GLY	ASP	SER	SER
GLY	GLY	VAL	VAL	ALA	LEU	SER	GLY	SER	ILE
ASN	ASN	ARG	ASP	GLN	GLN	LYS	ASP	PRO	GLY
GLY	GLY	ASP	ASP	ALA	ASP	GLN	THR	ARG	GLY
ASN	ASN	GLY	ARG	ASP	ALA	GLN	THR	ALA	GLY
GLY	GLY	THR	ARG	GLN	ASP	ASP	HIS	ASP	GLU
ASN	ASN	GLN	GLN	GLY	GLY	ALA	GLU	GLN	ILE
GLY	GLY	ALA	GLN	GLY	THR	THR	GLU	TRP	VAL
ASN	ASN	ALA	GLN	GLY	THR	THR	LYS	TRP	ASN
GLY	GLY	ALA	GLN	GLN	GLN	ALA	LEU	ASN	MET
ASN	ASN	GLY	GLY	GLY	GLU	GLY	GLY	GLY	GLU
GLY	GLY	THR	GLN	GLY	THR	GLY	GLY	GLY	GLY

- Molecule 4: Band 3 anion transport protein

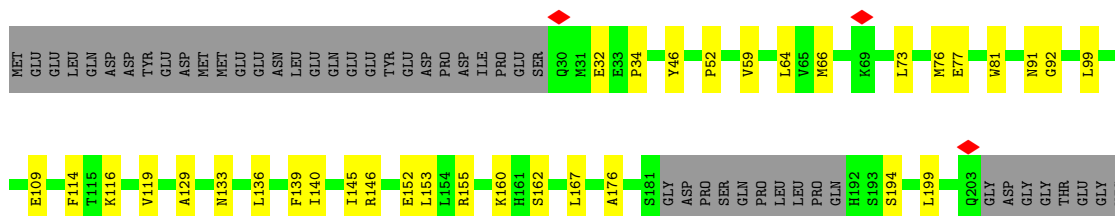


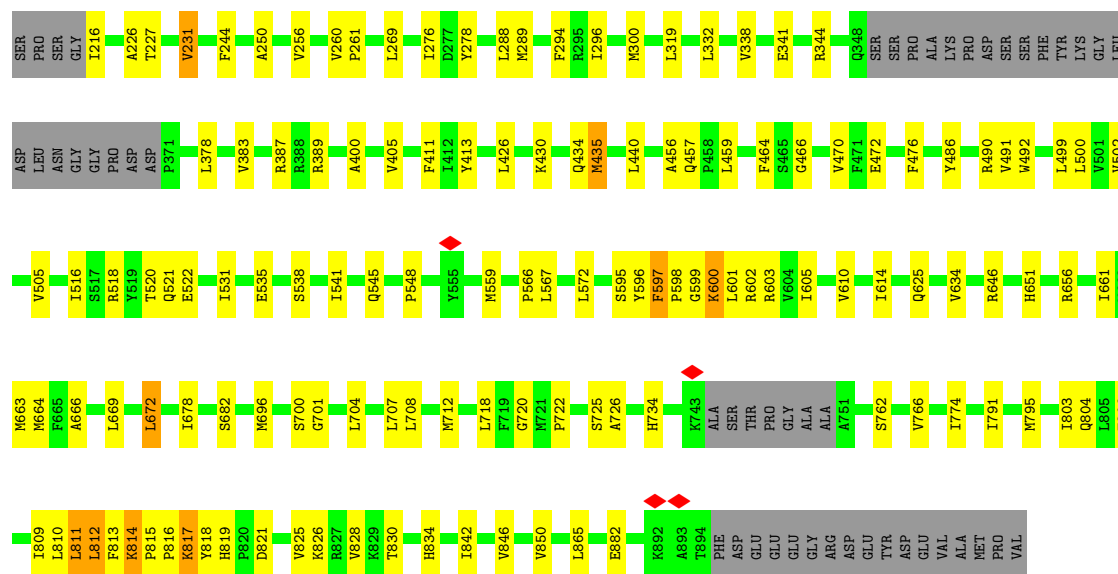
[illegible]

- Molecule 4: Band 3 anion transport protein



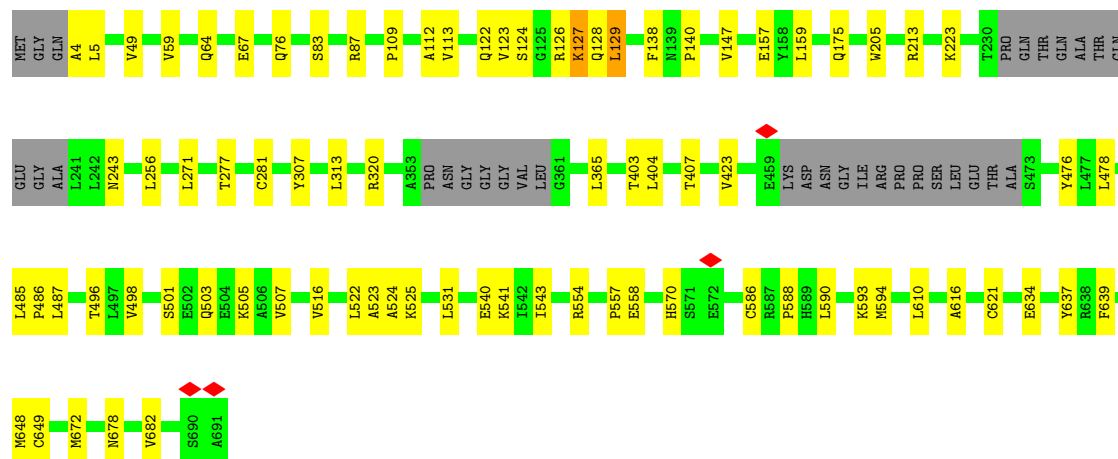
- Molecule 4: Band 3 anion transport protein





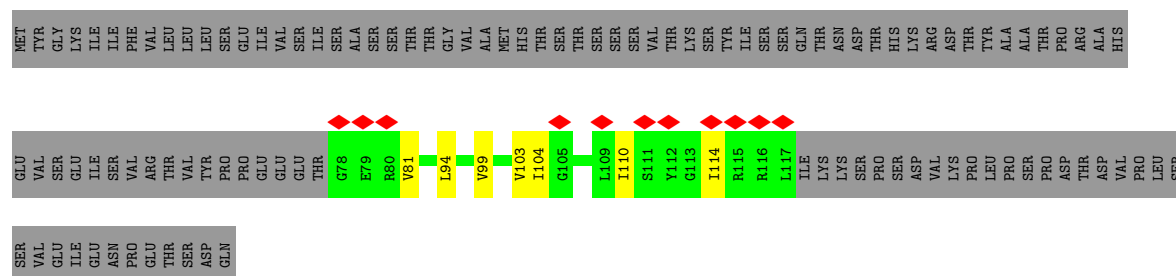
• Molecule 5: Protein 4.2

Chain X: 84% 11% 5%



• Molecule 6: Glycophorin-A

Chain N: 7% 22% 5% 73%



• Molecule 6: Glycophorin-A



MET	THR	GLY	LYS	ILE	ILE	PHE	VAL	LEU	LEU	LEU	SER	GLU	ILE	VAL	SER	ILE	SER	ALA	SER	THR	THR	GLY	VAL	ALA	MET	HIS	THR	SER	THR	SER	SER	SER	VAL	THR	LYS	SER	TYR	ILE	ILE	SER	SER	GLN	THR	ASN	ASP	THR	HIS	LYS	ARG	ASP	THR	TYR	ALA	THR	PRO	ARG	ALA	HIS
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GLU	VAL	SER	GLU	ILE	SER	VAL	ARG	THR	VAL	TYR	PRO	PRO	GLU	GLU	GLU	THR	G78	E79	F87	S88	E89	P90	E91	I92	T93	L94	V103	I104	I107	L108	L109	I110	I114	R115	R116	L117	ILE	LYS	LYS	SER	PRO	PRO	SER	ASP	VAL	LYS	LYS	PRO	LEU	PRO	SER	PRO	ASP	THR	ASP	VAL	PRO
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LEU	SER	SER	VAL	GLU	ILE	GLU	ASN	PRO	PRO	GLU	THR	SER	ASP	GLN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	710734	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF (cryoSPARC v3) followed by per particle defocus refinement and refinement of higher order aberrations (cryoSPARC v3)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.688	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	373.5, 373.5, 373.5	wwPDB
Map dimensions	900, 900, 900	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.415, 0.415, 0.415	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: PLC, PIO, AJP, CLR, NAG

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	K	0.17	0/3028	0.40	0/4121
2	L	0.17	0/3008	0.35	0/4075
2	Q	0.40	0/3025	0.62	0/4098
3	H	0.14	0/3490	0.34	0/4740
4	O	0.20	0/6489	0.40	0/8822
4	P	0.20	0/6556	0.40	0/8913
4	W	0.15	0/236	0.45	0/321
5	X	0.17	0/5281	0.36	0/7164
6	D	0.15	0/307	0.41	0/415
6	N	0.14	0/307	0.33	0/415
All	All	0.21	0/31727	0.41	0/43084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	K	2954	0	3064	34	0
2	L	2938	0	2978	24	0
2	Q	2954	0	2989	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	3431	0	3489	31	0
4	O	6339	0	6541	124	0
4	P	6406	0	6572	136	0
4	W	233	0	166	4	0
5	X	5174	0	5183	49	0
6	D	302	0	309	9	0
6	N	302	0	309	5	0
7	L	56	0	92	3	0
7	O	56	0	92	16	0
7	P	56	0	92	14	0
8	Q	75	0	0	7	0
9	O	14	0	13	0	0
9	P	14	0	13	0	0
10	O	42	0	64	3	0
10	P	42	0	64	1	0
11	P	94	0	88	31	0
12	H	77	0	0	0	0
12	K	54	0	0	1	0
12	L	89	0	0	0	0
12	O	11	0	0	0	0
12	P	53	0	0	0	0
12	Q	80	0	0	1	0
12	W	1	0	0	0	0
12	X	190	0	0	1	0
All	All	32037	0	32118	466	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 7.

All (466) 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:Q:190:TYR:HB2	12:Q:649:HOH:O	1.54	1.06
4:P:816:PRO:HG3	7:P:1003:CLR:H151	1.40	1.01
2:Q:318:PHE:O	2:Q:322:LEU:HB2	1.71	0.91
11:P:1006:PIO:H6BA	11:P:1006:PIO:H4A	1.63	0.80
2:Q:318:PHE:HA	2:Q:322:LEU:HB2	1.62	0.80
4:O:809:ILE:HA	4:O:812:LEU:HD12	1.65	0.78
4:P:227:THR:HG21	4:P:289:MET:HG3	1.65	0.77
2:Q:322:LEU:O	2:Q:323:ARG:HB2	1.85	0.76
4:P:815:PRO:HD2	4:P:818:TYR:HD1	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:598:PRO:HD2	4:P:601:LEU:HD23	1.67	0.76
5:X:59:VAL:HG12	5:X:123:VAL:HG22	1.70	0.73
4:P:597:PHE:HA	11:P:1006:PIO:H4AA	1.69	0.73
4:P:160:LYS:HE2	4:P:160:LYS:H	1.53	0.72
2:L:374:VAL:HG12	2:L:378:MET:HE2	1.72	0.71
2:Q:318:PHE:C	2:Q:322:LEU:HB2	2.15	0.71
2:Q:343:LEU:O	2:Q:347:VAL:HG23	1.90	0.71
4:O:831:TRP:HB3	7:O:1003:CLR:H111	1.72	0.71
4:P:813:PHE:HA	11:P:1005:PIO:H6A	1.73	0.70
2:Q:292:HIS:HD1	2:Q:294:PHE:HD2	1.37	0.70
2:Q:318:PHE:O	2:Q:322:LEU:CB	2.40	0.70
5:X:123:VAL:HB	5:X:126:ARG:HE	1.56	0.70
2:Q:377:LEU:CD1	8:Q:502:AJP:C83	2.70	0.70
2:Q:188:ILE:HD11	2:Q:377:LEU:HD23	1.73	0.70
2:Q:318:PHE:CA	2:Q:322:LEU:HB2	2.23	0.69
2:Q:377:LEU:HD11	8:Q:502:AJP:C83	2.22	0.69
4:O:84:LEU:HD23	4:O:97:PRO:HB2	1.74	0.69
1:K:57:MET:HE1	1:K:223:VAL:HG23	1.73	0.69
4:P:815:PRO:HA	11:P:1005:PIO:H2A	1.75	0.69
4:O:598:PRO:HD2	4:O:601:LEU:HD22	1.76	0.68
1:K:272:SER:OG	1:K:328:MET:SD	2.51	0.68
4:O:812:LEU:HB3	7:O:1003:CLR:H272	1.76	0.67
4:O:227:THR:HG21	4:O:289:MET:HG2	1.76	0.67
2:Q:253:THR:HG21	2:Q:301:SER:HB3	1.77	0.67
4:O:815:PRO:HA	11:P:1006:PIO:H2A	1.77	0.67
1:K:49:GLN:HE22	2:Q:52:PRO:HG3	1.60	0.66
3:H:25:LEU:HD21	3:H:63:GLU:HG3	1.77	0.66
2:L:377:LEU:HD21	7:L:502:CLR:H213	1.78	0.66
11:P:1006:PIO:H5B	11:P:1006:PIO:H6AA	1.76	0.66
4:P:499:LEU:HD13	7:P:1001:CLR:H273	1.79	0.65
1:K:249:VAL:HG22	1:K:274:VAL:HG12	1.78	0.64
2:Q:188:ILE:HD11	2:Q:377:LEU:CD2	2.27	0.64
2:L:1:MET:HG2	2:L:3:PHE:H	1.61	0.63
7:P:1003:CLR:H161	11:P:1005:PIO:H2AA	1.79	0.63
4:P:830:THR:HG21	7:P:1003:CLR:H152	1.81	0.63
4:P:815:PRO:HD2	4:P:818:TYR:CD1	2.34	0.63
4:P:545:GLN:HB3	10:P:1004:PLC:H51	1.80	0.63
4:P:821:ASP:OD1	4:P:826:LYS:NZ	2.31	0.62
4:P:810:LEU:HD23	4:P:813:PHE:HE2	1.65	0.62
4:P:459:LEU:HD12	4:P:696:MET:HE1	1.82	0.61
4:O:805:LEU:HD21	4:O:844:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:318:PHE:HA	2:Q:322:LEU:HG	1.82	0.61
6:D:108:LEU:HD13	4:P:378:LEU:HD13	1.82	0.60
4:O:521:GLN:OE1	4:O:691:LYS:NZ	2.33	0.60
4:O:596:TYR:HD1	4:P:813:PHE:HB2	1.65	0.60
7:P:1003:CLR:H231	11:P:1005:PIO:H3B	1.83	0.59
2:Q:318:PHE:HA	2:Q:322:LEU:CB	2.31	0.59
4:O:716:ALA:HB1	4:O:721:MET:HB2	1.84	0.59
2:L:346:ILE:HG23	2:L:358:MET:HG3	1.85	0.59
4:O:139:PHE:HB3	4:O:145:ILE:HG12	1.83	0.59
7:P:1003:CLR:H17	11:P:1005:PIO:H3C	1.84	0.59
2:Q:322:LEU:HD13	2:Q:324:ILE:HD12	1.85	0.59
6:N:81:VAL:O	4:O:656:ARG:NH1	2.36	0.59
4:O:500:LEU:HD21	4:O:672:LEU:HD12	1.85	0.59
4:P:66:MET:HB2	4:P:176:ALA:HB2	1.85	0.58
4:O:834:HIS:ND1	7:O:1003:CLR:H181	2.18	0.58
4:O:815:PRO:HD2	4:O:818:TYR:HD1	1.68	0.58
4:P:600:LYS:HZ1	11:P:1006:PIO:H4	1.68	0.58
4:P:803:ILE:HG22	4:P:806:PHE:H	1.68	0.58
1:K:117:THR:O	1:K:121:MET:HG3	2.03	0.58
7:O:1003:CLR:H263	11:P:1006:PIO:H4B	1.86	0.58
5:X:4:ALA:N	7:O:1003:CLR:H1	2.01	0.57
4:O:257:GLU:OE2	4:O:257:GLU:N	2.34	0.57
4:P:341:GLU:OE1	4:P:344:ARG:NH1	2.37	0.57
4:P:811:LEU:HA	4:P:814:LYS:HD3	1.85	0.57
4:W:11:MET:HE2	4:W:11:MET:HA	1.86	0.57
4:P:426:LEU:HD22	4:P:430:LYS:HZ1	1.68	0.57
1:K:56:VAL:HG22	2:L:220:MET:HE3	1.85	0.57
4:O:505:VAL:HG21	4:O:707:LEU:HB2	1.86	0.57
4:O:59:VAL:HB	4:O:81:TRP:HB2	1.86	0.57
4:O:122:ASP:OD2	4:O:246:ARG:NH2	2.37	0.57
4:P:663:MET:HA	4:P:666:ALA:HB3	1.86	0.57
1:K:220:TRP:HB3	1:K:245:LEU:HD11	1.87	0.57
5:X:126:ARG:HH12	5:X:129:LEU:HB2	1.69	0.56
5:X:590:LEU:O	5:X:678:ASN:ND2	2.37	0.56
4:P:226:ALA:HB2	4:P:260:VAL:HG23	1.86	0.56
4:P:491:VAL:HG22	4:P:718:LEU:HA	1.88	0.56
4:P:846:VAL:O	4:P:850:VAL:HG23	2.06	0.56
4:O:596:TYR:CD1	4:P:813:PHE:HB2	2.39	0.56
2:Q:339:VAL:O	2:Q:343:LEU:HG	2.06	0.56
2:L:289:MET:HG2	2:L:354:SER:HB2	1.87	0.56
1:K:285:CYS:HA	1:K:288:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:516:VAL:HG12	5:X:522:LEU:HD23	1.88	0.56
3:H:410:VAL:HG13	4:W:31:MET:HE1	1.88	0.55
4:P:599:GLY:O	4:P:603:ARG:HG3	2.06	0.55
4:O:581:THR:HB	4:O:617:MET:HG3	1.88	0.55
4:P:834:HIS:ND1	7:P:1003:CLR:H181	2.22	0.55
2:Q:286:CYS:HB3	2:Q:291:ILE:HG21	1.88	0.55
4:P:559:MET:HE1	4:P:567:LEU:HD11	1.87	0.55
4:O:175:PRO:HB2	4:O:233:ARG:HH22	1.71	0.55
4:P:600:LYS:HZ3	4:P:600:LYS:H	1.55	0.55
2:Q:144:MET:HB2	2:Q:383:LEU:HD11	1.88	0.55
5:X:498:VAL:HG12	5:X:540:GLU:HG3	1.89	0.55
7:O:1003:CLR:H232	11:P:1006:PIO:H4B	1.89	0.55
4:P:518:ARG:HG2	4:P:522:GLU:HG3	1.88	0.55
1:K:153:LEU:HD23	1:K:376:ILE:HD12	1.89	0.54
6:D:87:PHE:HB3	6:D:91:GLU:HB3	1.88	0.54
6:D:90:PRO:O	6:D:94:LEU:HG	2.07	0.54
4:P:76:MET:HE3	4:P:77:GLU:H	1.72	0.54
4:O:273:ALA:HB3	4:O:276:ILE:HD12	1.88	0.54
4:O:440:LEU:HD11	4:O:464:PHE:HB2	1.90	0.54
4:P:815:PRO:HB2	4:P:817:LYS:HD3	1.88	0.54
4:P:828:VAL:HG13	4:P:882:GLU:HG2	1.90	0.54
4:P:76:MET:HE3	4:P:77:GLU:N	2.23	0.54
4:P:91:ASN:OD1	4:P:91:ASN:N	2.41	0.54
4:O:440:LEU:HD13	4:O:722:PRO:HG2	1.90	0.54
2:Q:73:LYS:HD3	2:Q:202:GLU:HG3	1.90	0.53
5:X:621:CYS:HB3	5:X:639:PHE:CZ	2.43	0.53
4:P:160:LYS:HE2	4:P:160:LYS:N	2.23	0.53
4:P:598:PRO:HA	11:P:1006:PIO:O2	2.09	0.53
3:H:268:LYS:HB3	3:H:272:GLU:HA	1.90	0.53
4:O:400:ALA:HA	4:O:405:VAL:HG21	1.90	0.53
3:H:237:GLN:CD	3:H:237:GLN:H	2.16	0.53
5:X:478:LEU:HB3	5:X:496:THR:HB	1.89	0.53
4:O:791:ILE:O	4:O:795:MET:HG3	2.08	0.53
5:X:523:ALA:HB1	5:X:557:PRO:HG2	1.90	0.53
4:O:484:LEU:HD13	4:O:663:MET:HE2	1.90	0.53
5:X:67:GLU:H	5:X:67:GLU:CD	2.15	0.53
4:P:92:GLY:HA2	4:P:167:LEU:HD23	1.91	0.53
1:K:58:ALA:HB2	1:K:121:MET:HG2	1.90	0.53
4:P:682:SER:HA	4:P:726:ALA:HB3	1.91	0.53
4:P:811:LEU:HD23	4:P:814:LYS:HD3	1.91	0.53
2:Q:292:HIS:ND1	2:Q:294:PHE:HD2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:434:GLN:HE22	4:P:476:PHE:HE1	1.58	0.52
4:P:486:TYR:CZ	4:P:490:ARG:HD2	2.44	0.52
4:P:596:TYR:O	4:P:597:PHE:HB2	2.09	0.52
1:K:123:VAL:HG11	1:K:143:VAL:HA	1.90	0.52
2:Q:286:CYS:HB3	2:Q:291:ILE:CG2	2.39	0.52
4:P:834:HIS:HE1	7:P:1003:CLR:H162	1.75	0.52
4:O:231:VAL:HG12	4:O:268:LEU:HB2	1.91	0.52
4:P:531:ILE:O	4:P:535:GLU:HG2	2.09	0.52
4:O:581:THR:HG23	4:O:790:GLY:HA3	1.92	0.52
4:O:62:GLN:HB2	4:O:230:LEU:HD23	1.93	0.51
4:O:418:SER:HB2	4:O:792:PHE:HZ	1.73	0.51
4:P:119:VAL:HG12	4:P:244:PHE:HB3	1.91	0.51
4:P:541:ILE:O	4:P:545:GLN:HG3	2.10	0.51
4:P:708:LEU:O	4:P:712:MET:HG3	2.11	0.51
4:P:289:MET:HA	4:P:289:MET:HE2	1.92	0.51
4:P:825:VAL:HG12	4:P:826:LYS:HD3	1.92	0.51
4:O:727:THR:OG1	4:O:730:ARG:NH1	2.43	0.51
4:P:136:LEU:HD23	4:P:139:PHE:HD2	1.74	0.51
4:P:52:PRO:HG2	4:P:300:MET:HE2	1.93	0.51
4:P:400:ALA:HA	4:P:405:VAL:HG21	1.92	0.51
5:X:67:GLU:OE1	5:X:67:GLU:N	2.42	0.51
5:X:639:PHE:CD2	5:X:648:MET:HG3	2.45	0.51
1:K:269:TYR:OH	1:K:306:ILE:HD12	2.11	0.51
1:K:406:VAL:O	2:L:266:LYS:NZ	2.42	0.51
4:O:60:GLU:OE2	4:O:62:GLN:NE2	2.38	0.51
4:O:435:MET:HE3	4:O:722:PRO:HG3	1.92	0.51
2:Q:120:PHE:HB3	2:Q:174:ILE:HD11	1.93	0.51
1:K:70:ARG:HG3	1:K:202:ALA:HB2	1.93	0.51
4:O:341:GLU:HG3	4:P:199:LEU:HD21	1.91	0.51
4:P:734:HIS:NE2	4:P:762:SER:OG	2.37	0.51
1:K:154:ARG:NH2	12:K:502:HOH:O	2.34	0.50
5:X:485:LEU:HD12	5:X:486:PRO:HD2	1.92	0.50
4:P:830:THR:CG2	7:P:1003:CLR:H152	2.40	0.50
5:X:213:ARG:NH2	12:X:723:HOH:O	2.44	0.50
4:P:456:ALA:HB2	4:P:704:LEU:HD23	1.94	0.50
2:Q:73:LYS:HG3	2:Q:74:LYS:HG3	1.93	0.50
3:H:380:LYS:NZ	4:W:29:SER:O	2.34	0.50
4:O:596:TYR:O	4:O:597:PHE:HB2	2.12	0.50
4:P:231:VAL:HG13	4:P:278:TYR:HB3	1.93	0.50
4:P:678:ILE:HG12	4:P:725:SER:HB2	1.94	0.50
2:Q:263:HIS:CE1	2:Q:264:ARG:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:123:VAL:HG23	5:X:126:ARG:HH21	1.76	0.50
4:P:809:ILE:HA	4:P:812:LEU:HD12	1.93	0.50
2:L:59:VAL:HA	2:Q:220:MET:SD	2.52	0.50
3:H:380:LYS:HE2	3:H:414:MET:HE2	1.94	0.50
4:O:581:THR:HG21	4:O:787:VAL:HA	1.93	0.50
4:O:830:THR:HB	7:O:1003:CLR:H8	1.92	0.50
4:O:120:LEU:HD23	4:O:123:LEU:HD22	1.93	0.49
4:O:472:GLU:OE1	4:O:486:TYR:OH	2.23	0.49
4:P:810:LEU:HA	4:P:813:PHE:CE2	2.47	0.49
1:K:61:GLY:HA3	1:K:216:LEU:HG	1.95	0.49
6:D:79:GLU:OE2	4:P:656:ARG:NH1	2.45	0.49
4:P:66:MET:HG3	4:P:73:LEU:HD22	1.93	0.49
5:X:476:TYR:HB3	5:X:498:VAL:HG22	1.94	0.49
4:O:529:SER:OG	4:O:799:SER:OG	2.28	0.49
2:Q:292:HIS:ND1	2:Q:293:PRO:HD2	2.28	0.49
3:H:358:LEU:HB3	3:H:393:THR:HG21	1.94	0.49
4:O:815:PRO:HG3	11:P:1006:PIO:O1A	2.12	0.49
2:L:120:PHE:HB3	2:L:174:ILE:HD11	1.94	0.49
2:Q:318:PHE:HA	2:Q:322:LEU:CG	2.43	0.49
3:H:309:ILE:HD11	3:H:321:VAL:HG13	1.95	0.49
4:O:73:LEU:HD13	4:O:159:LEU:HD11	1.94	0.49
4:P:152:GLU:OE1	4:P:155:ARG:NH2	2.46	0.49
2:L:24:VAL:HG12	2:Q:293:PRO:HG2	1.94	0.48
2:L:64:GLY:HA2	2:L:214:GLY:HA2	1.94	0.48
4:O:195:LEU:HD21	4:P:338:VAL:HG13	1.95	0.48
5:X:64:GLN:NE2	5:X:76:GLN:OE1	2.43	0.48
5:X:616:ALA:HB3	5:X:672:MET:HE2	1.94	0.48
4:O:597:PHE:HA	11:P:1005:PIO:H5AA	1.96	0.48
2:L:144:MET:HB2	2:L:383:LEU:HD11	1.94	0.48
1:K:217:TRP:NE1	1:K:245:LEU:HB3	2.28	0.48
3:H:133:ASN:HA	3:H:171:LYS:HD2	1.94	0.48
4:O:140:ILE:HD11	4:O:150:ARG:HB2	1.94	0.48
4:O:486:TYR:CZ	4:O:490:ARG:HD2	2.49	0.48
4:O:537:PHE:HE1	10:O:1004:PLC:H9A1	1.79	0.48
5:X:157:GLU:HG2	5:X:423:VAL:HA	1.95	0.48
7:P:1003:CLR:H162	7:P:1003:CLR:H221	1.56	0.48
4:O:558:LEU:HD12	4:O:564:GLN:HG3	1.96	0.48
4:P:810:LEU:HD23	4:P:813:PHE:CE2	2.46	0.48
2:Q:347:VAL:HG21	8:Q:501:AJP:C03	2.44	0.48
4:O:559:MET:HE3	4:O:559:MET:HA	1.95	0.48
4:P:426:LEU:HD22	4:P:430:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:597:PHE:HA	11:P:1006:PIO:C4A	2.40	0.48
4:O:636:ASP:OD2	4:O:639:LYS:NZ	2.45	0.48
4:O:780:LEU:HA	4:O:783:ILE:HD12	1.95	0.48
4:P:669:LEU:HD12	4:P:669:LEU:H	1.79	0.48
4:P:59:VAL:HB	4:P:81:TRP:HB2	1.94	0.47
4:P:500:LEU:HD21	4:P:672:LEU:HG	1.96	0.47
4:O:596:TYR:HB3	4:O:597:PHE:HD2	1.79	0.47
4:O:834:HIS:CE1	7:O:1003:CLR:H162	2.49	0.47
4:P:472:GLU:OE1	4:P:486:TYR:OH	2.21	0.47
2:L:24:VAL:CG1	2:Q:293:PRO:HG2	2.44	0.47
2:Q:322:LEU:CD1	2:Q:324:ILE:HD12	2.44	0.47
2:Q:347:VAL:O	2:Q:351:MET:HG2	2.14	0.47
4:P:440:LEU:HD13	4:P:722:PRO:HG2	1.97	0.47
11:P:1005:PIO:H5B	11:P:1005:PIO:H6AA	1.96	0.47
11:P:1006:PIO:H4A	11:P:1006:PIO:H3B	1.96	0.47
2:L:243:THR:HA	2:L:283:VAL:HG11	1.97	0.47
6:D:90:PRO:HA	6:D:93:THR:HG22	1.97	0.47
6:D:103:VAL:O	6:D:107:ILE:HD12	2.15	0.47
4:O:815:PRO:CA	11:P:1006:PIO:H2A	2.44	0.47
4:P:791:ILE:O	4:P:795:MET:HG3	2.15	0.47
11:P:1006:PIO:H5A	11:P:1006:PIO:H8BA	1.96	0.47
3:H:53:SER:HA	3:H:93:VAL:HG11	1.96	0.47
5:X:140:PRO:HG2	5:X:159:LEU:HD22	1.97	0.47
5:X:634:GLU:OE1	4:P:46:TYR:OH	2.28	0.47
5:X:223:LYS:HD3	5:X:271:LEU:HD22	1.97	0.47
4:O:814:LYS:HZ1	4:O:819:HIS:N	2.12	0.47
4:P:597:PHE:HB3	4:P:601:LEU:HD23	1.97	0.47
1:K:108:ILE:HD12	2:L:293:PRO:HG2	1.97	0.47
7:L:501:CLR:H162	7:L:501:CLR:H222	1.66	0.46
4:O:217:LEU:HD22	4:O:258:LEU:HD11	1.97	0.46
4:O:825:VAL:HG12	4:O:826:LYS:HE2	1.96	0.46
4:O:831:TRP:HB3	7:O:1003:CLR:H193	1.97	0.46
4:P:815:PRO:HA	11:P:1005:PIO:C2A	2.43	0.46
3:H:460:LYS:HA	3:H:460:LYS:HD3	1.57	0.46
1:K:58:ALA:HA	1:K:62:LEU:HD12	1.98	0.46
3:H:91:ASP:O	3:H:95:ARG:HG3	2.15	0.46
4:O:112:ARG:HG3	4:O:112:ARG:HH11	1.81	0.46
4:O:680:LEU:HD11	4:O:864:ILE:HG13	1.98	0.46
3:H:424:LEU:HD11	3:H:456:LEU:HD23	1.98	0.46
4:O:146:ARG:NH2	4:O:180:ARG:HH12	2.13	0.46
10:O:1004:PLC:H2A1	10:O:1004:PLC:H5'2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:548:PRO:HD2	4:P:566:PRO:HB3	1.98	0.46
2:Q:222:TRP:HB3	2:Q:247:LEU:HD11	1.97	0.46
4:O:82:VAL:O	4:O:84:LEU:N	2.48	0.46
4:O:153:LEU:HD22	4:O:269:LEU:HD13	1.97	0.46
4:P:440:LEU:HD11	4:P:464:PHE:HB2	1.98	0.46
3:H:166:TYR:OH	3:H:170:GLY:O	2.27	0.46
3:H:387:MET:HE2	3:H:387:MET:HB3	1.76	0.46
5:X:313:LEU:HD13	5:X:525:LYS:HD3	1.97	0.46
2:L:60:MET:SD	2:L:225:PHE:HB2	2.56	0.46
4:P:505:VAL:HG21	4:P:707:LEU:HB2	1.98	0.46
4:O:599:GLY:N	11:P:1005:PIO:O3	2.49	0.46
7:O:1001:CLR:H162	7:O:1001:CLR:H221	1.50	0.46
4:P:456:ALA:HB3	4:P:701:GLY:HA3	1.97	0.46
2:Q:12:LEU:O	2:Q:16:MET:HG2	2.16	0.45
2:Q:324:ILE:HD11	8:Q:502:AJP:C10	2.46	0.45
5:X:501:SER:OG	5:X:503:GLN:O	2.34	0.45
4:O:439:GLU:HG2	4:O:646:ARG:HH12	1.80	0.45
5:X:307:TYR:HE2	5:X:404:LEU:HD21	1.81	0.45
2:L:67:PHE:O	2:L:211:ALA:HA	2.16	0.45
5:X:320:ARG:HH11	5:X:320:ARG:HB2	1.80	0.45
4:P:383:VAL:HG12	4:P:387:ARG:HE	1.80	0.45
5:X:507:VAL:HG22	5:X:570:HIS:HB3	1.98	0.45
4:P:105:TRP:O	4:P:109:GLU:HG2	2.17	0.45
2:L:222:TRP:HB3	2:L:247:LEU:HD11	1.97	0.45
11:P:1005:PIO:C1B	11:P:1005:PIO:H4AA	2.46	0.45
5:X:127:LYS:HZ2	4:O:817:LYS:HE2	1.82	0.45
4:O:331:ALA:HB1	4:P:99:LEU:HD13	1.98	0.45
4:O:423:PHE:HD2	4:O:469:LEU:HD22	1.82	0.45
4:O:588:LEU:HD13	4:O:609:GLY:HA2	1.98	0.45
4:O:595:SER:HB2	4:P:818:TYR:CD2	2.51	0.45
4:O:661:ILE:HD11	7:O:1001:CLR:H193	1.98	0.45
2:Q:19:LEU:HD13	2:Q:96:ILE:HG21	1.99	0.45
4:O:325:ASP:OD1	4:O:325:ASP:N	2.50	0.45
2:Q:179:ALA:HB2	2:Q:334:HIS:HB2	1.97	0.45
5:X:649:CYS:O	4:P:32:GLU:HB3	2.16	0.45
4:P:522:GLU:OE2	4:P:804:GLN:N	2.50	0.45
2:Q:277:LEU:HB2	2:Q:333:LEU:HD11	1.98	0.45
4:W:31:MET:HE3	4:W:31:MET:HB2	1.87	0.45
5:X:320:ARG:HB2	5:X:320:ARG:NH1	2.31	0.45
4:P:129:ALA:O	4:P:133:ASN:ND2	2.46	0.45
3:H:393:THR:O	3:H:393:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:1005:PIO:H7BA	11:P:1005:PIO:H5A	2.00	0.44
4:O:120:LEU:HB2	4:O:245:VAL:HG22	2.00	0.44
4:O:595:SER:HB2	4:P:818:TYR:CG	2.52	0.44
2:Q:394:GLN:CD	2:Q:394:GLN:H	2.25	0.44
4:O:558:LEU:H	4:O:558:LEU:HG	1.53	0.44
4:P:146:ARG:HE	4:P:146:ARG:HB2	1.69	0.44
2:Q:172:MET:HG2	2:Q:365:LEU:HD13	1.99	0.44
6:D:110:ILE:O	6:D:114:ILE:HG12	2.18	0.44
4:O:813:PHE:HA	11:P:1006:PIO:C6A	2.48	0.44
4:P:413:TYR:HA	4:P:766:VAL:HG13	1.99	0.44
4:P:457:GLN:HE21	4:P:700:SER:HB3	1.83	0.44
2:L:179:ALA:HB2	2:L:334:HIS:HB2	2.00	0.44
6:N:104:ILE:HD13	4:O:502:VAL:HG11	1.99	0.44
4:O:146:ARG:HH22	4:O:180:ARG:HH12	1.65	0.44
4:O:830:THR:HG21	7:O:1003:CLR:H152	2.00	0.44
4:P:153:LEU:HD22	4:P:269:LEU:HD13	2.00	0.44
3:H:226:LEU:HD13	3:H:261:ARG:HG3	1.98	0.44
4:O:308:LEU:HD12	4:O:308:LEU:HA	1.83	0.44
1:K:164:ASP:HB3	1:K:167:MET:HB2	2.00	0.44
4:O:82:VAL:HG11	4:O:219:LYS:HG3	2.00	0.44
4:O:510:SER:HB2	4:O:703:HIS:CE1	2.53	0.43
4:O:516:ILE:HG23	4:O:520:THR:HB	1.99	0.43
7:O:1003:CLR:H161	11:P:1006:PIO:H2B	1.99	0.43
4:P:139:PHE:HB3	4:P:145:ILE:HG12	1.99	0.43
7:P:1003:CLR:H232	11:P:1005:PIO:H4A	2.00	0.43
1:K:411:PRO:O	3:H:153:GLN:NE2	2.49	0.43
5:X:594:MET:HE3	5:X:682:VAL:HB	1.99	0.43
6:D:89:GLU:HG3	4:P:651:HIS:CD2	2.53	0.43
4:O:596:TYR:CZ	4:P:814:LYS:HD2	2.53	0.43
1:K:114:ARG:HD3	1:K:226:PRO:HB3	2.00	0.43
1:K:267:MET:HG3	1:K:271:HIS:CE1	2.53	0.43
2:L:57:VAL:O	2:L:61:ILE:HG12	2.17	0.43
2:Q:16:MET:HE1	2:Q:93:TRP:CE3	2.54	0.43
4:O:548:PRO:HD2	4:O:566:PRO:HB3	1.99	0.43
4:P:492:TRP:CE2	4:P:664:MET:HG2	2.53	0.43
7:P:1001:CLR:H272	7:P:1001:CLR:H231	1.87	0.43
4:P:516:ILE:O	4:P:521:GLN:NE2	2.49	0.43
4:P:538:SER:HA	4:P:541:ILE:HD12	2.01	0.43
4:P:815:PRO:CD	4:P:818:TYR:HD1	2.27	0.43
4:P:250:ALA:HB1	4:P:261:PRO:HB2	2.00	0.43
2:Q:347:VAL:HG12	2:Q:351:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:5:LEU:HD12	5:X:5:LEU:HA	1.90	0.43
4:O:194:SER:O	4:O:198:GLN:HG3	2.19	0.43
4:O:834:HIS:HE1	7:O:1003:CLR:H162	1.83	0.43
2:Q:314:LEU:HD23	2:Q:314:LEU:HA	1.90	0.43
2:Q:322:LEU:HD22	2:Q:322:LEU:HA	1.80	0.43
4:O:818:TYR:CG	4:P:595:SER:HB2	2.53	0.43
4:P:634:VAL:HG11	4:P:774:ILE:HA	2.01	0.43
4:P:817:LYS:HB2	4:P:817:LYS:HE3	1.64	0.43
4:P:818:TYR:O	4:P:819:HIS:C	2.61	0.43
3:H:26:ASP:OD1	5:X:83:SER:OG	2.28	0.43
5:X:126:ARG:NH1	5:X:129:LEU:HB2	2.33	0.43
4:O:814:LYS:HA	4:O:815:PRO:HD3	1.93	0.43
2:Q:219:TRP:CD1	2:Q:247:LEU:HD22	2.54	0.42
3:H:384:VAL:O	3:H:388:GLU:HG3	2.19	0.42
5:X:138:PHE:HB3	5:X:147:VAL:HG21	2.01	0.42
4:O:292:ARG:HH11	4:O:352:ALA:HB1	1.83	0.42
4:P:842:ILE:O	4:P:846:VAL:HG23	2.18	0.42
1:K:68:ASN:O	1:K:68:ASN:ND2	2.52	0.42
2:Q:285:THR:O	2:Q:289:MET:HE3	2.19	0.42
7:L:502:CLR:H222	7:L:502:CLR:H162	1.69	0.42
2:Q:180:TYR:HA	2:Q:183:LEU:HD12	2.01	0.42
4:O:548:PRO:O	4:O:553:TYR:OH	2.31	0.42
4:O:680:LEU:HD23	4:O:680:LEU:HA	1.86	0.42
4:P:319:LEU:HD23	4:P:319:LEU:HA	1.88	0.42
4:P:865:LEU:HD23	4:P:865:LEU:HA	1.87	0.42
11:P:1005:PIO:H6AA	11:P:1005:PIO:C5B	2.49	0.42
1:K:387:LEU:O	1:K:393:TRP:NE1	2.42	0.42
5:X:243:ASN:ND2	5:X:558:GLU:OE2	2.53	0.42
5:X:588:PRO:HB2	5:X:610:LEU:HD11	2.01	0.42
6:N:94:LEU:HD23	6:N:94:LEU:HA	1.90	0.42
7:P:1003:CLR:H25	11:P:1005:PIO:H6AA	2.01	0.42
2:Q:101:LEU:HD12	2:Q:101:LEU:HA	1.92	0.42
5:X:87:ARG:HA	5:X:87:ARG:HD2	1.88	0.42
4:O:469:LEU:O	4:O:473:GLU:HG3	2.19	0.42
1:K:118:MET:SD	1:K:226:PRO:HG2	2.59	0.42
4:O:73:LEU:HD23	4:O:184:PRO:HG3	2.01	0.42
4:P:109:GLU:HG3	4:P:276:ILE:HG12	2.02	0.42
2:Q:324:ILE:HD11	8:Q:502:AJP:C08	2.50	0.42
3:H:367:ARG:NH1	3:H:400:VAL:O	2.51	0.42
4:P:435:MET:HE3	4:P:722:PRO:HG3	2.01	0.42
5:X:593:LYS:HB2	5:X:593:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:99:VAL:O	6:N:103:VAL:HG12	2.20	0.42
4:O:332:LEU:HD12	4:O:332:LEU:HA	1.87	0.42
4:O:816:PRO:HG3	7:O:1003:CLR:H151	2.01	0.42
4:P:466:GLY:O	4:P:470:VAL:HG23	2.19	0.42
2:Q:64:GLY:HA3	2:Q:218:LEU:HG	2.00	0.42
5:X:524:ALA:HB1	5:X:554:ARG:HD2	2.02	0.42
3:H:20:ALA:HA	3:H:60:MET:HE3	2.02	0.42
3:H:181:ALA:O	3:H:218:ASN:ND2	2.46	0.42
4:O:636:ASP:OD1	4:O:636:ASP:N	2.48	0.42
1:K:397:HIS:HB3	1:K:400:LYS:HG2	2.03	0.41
2:Q:292:HIS:CE1	2:Q:293:PRO:HD2	2.55	0.41
5:X:487:LEU:N	5:X:586:CYS:O	2.47	0.41
5:X:637:TYR:HB3	4:P:34:PRO:HB2	2.02	0.41
4:O:660:PRO:HB2	4:O:662:TRP:CD1	2.55	0.41
4:O:813:PHE:HA	11:P:1006:PIO:H6A	2.02	0.41
4:O:814:LYS:NZ	4:O:819:HIS:HD2	2.17	0.41
4:P:389:ARG:HG2	4:P:456:ALA:HA	2.03	0.41
4:P:516:ILE:HG23	4:P:520:THR:HB	2.02	0.41
2:L:128:SER:OG	2:L:148:GLU:OE2	2.30	0.41
8:Q:502:AJP:C81	8:Q:502:AJP:O82	2.67	0.41
3:H:255:VAL:HG21	3:H:287:ILE:HD13	2.01	0.41
4:O:160:LYS:HA	4:O:160:LYS:HD2	1.69	0.41
4:O:818:TYR:CD2	4:P:595:SER:HB2	2.55	0.41
4:P:389:ARG:HA	4:P:389:ARG:HD2	1.85	0.41
4:O:540:LEU:HD22	4:O:578:MET:SD	2.60	0.41
4:P:605:ILE:HD13	4:P:605:ILE:HA	1.92	0.41
4:P:646:ARG:NH1	4:P:720:GLY:O	2.50	0.41
4:P:810:LEU:HA	4:P:813:PHE:CD2	2.56	0.41
4:O:430:LYS:HD2	4:O:473:GLU:HA	2.02	0.41
4:P:296:ILE:O	4:P:300:MET:HE3	2.21	0.41
3:H:214:ALA:HA	3:H:254:MET:HG2	2.01	0.41
4:P:598:PRO:HD2	4:P:601:LEU:CD2	2.46	0.41
4:P:811:LEU:HA	4:P:811:LEU:HD23	1.77	0.41
1:K:417:PHE:CD2	3:H:54:LYS:HD2	2.56	0.41
2:L:67:PHE:HA	2:L:70:THR:HG23	2.03	0.41
2:Q:292:HIS:CG	2:Q:293:PRO:HD2	2.56	0.41
2:Q:299:ILE:HD11	8:Q:501:AJP:C08	2.51	0.41
2:Q:343:LEU:HA	2:Q:346:ILE:HD12	2.01	0.41
3:H:219:LEU:HD13	3:H:254:MET:HE2	2.03	0.41
3:H:257:LEU:O	3:H:261:ARG:HG2	2.21	0.41
4:O:154:LEU:O	4:O:158:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:466:GLY:O	4:O:470:VAL:HG23	2.20	0.41
5:X:256:LEU:HD23	5:X:256:LEU:HA	1.91	0.41
4:O:545:GLN:HB3	10:O:1004:PLC:H51	2.03	0.41
1:K:115:LEU:HD21	1:K:166:HIS:HB3	2.03	0.41
1:K:242[A]:TYR:CE2	2:Q:91:LEU:HD13	2.56	0.41
2:L:373:VAL:O	2:L:377:LEU:HG	2.20	0.41
2:Q:384:LYS:O	2:Q:385:LEU:C	2.64	0.41
3:H:14:THR:HG22	3:H:18:ARG:NH1	2.35	0.41
3:H:343:HIS:HD2	3:H:377:ILE:HD12	1.86	0.41
5:X:113:VAL:HG13	5:X:205:TRP:HB2	2.03	0.41
4:O:245:VAL:HB	4:O:265:LEU:HB2	2.03	0.41
4:O:433:ASN:HB3	4:O:642:ASN:HB2	2.01	0.41
4:O:491:VAL:HG22	4:O:718:LEU:HA	2.02	0.41
4:O:682:SER:HA	4:O:726:ALA:HB3	2.03	0.41
4:P:411:PHE:CD1	4:P:610:VAL:HG11	2.56	0.41
4:P:490:ARG:NH2	4:P:722:PRO:HA	2.36	0.41
2:L:250:CYS:SG	2:L:279:GLY:N	2.94	0.41
4:O:811:LEU:HD22	4:O:814:LYS:HZ2	1.85	0.41
4:O:816:PRO:CG	7:O:1003:CLR:H72	2.51	0.41
4:O:849:VAL:O	4:O:853:THR:HG23	2.21	0.41
1:K:161:PHE:CD1	1:K:369:GLU:HG3	2.57	0.40
1:K:295:MET:HB3	2:Q:17:ILE:HG12	2.03	0.40
5:X:122:GLN:HG3	5:X:128:GLN:HG3	2.03	0.40
4:P:288:LEU:HG	4:P:294:PHE:CD1	2.56	0.40
4:P:812:LEU:HB3	7:P:1003:CLR:H241	2.03	0.40
4:P:815:PRO:CB	11:P:1005:PIO:H3	2.51	0.40
3:H:301:LYS:NZ	3:H:333:ASP:OD2	2.54	0.40
5:X:109:PRO:HG2	5:X:112:ALA:HB2	2.03	0.40
6:N:110:ILE:O	6:N:114:ILE:HG12	2.21	0.40
4:O:106:SER:HB3	4:O:280:GLN:HB3	2.02	0.40
4:O:291:GLU:OE1	4:O:293:VAL:HB	2.22	0.40
4:O:559:MET:HE1	4:O:567:LEU:HD11	2.03	0.40
1:K:154:ARG:CZ	1:K:169:LEU:HD13	2.52	0.40
2:Q:295:GLY:HA2	2:Q:298:ILE:HD12	2.03	0.40
4:P:597:PHE:HB3	4:P:598:PRO:HD2	2.03	0.40
5:X:365:LEU:HD23	5:X:365:LEU:HA	1.78	0.40
6:D:104:ILE:HD13	4:P:502:VAL:HG11	2.03	0.40
4:O:542:LYS:HA	4:O:545:GLN:HG3	2.04	0.40
4:O:572:LEU:HB3	4:P:572:LEU:HB3	2.04	0.40
4:O:597:PHE:HB3	4:O:598:PRO:HD2	2.03	0.40
4:P:64:LEU:HG	4:P:73:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:389:ARG:NH1	4:P:456:ALA:O	2.54	0.40
1:K:189:LYS:HA	1:K:190:PRO:HD3	1.94	0.40
2:Q:158:LEU:HD12	2:Q:162:ILE:HB	2.03	0.40
5:X:541:LYS:HD3	5:X:543:ILE:HD11	2.04	0.40
4:O:272:GLU:H	4:O:272:GLU:CD	2.29	0.40
4:P:614:ILE:HD11	4:P:791:ILE:HG13	2.03	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	K	371/417 (89%)	366 (99%)	5 (1%)	0	100	100
2	L	384/409 (94%)	380 (99%)	4 (1%)	0	100	100
2	Q	386/409 (94%)	376 (97%)	8 (2%)	2 (0%)	24	37
3	H	449/1881 (24%)	438 (98%)	11 (2%)	0	100	100
4	O	796/911 (87%)	780 (98%)	14 (2%)	2 (0%)	36	50
4	P	804/911 (88%)	790 (98%)	13 (2%)	1 (0%)	48	64
4	W	30/911 (3%)	26 (87%)	4 (13%)	0	100	100
5	X	650/691 (94%)	643 (99%)	7 (1%)	0	100	100
6	D	38/150 (25%)	37 (97%)	1 (3%)	0	100	100
6	N	38/150 (25%)	35 (92%)	3 (8%)	0	100	100
All	All	3946/6840 (58%)	3871 (98%)	70 (2%)	5 (0%)	49	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	2	ARG

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Mol	Chain	Res	Type
4	O	83	GLN
2	Q	292	HIS
4	P	597	PHE
4	O	597	PHE

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	K	318/348 (91%)	309 (97%)	9 (3%)	38	60
2	L	307/328 (94%)	305 (99%)	2 (1%)	76	88
2	Q	308/328 (94%)	301 (98%)	7 (2%)	44	66
3	H	367/1594 (23%)	359 (98%)	8 (2%)	45	67
4	O	689/786 (88%)	670 (97%)	19 (3%)	38	60
4	P	692/786 (88%)	673 (97%)	19 (3%)	39	62
4	W	20/786 (2%)	20 (100%)	0	100	100
5	X	559/588 (95%)	548 (98%)	11 (2%)	48	70
6	D	31/136 (23%)	30 (97%)	1 (3%)	34	56
6	N	31/136 (23%)	31 (100%)	0	100	100
All	All	3322/5816 (57%)	3246 (98%)	76 (2%)	44	66

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	LEU
1	K	34[A]	TYR
1	K	34[B]	TYR
1	K	42	LYS
1	K	153	LEU
1	K	249	VAL
1	K	311	CYS
1	K	330	SER
1	K	364	LEU

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Mol	Chain	Res	Type
2	L	269	MET
2	L	306	VAL
2	Q	190	TYR
2	Q	191	ARG
2	Q	291	ILE
2	Q	321	LYS
2	Q	322	LEU
2	Q	377	LEU
2	Q	378	MET
3	H	76	LYS
3	H	223	GLN
3	H	334	ILE
3	H	356	VAL
3	H	417	LEU
3	H	432	VAL
3	H	437	VAL
3	H	460	LYS
5	X	49	VAL
5	X	124	SER
5	X	127	LYS
5	X	129	LEU
5	X	175	GLN
5	X	277	THR
5	X	281	CYS
5	X	403	THR
5	X	407	THR
5	X	505	LYS
5	X	531	LEU
6	D	108	LEU
4	O	73	LEU
4	O	91	ASN
4	O	135	LEU
4	O	148	GLN
4	O	499	LEU
4	O	503	LEU
4	O	517	SER
4	O	558	LEU
4	O	600	LYS
4	O	601	LEU
4	O	602	ARG
4	O	629	THR
4	O	676	ILE

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Mol	Chain	Res	Type
4	O	740	VAL
4	O	810	LEU
4	O	811	LEU
4	O	813	PHE
4	O	814	LYS
4	O	817	LYS
4	P	114	PHE
4	P	116	LYS
4	P	140	ILE
4	P	162	SER
4	P	194	SER
4	P	216	ILE
4	P	231	VAL
4	P	256	VAL
4	P	332	LEU
4	P	435	MET
4	P	600	LYS
4	P	602	ARG
4	P	625	GLN
4	P	661	ILE
4	P	672	LEU
4	P	811	LEU
4	P	812	LEU
4	P	814	LYS
4	P	817	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	49	GLN
1	K	362	GLN
1	K	389	ASN
1	K	405	GLN
2	L	109	ASN
2	Q	98	GLN
2	Q	154	HIS
3	H	282	ASN
5	X	154	GLN
5	X	220	HIS
5	X	225	GLN
5	X	492	GLN
5	X	532	HIS

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Mol	Chain	Res	Type
5	X	559	ASN
4	O	192	HIS
4	O	198	GLN
4	O	545	GLN
4	O	683	GLN
4	O	819	HIS
4	O	884	GLN
4	P	163	HIS
4	P	198	GLN
4	P	339	GLN
4	P	374	GLN
4	P	434	GLN
4	P	457	GLN
4	P	752	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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
11	PIO	P	1006	-	47,47,47	0.48	0	62,65,65	0.45	0
7	CLR	O	1001	-	31,31,31	0.39	0	48,48,48	0.70	0
11	PIO	P	1005	-	47,47,47	0.48	0	62,65,65	0.47	0
10	PLC	O	1004	-	41,41,41	0.51	0	47,49,49	0.52	0
7	CLR	L	501	-	31,31,31	0.40	0	48,48,48	0.66	0
7	CLR	P	1001	-	31,31,31	0.40	0	48,48,48	0.53	0
8	AJP	Q	502	-	49,49,95	0.40	0	75,80,149	0.38	0
7	CLR	P	1003	-	31,31,31	0.32	0	48,48,48	0.44	0
7	CLR	O	1003	-	31,31,31	0.30	0	48,48,48	0.41	0
8	AJP	Q	501	-	37,37,95	0.48	0	58,62,149	0.59	1 (1%)
9	NAG	P	1002	4	14,14,15	0.25	0	17,19,21	0.40	0
9	NAG	O	1002	4	14,14,15	0.45	0	17,19,21	0.62	0
10	PLC	P	1004	-	41,41,41	0.52	0	47,49,49	0.51	0
7	CLR	L	502	-	31,31,31	0.44	0	48,48,48	0.83	1 (2%)

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
11	PIO	P	1006	-	-	18/44/68/68	0/1/1/1
7	CLR	O	1001	-	-	8/10/68/68	0/4/4/4
11	PIO	P	1005	-	-	27/44/68/68	0/1/1/1
10	PLC	O	1004	-	-	17/45/45/45	-
7	CLR	L	501	-	-	6/10/68/68	0/4/4/4
7	CLR	P	1001	-	-	8/10/68/68	0/4/4/4
8	AJP	Q	502	-	-	4/6/121/220	0/7/7/11
7	CLR	P	1003	-	-	9/10/68/68	0/4/4/4
7	CLR	O	1003	-	-	8/10/68/68	0/4/4/4
8	AJP	Q	501	-	-	-	0/6/6/11
9	NAG	P	1002	4	-	0/6/23/26	0/1/1/1
9	NAG	O	1002	4	-	2/6/23/26	0/1/1/1
10	PLC	P	1004	-	-	18/45/45/45	-
7	CLR	L	502	-	-	2/10/68/68	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	502	CLR	C16-C15-C14	-3.02	99.23	105.14
8	Q	501	AJP	C19-C24-C23	-2.37	111.58	114.40

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	O	1004	PLC	C4-O4P-P-O2P
10	O	1004	PLC	C4-O4P-P-O3P
10	P	1004	PLC	O4P-C4-C5-N
10	P	1004	PLC	C1'-C'-O2-C2
10	P	1004	PLC	C4-O4P-P-O2P
11	P	1005	PIO	C1-O1-P1-O12
11	P	1005	PIO	C1C-O13-P1-O1
11	P	1005	PIO	C1C-O13-P1-O11
11	P	1005	PIO	C2A-C1A-O2C-C2C
11	P	1006	PIO	C1C-O13-P1-O1
11	P	1006	PIO	C1C-O13-P1-O12
11	P	1006	PIO	C2A-C1A-O2C-C2C
7	O	1003	CLR	C21-C20-C22-C23
11	P	1005	PIO	O1B-C1B-O3C-C3C
7	O	1003	CLR	C13-C17-C20-C22
10	P	1004	PLC	O'-C'-O2-C2
11	P	1006	PIO	O1A-C1A-O2C-C2C
7	O	1001	CLR	C21-C20-C22-C23
7	P	1001	CLR	C21-C20-C22-C23
7	P	1003	CLR	C21-C20-C22-C23
7	O	1003	CLR	C16-C17-C20-C21
7	P	1003	CLR	C16-C17-C20-C21
7	O	1003	CLR	C13-C17-C20-C21
7	P	1003	CLR	C13-C17-C20-C22
11	P	1005	PIO	C2B-C1B-O3C-C3C
11	P	1005	PIO	O1A-C1A-O2C-C2C
9	O	1002	NAG	O5-C5-C6-O6
7	O	1001	CLR	C13-C17-C20-C21
7	P	1001	CLR	C13-C17-C20-C21
7	P	1003	CLR	C13-C17-C20-C21
7	O	1001	CLR	C17-C20-C22-C23
7	P	1001	CLR	C13-C17-C20-C22
8	Q	502	AJP	O31-C30-C32-O33
7	P	1003	CLR	C17-C20-C22-C23
11	P	1006	PIO	C1A-C2A-C3A-C4A
11	P	1006	PIO	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
11	P	1006	PIO	C2B-C1B-O3C-C3C
8	Q	502	AJP	C29-C30-C32-O33
7	O	1001	CLR	C16-C17-C20-C21
7	P	1001	CLR	C16-C17-C20-C21
10	P	1004	PLC	C4-C5-N-C8
7	P	1001	CLR	C17-C20-C22-C23
11	P	1006	PIO	O1B-C1B-O3C-C3C
7	O	1003	CLR	C16-C17-C20-C22
7	O	1001	CLR	C13-C17-C20-C22
9	O	1002	NAG	C4-C5-C6-O6
7	O	1001	CLR	C22-C23-C24-C25
7	O	1001	CLR	C16-C17-C20-C22
7	L	501	CLR	C22-C23-C24-C25
7	P	1003	CLR	C20-C22-C23-C24
10	P	1004	PLC	CB-C1B-C2B-C3B
7	P	1001	CLR	C16-C17-C20-C22
7	P	1003	CLR	C16-C17-C20-C22
7	O	1001	CLR	C20-C22-C23-C24
7	L	501	CLR	C20-C22-C23-C24
7	P	1001	CLR	C20-C22-C23-C24
10	P	1004	PLC	C'-C1'-C2'-C3'
7	P	1001	CLR	C22-C23-C24-C25
11	P	1005	PIO	C1A-C2A-C3A-C4A
11	P	1005	PIO	C2B-C3B-C4B-C5B
11	P	1005	PIO	C4B-C5B-C6B-C7B
11	P	1006	PIO	C2B-C3B-C4B-C5B
7	P	1003	CLR	C23-C24-C25-C27
10	P	1004	PLC	C4-C5-N-C6
10	P	1004	PLC	C4-C5-N-C7
7	L	502	CLR	C20-C22-C23-C24
7	O	1003	CLR	C22-C23-C24-C25
11	P	1005	PIO	O2C-C2C-C3C-O3C
7	P	1003	CLR	C23-C24-C25-C26
11	P	1006	PIO	O13-C1C-C2C-C3C
10	P	1004	PLC	C1B-C2B-C3B-C4B
11	P	1005	PIO	C1C-C2C-C3C-O3C
11	P	1005	PIO	C3A-C4A-C5A-C6A
11	P	1005	PIO	C1C-C2C-O2C-C1A
10	O	1004	PLC	C1B-CB-O3-C3
10	O	1004	PLC	C5B-C6B-C7B-C8B
11	P	1006	PIO	C5A-C6A-C7A-C8A
10	P	1004	PLC	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
11	P	1005	PIO	O13-C1C-C2C-C3C
10	O	1004	PLC	O3P-C1-C2-O2
10	P	1004	PLC	O2-C2-C3-O3
7	O	1003	CLR	C17-C20-C22-C23
10	O	1004	PLC	C4'-C5'-C6'-C7'
10	O	1004	PLC	OB-CB-O3-C3
10	O	1004	PLC	C6B-C7B-C8B-C9B
11	P	1006	PIO	O13-C1C-C2C-O2C
10	P	1004	PLC	C1-C2-C3-O3
10	P	1004	PLC	C6B-C7B-C8B-C9B
11	P	1005	PIO	C2A-C3A-C4A-C5A
11	P	1006	PIO	C2C-C1C-O13-P1
11	P	1005	PIO	C5-O5-P5-O53
10	O	1004	PLC	C1'-C'-O2-C2
10	O	1004	PLC	C7'-C8'-C9'-CA'
10	O	1004	PLC	O'-C'-O2-C2
10	O	1004	PLC	C2B-C3B-C4B-C5B
11	P	1005	PIO	C1-O1-P1-O13
11	P	1005	PIO	C1C-O13-P1-O12
11	P	1006	PIO	C1C-O13-P1-O11
10	O	1004	PLC	O3P-C1-C2-C3
11	P	1005	PIO	O13-C1C-C2C-O2C
7	L	501	CLR	C16-C17-C20-C22
7	L	501	CLR	C13-C17-C20-C21
7	L	502	CLR	C22-C23-C24-C25
10	O	1004	PLC	C'-C1'-C2'-C3'
11	P	1005	PIO	C4-O4-P4-O42
7	L	501	CLR	C13-C17-C20-C22
11	P	1005	PIO	C5B-C6B-C7B-C8B
11	P	1005	PIO	C4A-C5A-C6A-C7A
10	P	1004	PLC	O3P-C1-C2-O2
7	L	501	CLR	C16-C17-C20-C21
11	P	1006	PIO	C1C-C2C-O2C-C1A
10	O	1004	PLC	C1B-C2B-C3B-C4B
7	O	1003	CLR	C23-C24-C25-C26
8	Q	502	AJP	O31-C26-O25-C23
10	P	1004	PLC	C1'-C2'-C3'-C4'
10	O	1004	PLC	C2B-C1B-CB-O3
11	P	1006	PIO	O2C-C1A-C2A-C3A
11	P	1005	PIO	O3C-C1B-C2B-C3B
11	P	1006	PIO	C3A-C4A-C5A-C6A
10	P	1004	PLC	C2-C1-O3P-P

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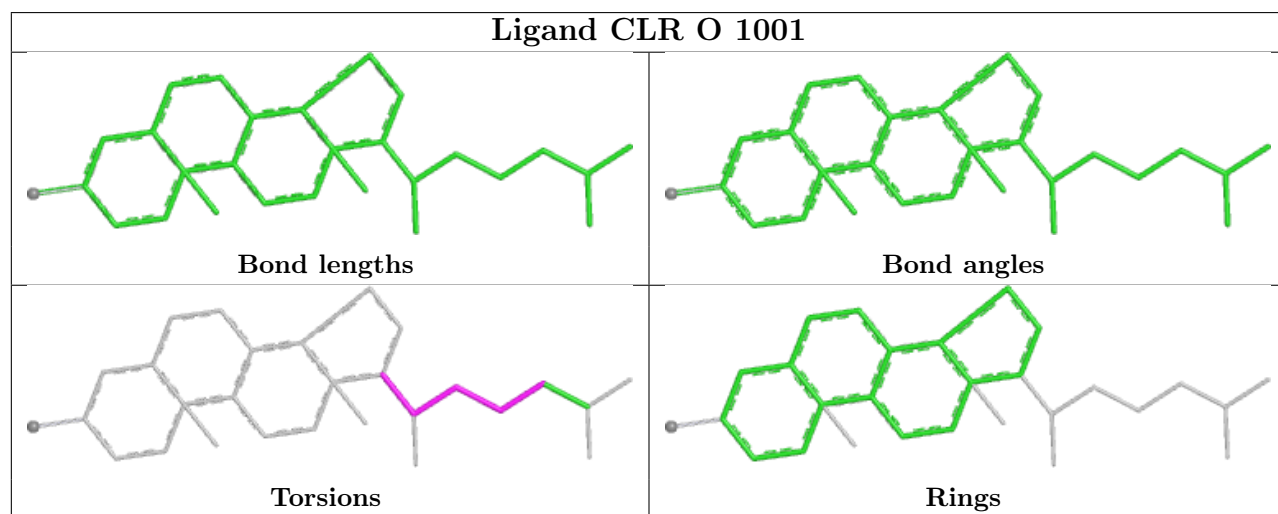
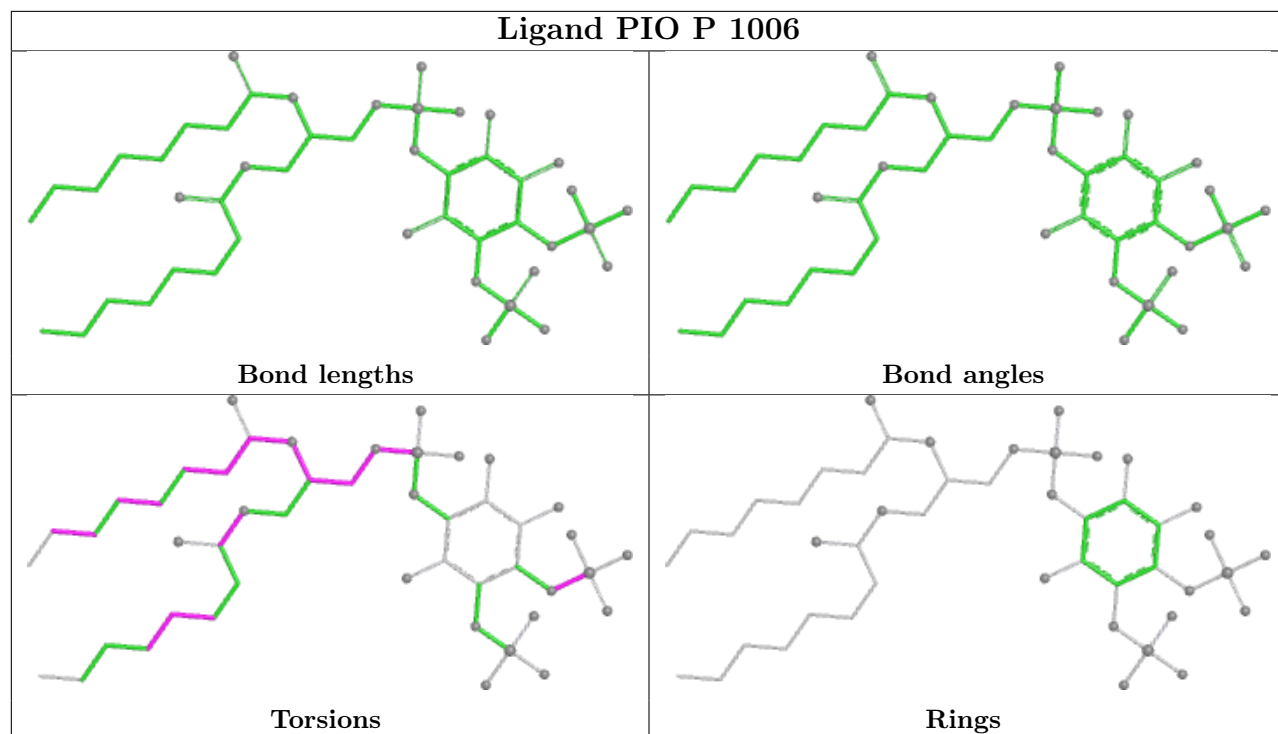
Mol	Chain	Res	Type	Atoms
11	P	1006	PIO	C4-O4-P4-O42
11	P	1005	PIO	O1B-C1B-C2B-C3B
11	P	1005	PIO	O2C-C1A-C2A-C3A
10	O	1004	PLC	C2B-C1B-CB-OB
8	Q	502	AJP	C27-C26-O25-C23
10	P	1004	PLC	C3B-C4B-C5B-C6B
11	P	1005	PIO	O1A-C1A-C2A-C3A

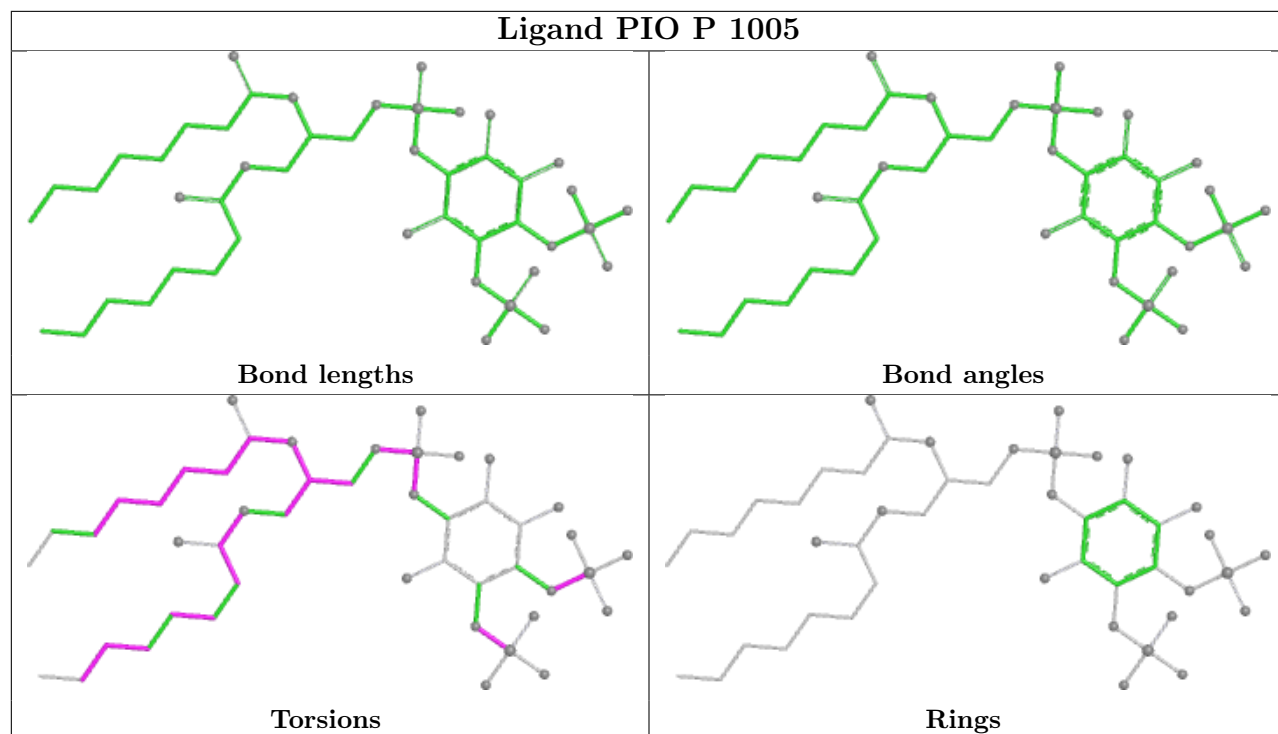
There are no ring outliers.

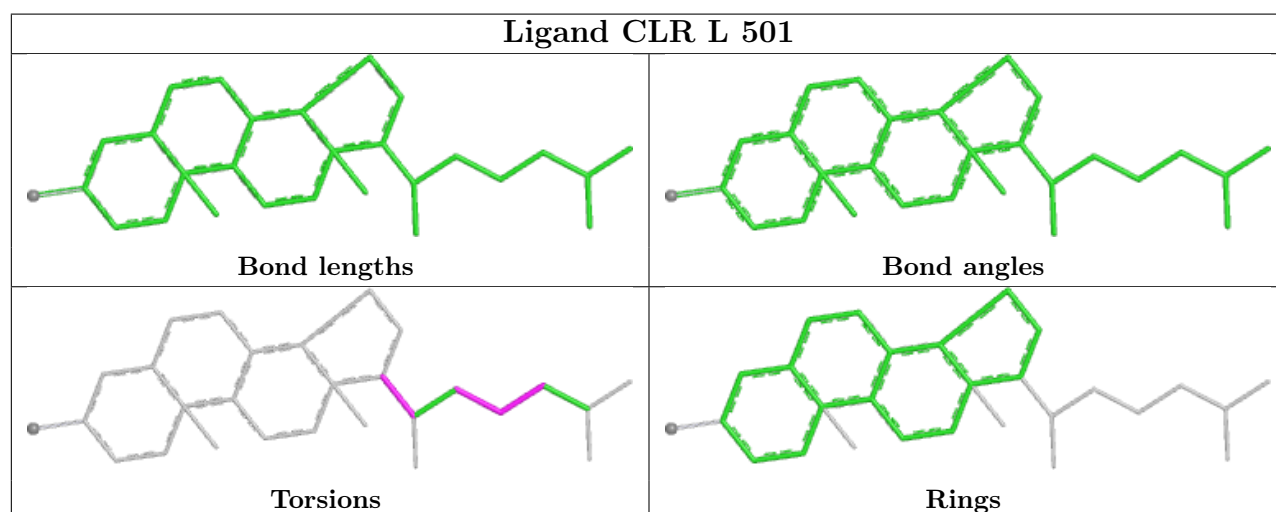
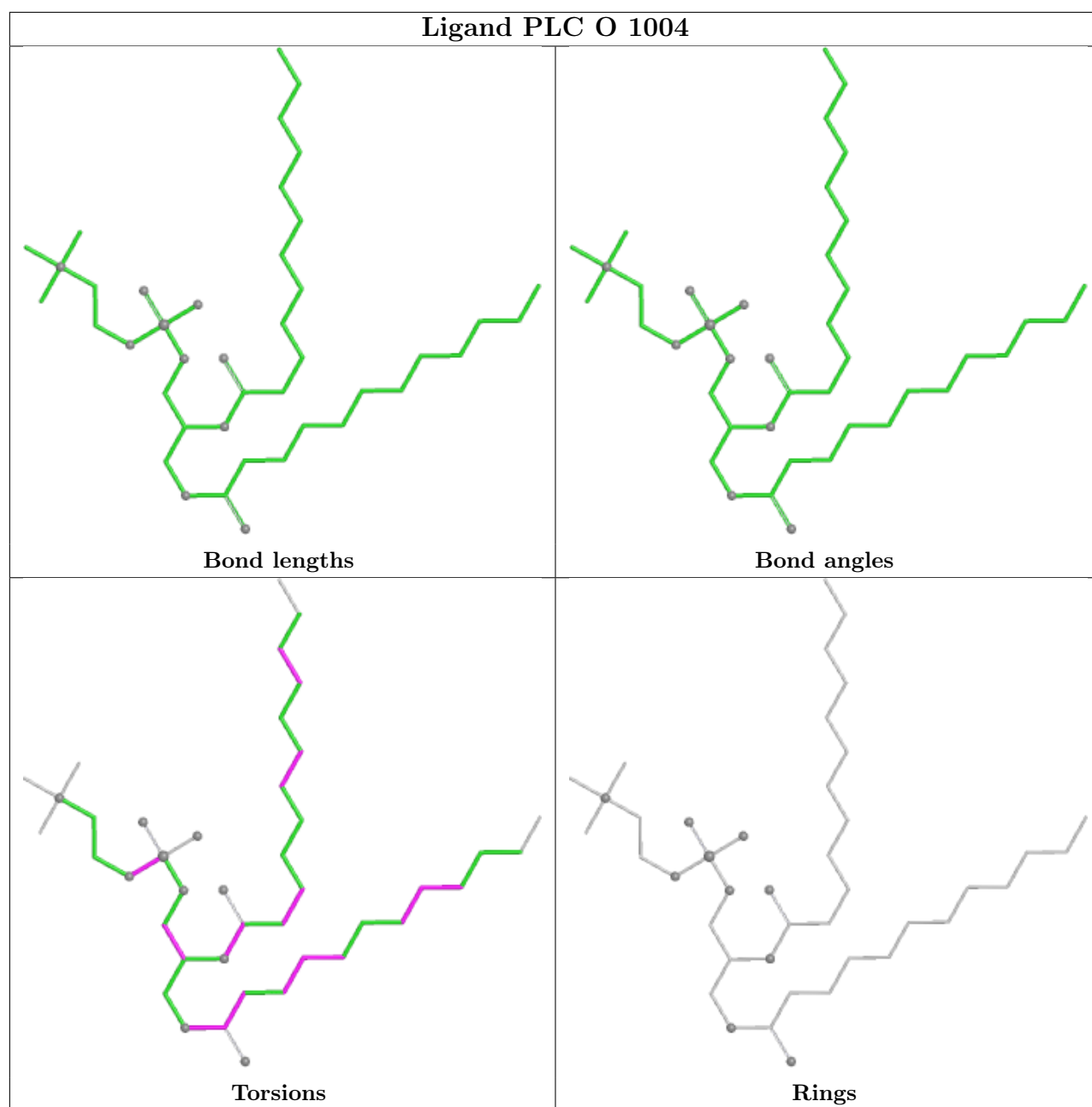
12 monomers are involved in 67 short contacts:

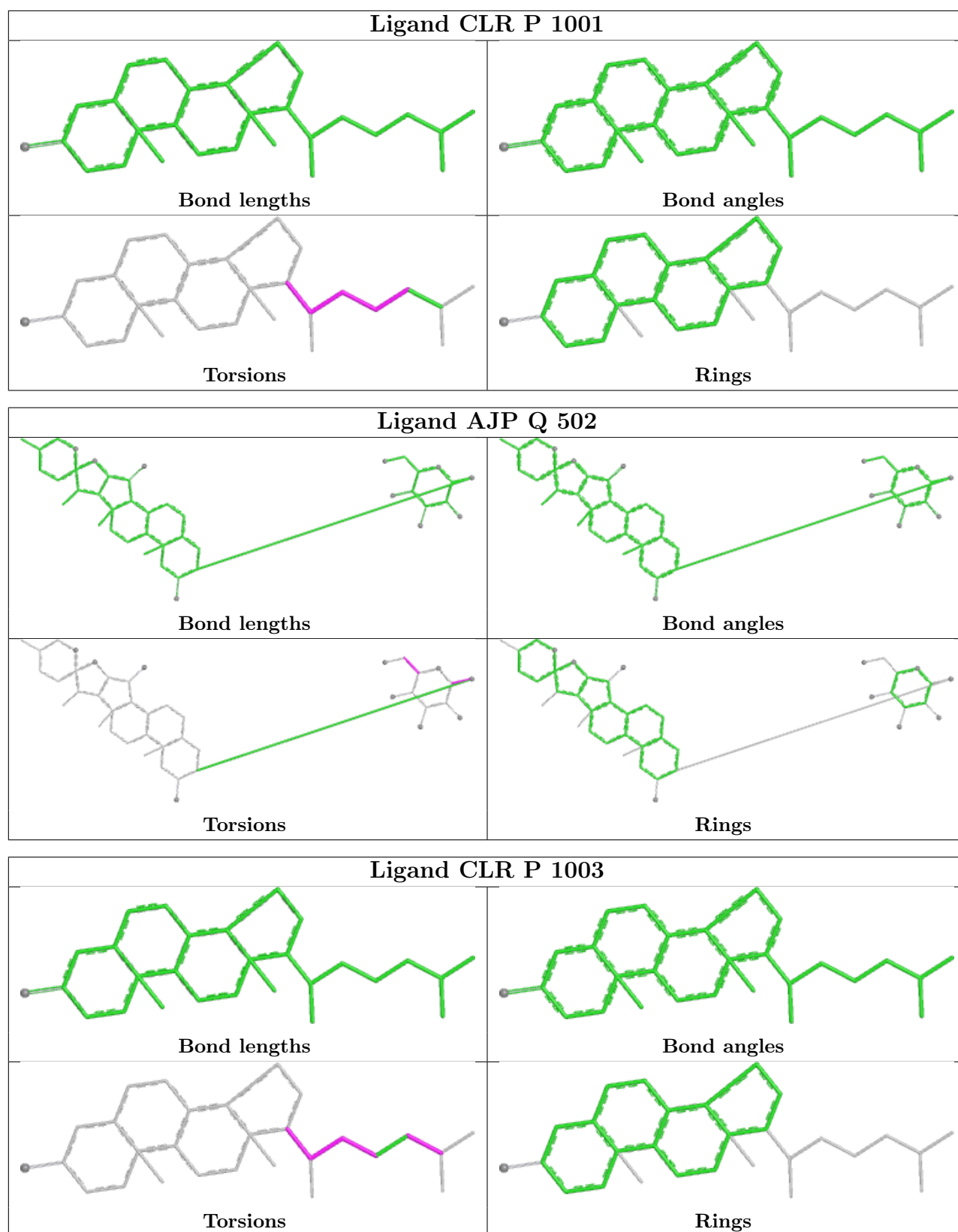
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	1006	PIO	16	0
7	O	1001	CLR	2	0
11	P	1005	PIO	15	0
10	O	1004	PLC	3	0
7	L	501	CLR	1	0
7	P	1001	CLR	2	0
8	Q	502	AJP	5	0
7	P	1003	CLR	12	0
7	O	1003	CLR	14	0
8	Q	501	AJP	2	0
10	P	1004	PLC	1	0
7	L	502	CLR	2	0

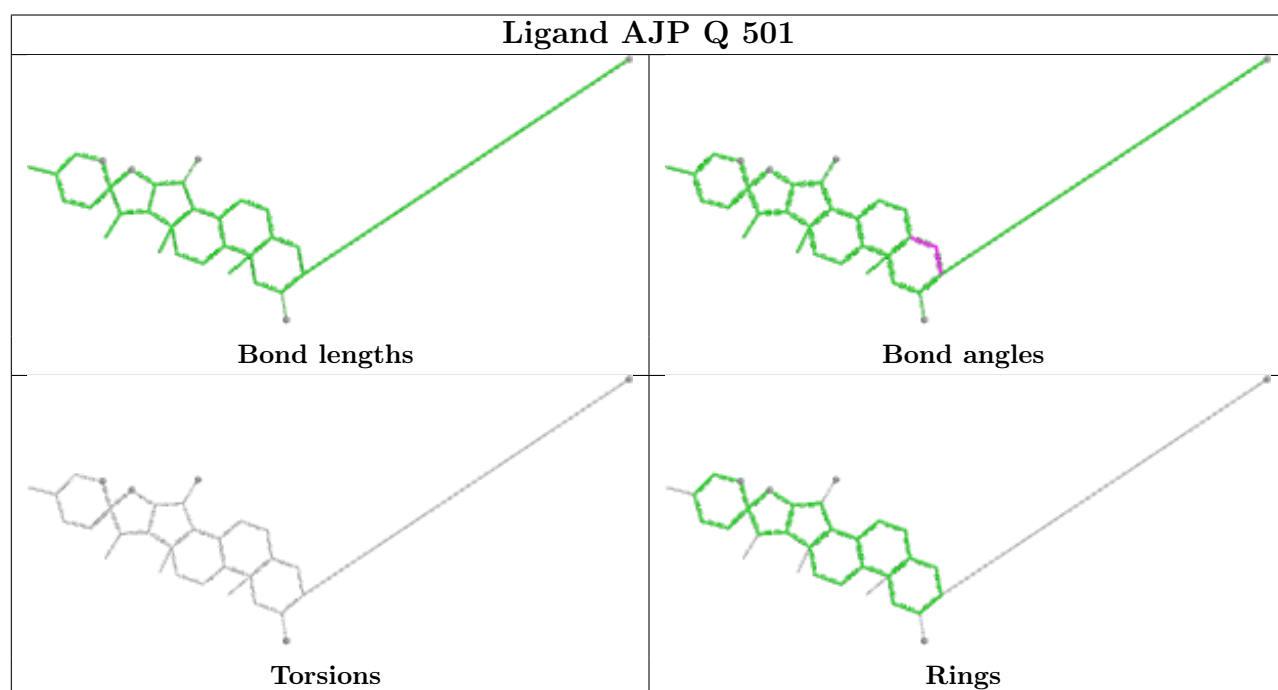
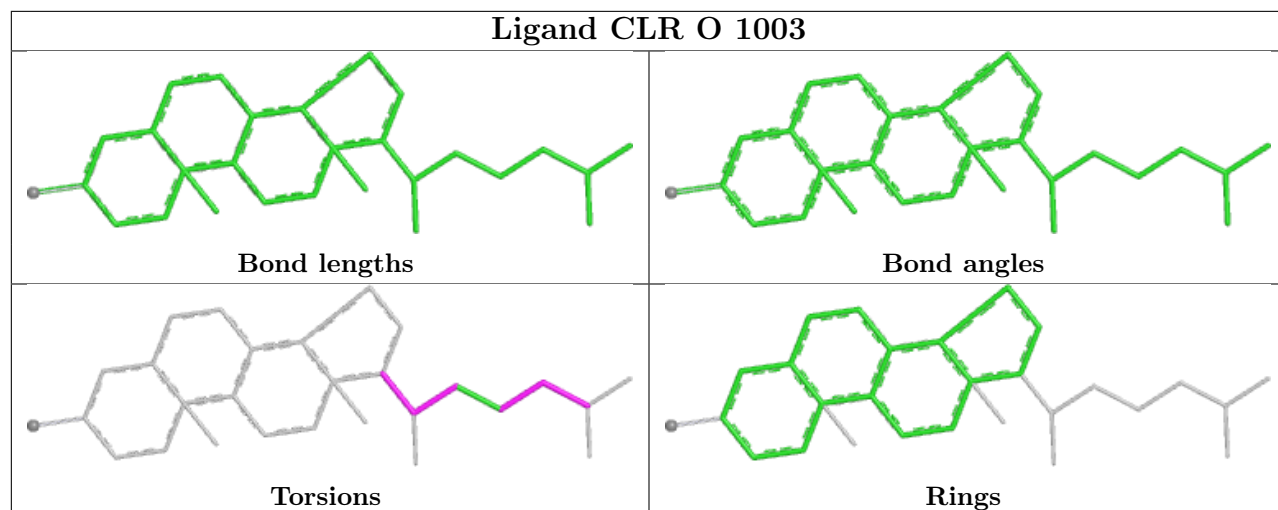
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

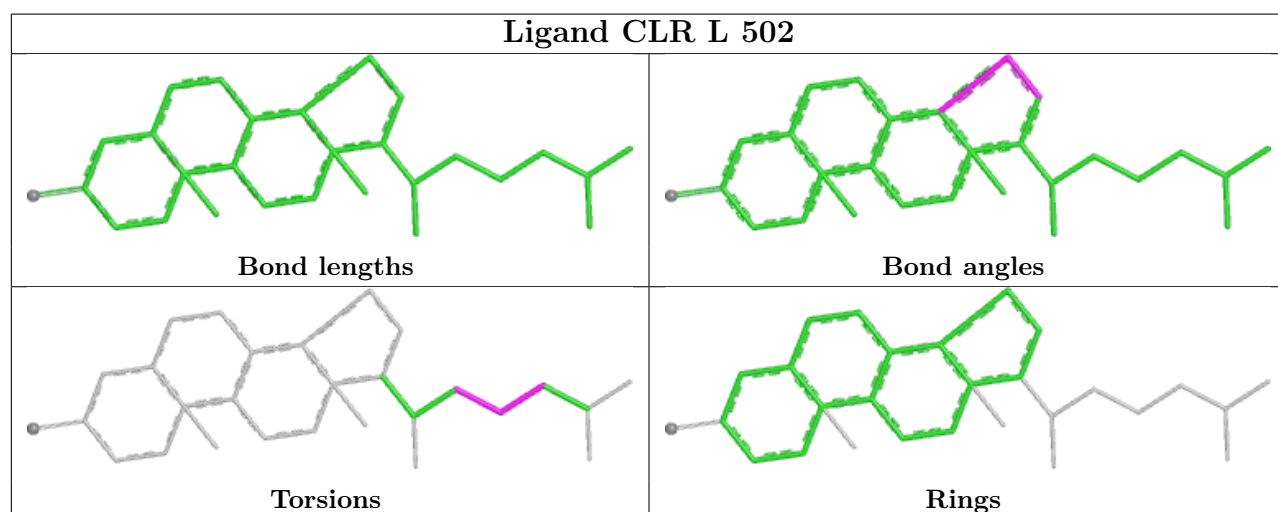
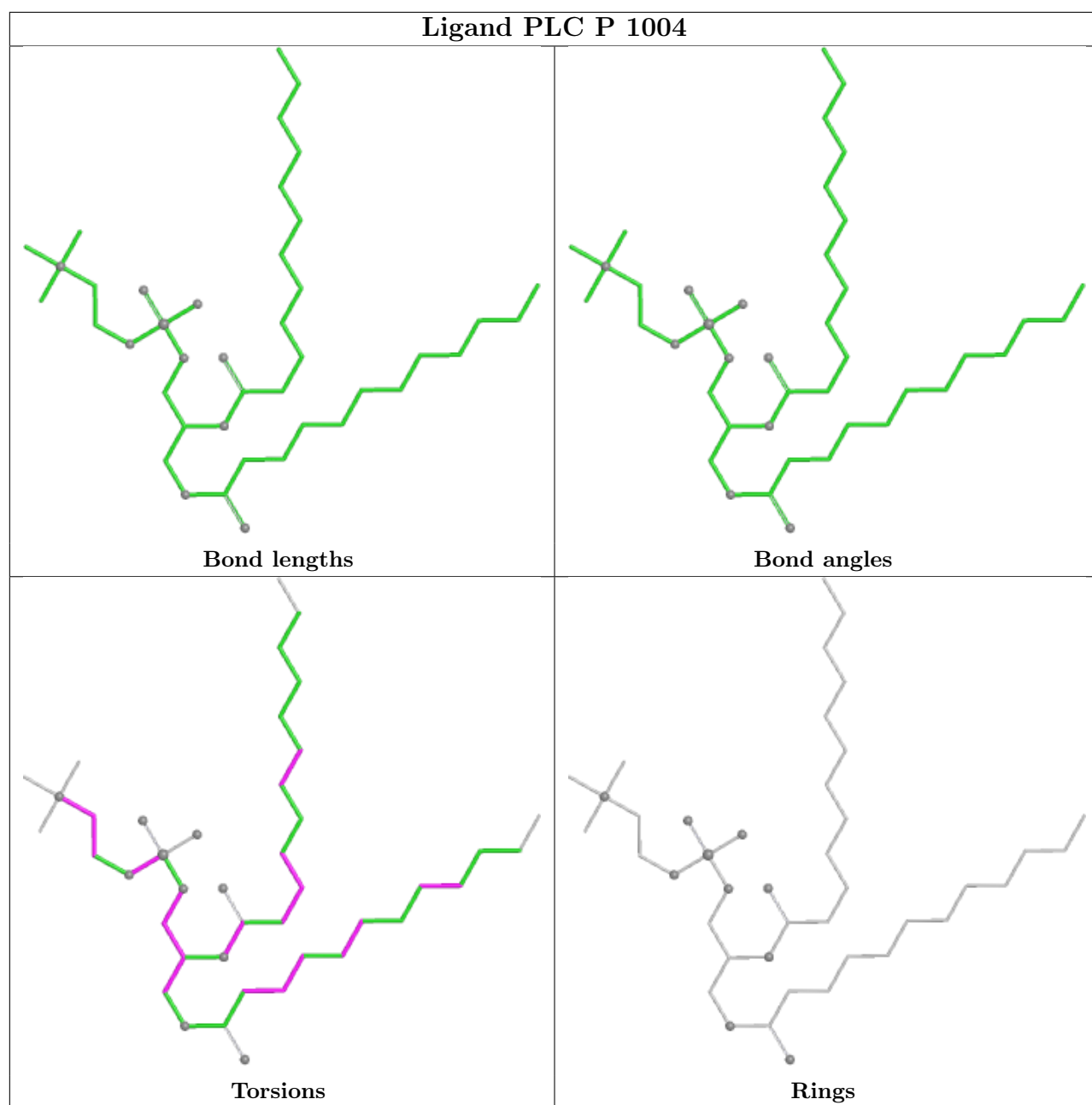












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

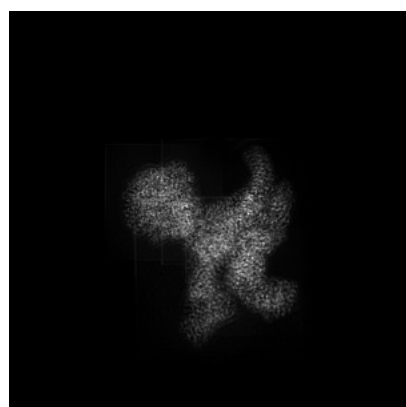
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26943. These allow visual inspection of the internal detail of the map and identification of artifacts.

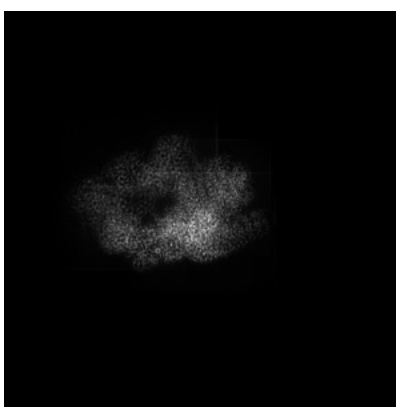
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

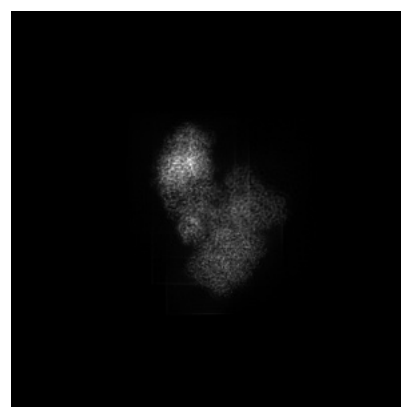
6.1.1 Primary map



X



Y



Z

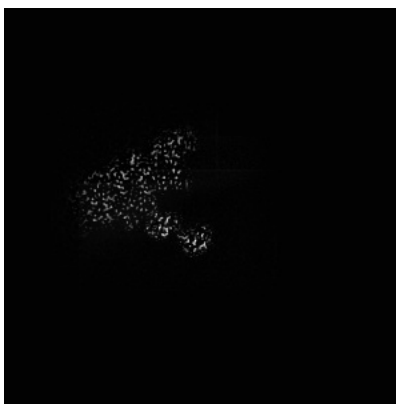
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

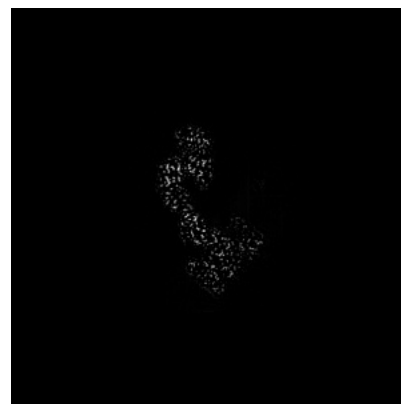
6.2.1 Primary map



X Index: 450



Y Index: 450



Z Index: 450

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

6.3 Largest variance slices [i](#)

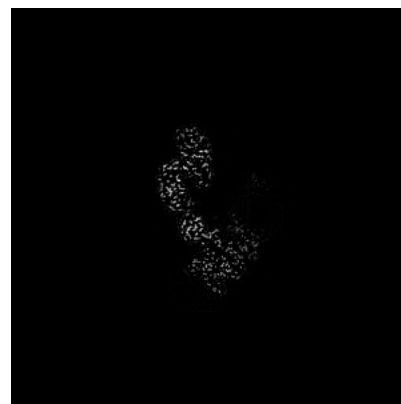
6.3.1 Primary map



X Index: 405



Y Index: 555

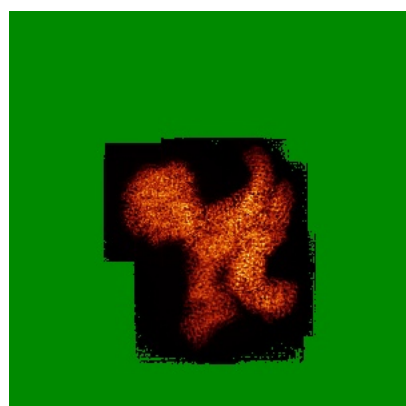


Z Index: 441

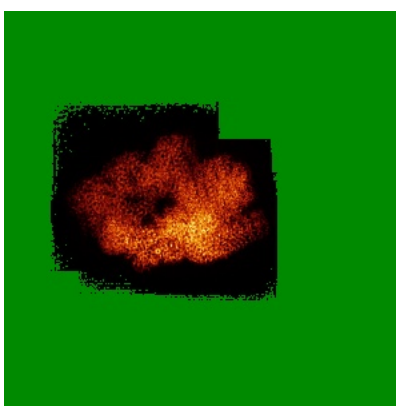
The images above show the largest variance slices of the map in three orthogonal directions.

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

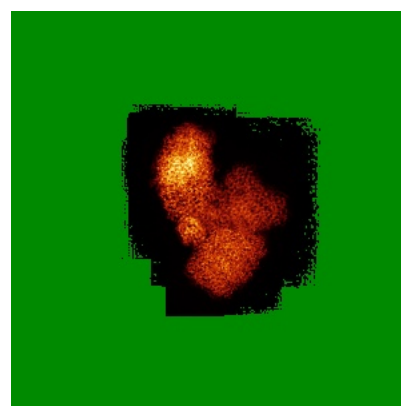
6.4.1 Primary map



X



Y

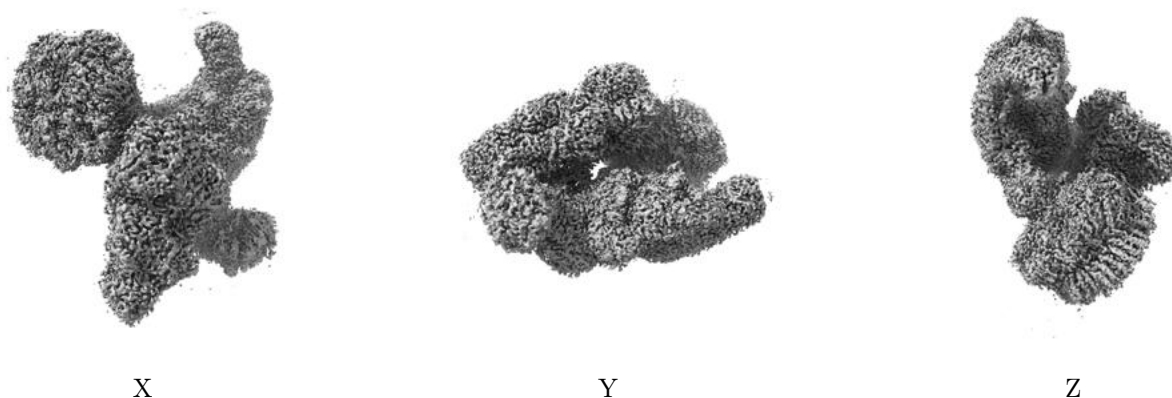


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

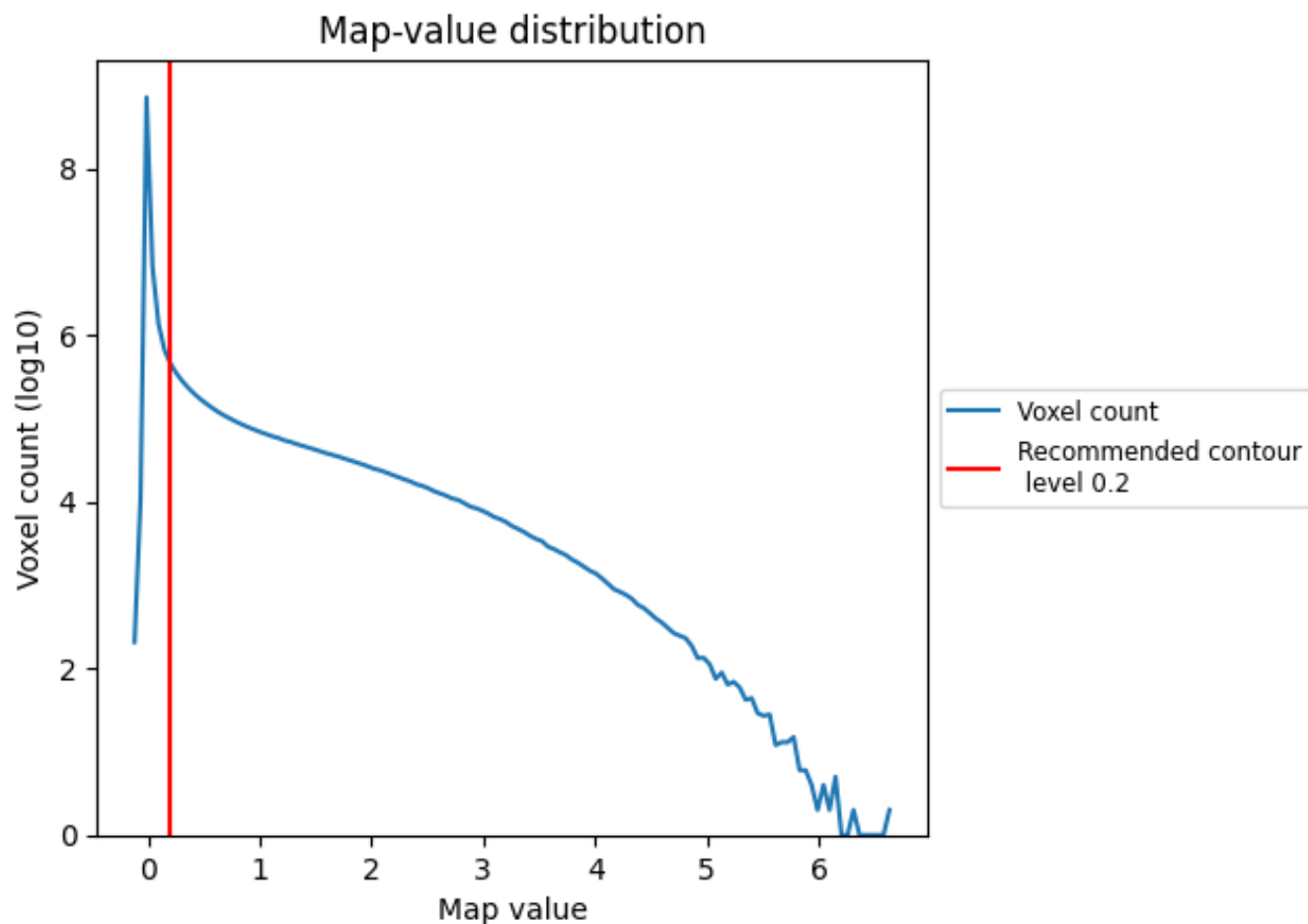
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

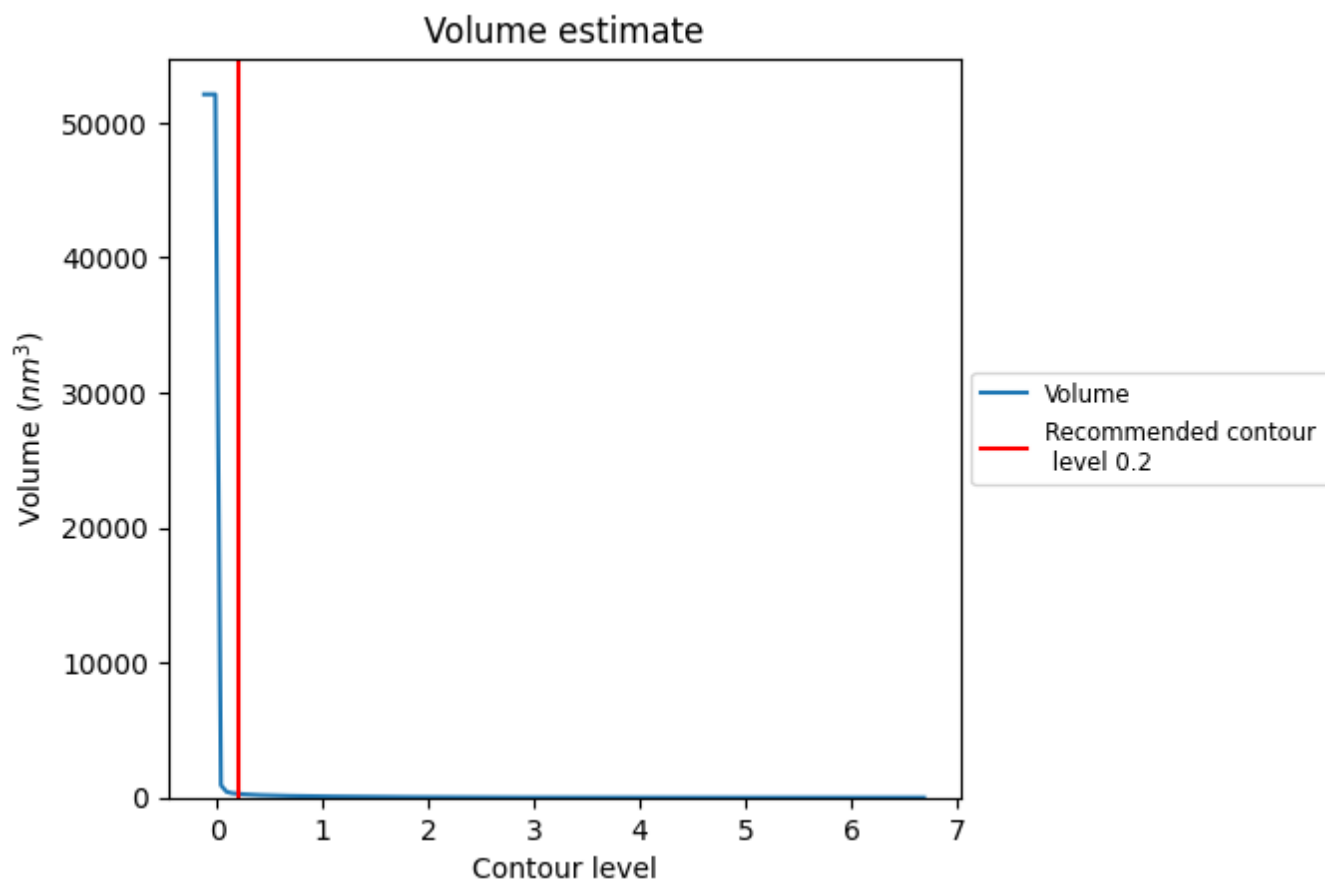
This section contains the results of statistical analysis of the map.

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.

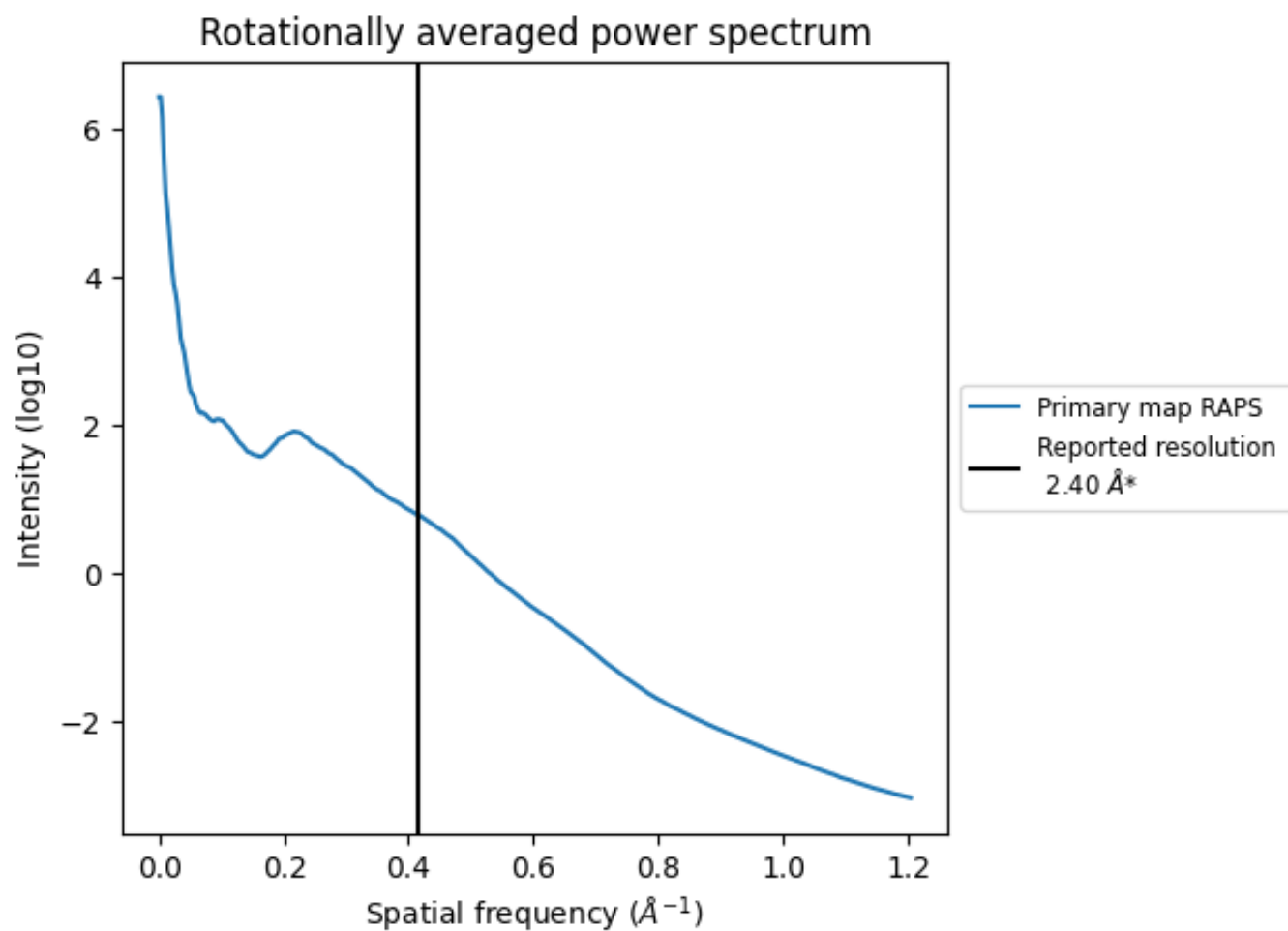
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 275 nm^3 ; this corresponds to an approximate mass of 249 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 ⓘ

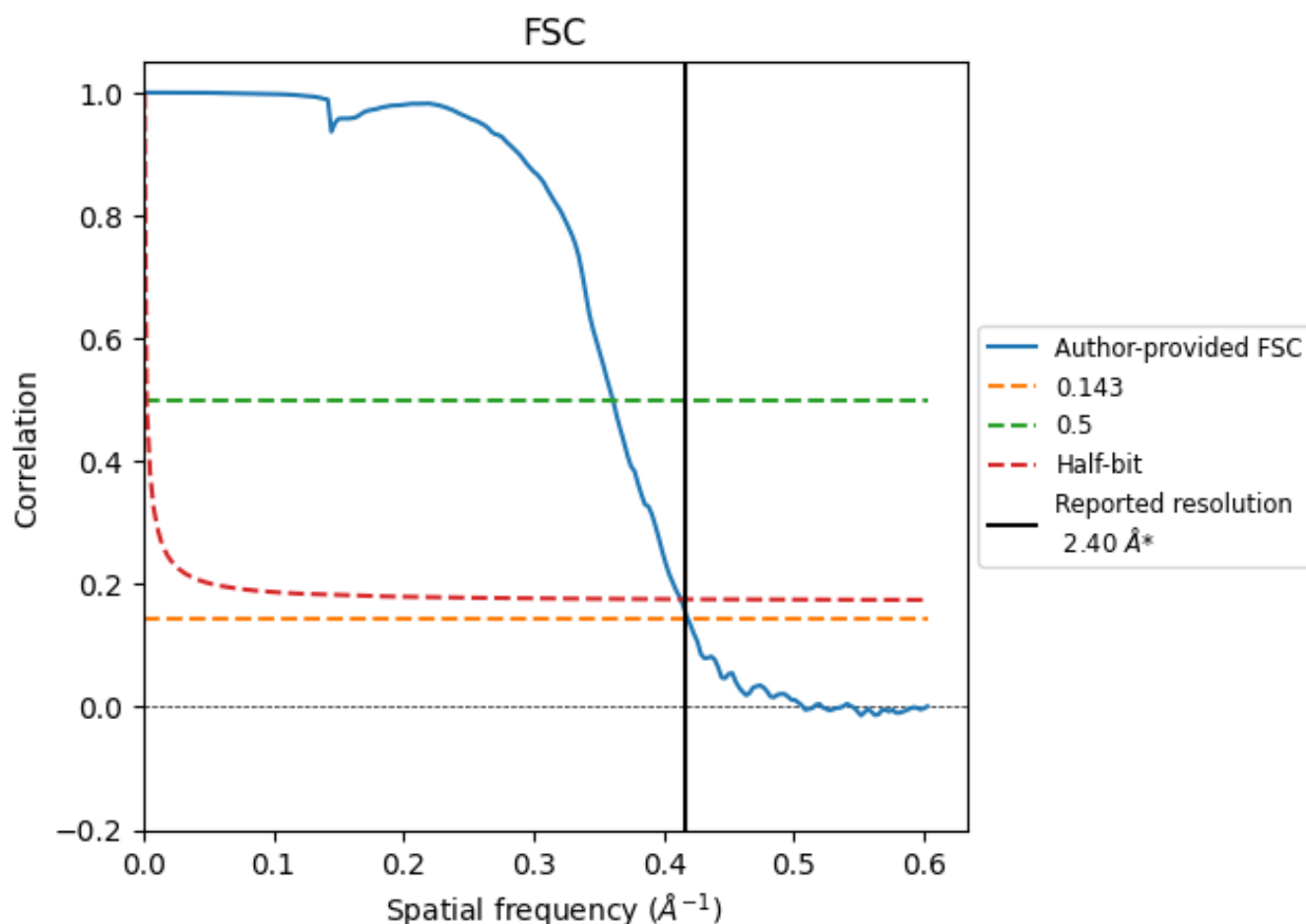


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.77	2.42
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

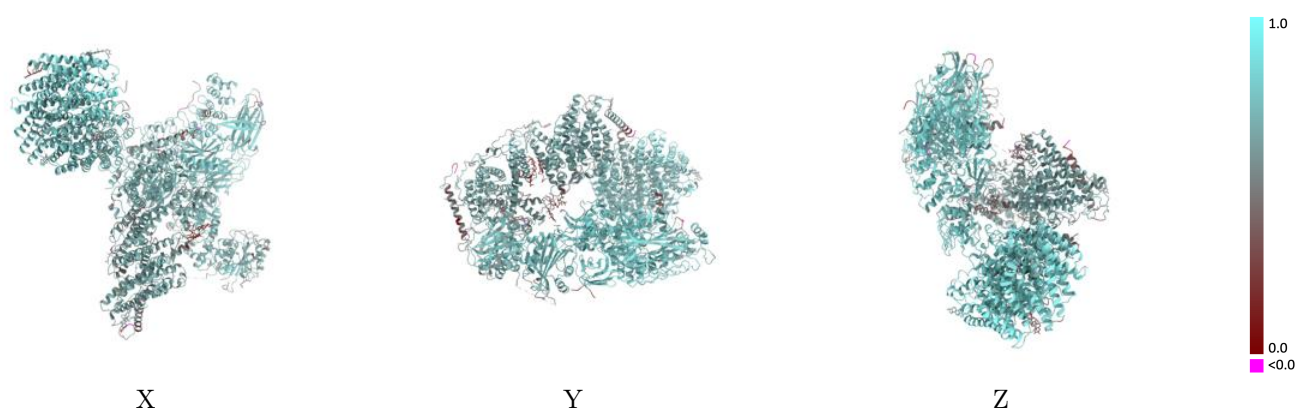
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26943 and PDB model 7V0K. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

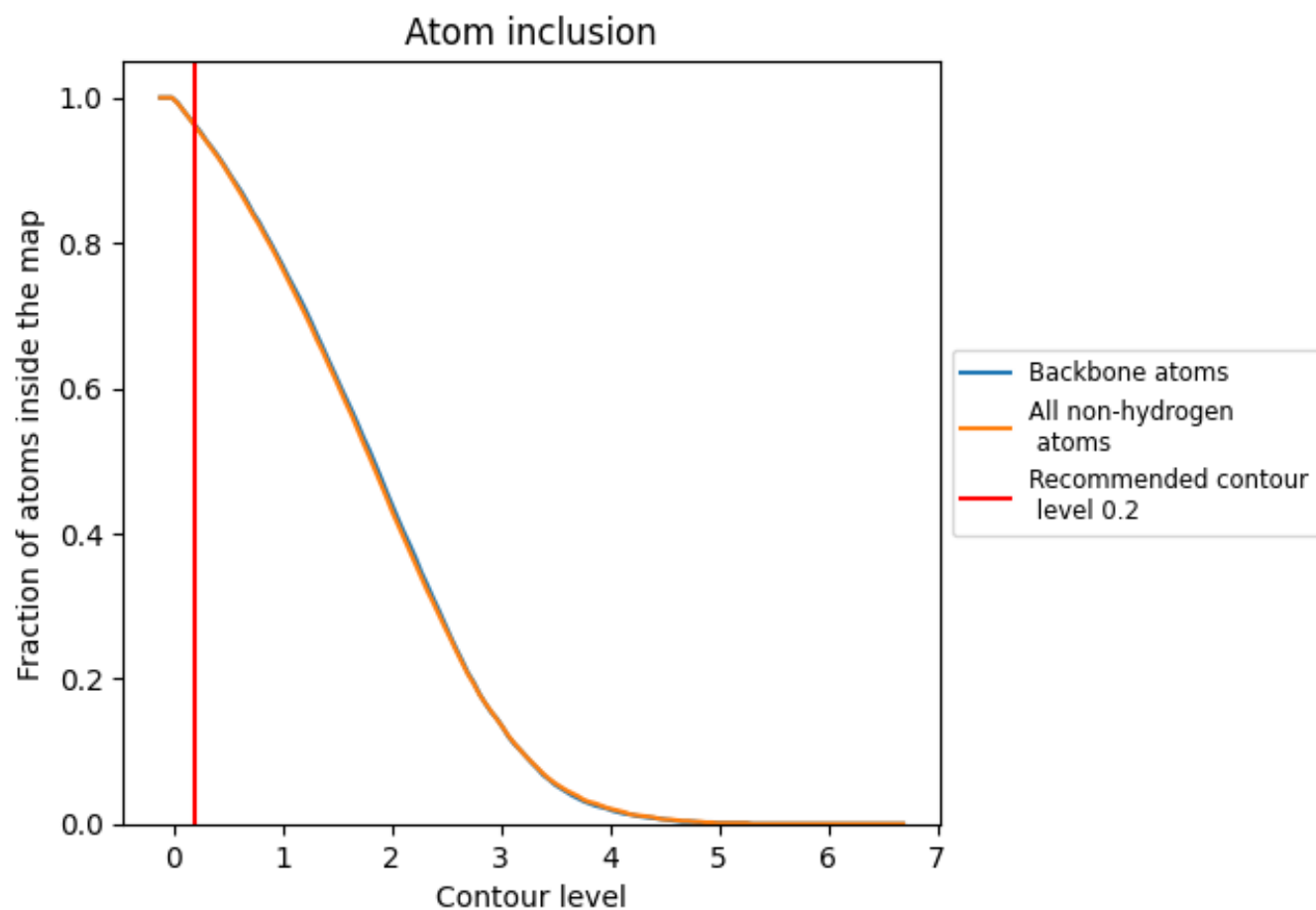


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.7030
D	0.7980	0.4420
H	0.9920	0.7510
K	0.9750	0.7460
L	0.9920	0.8060
N	0.6500	0.3790
O	0.9420	0.6240
P	0.9490	0.6390
Q	0.9840	0.7880
W	0.8360	0.6070
X	0.9760	0.7540

