



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:56 AM UTC

PDB ID : 7QHS / pdb_00007qhs
EMDB ID : EMD-13978
Title : S. cerevisiae CMGE nucleating origin DNA melting
Authors : Lewis, J.S.; Sousa, J.S.; Costa, A.
Deposited on : 2021-12-14
Resolution : 3.30 Å(reported)
Based on initial models : 6HV9, 6SKL

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:

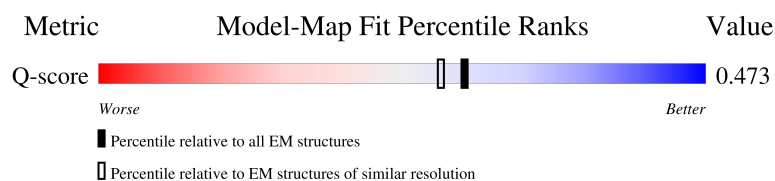
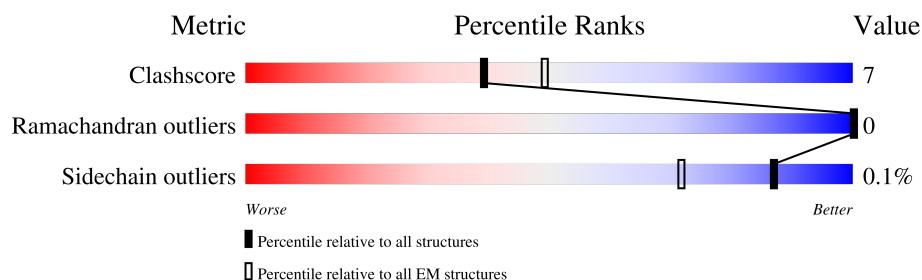
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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.



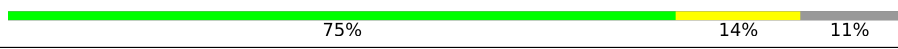
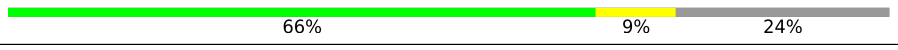
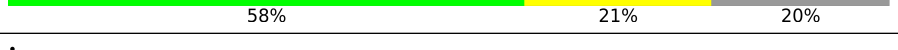
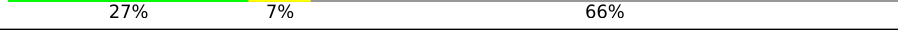
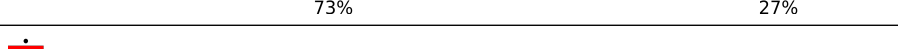
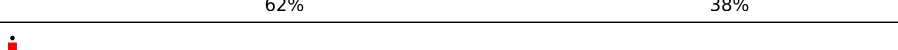
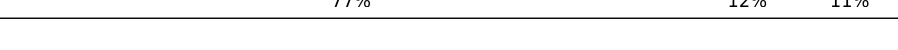
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	2	868	 66% 10% 24%
2	3	1006	 56% 7% 37%
3	4	933	 47% 18% 35%
4	6	1017	 52% 10% 38%

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Mol	Chain	Length	Quality of chain
5	7	845	
6	H	208	
7	I	213	
8	C	229	
9	D	294	
10	E	657	
11	F	689	
12	G	2222	
13	A	26	
14	B	26	
15	5	775	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 53670 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	660	Total	C	N	O	S	0	0
			5231	3284	937	991	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	633	Total	C	N	O	S	0	0
			4958	3119	882	944	13		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		

- Molecule 5 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	658	Total	C	N	O	S	0	0
			5181	3268	897	987	29		

- Molecule 6 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	208	Total	C	N	O	S	0	0
			1697	1065	290	332	10		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	189	Total	C	N	O	S	0	0
			1581	1018	277	282	4		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	173	Total	C	N	O	S	0	0
			1398	911	224	256	7		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	TRP	-	expression tag	UNP Q12146
C	-33	SER	-	expression tag	UNP Q12146
C	-32	HIS	-	expression tag	UNP Q12146
C	-31	PRO	-	expression tag	UNP Q12146
C	-30	GLN	-	expression tag	UNP Q12146
C	-29	PHE	-	expression tag	UNP Q12146
C	-28	GLU	-	expression tag	UNP Q12146
C	-27	LYS	-	expression tag	UNP Q12146
C	-26	GLY	-	expression tag	UNP Q12146
C	-25	GLY	-	expression tag	UNP Q12146
C	-24	GLY	-	expression tag	UNP Q12146
C	-23	SER	-	expression tag	UNP Q12146
C	-22	GLY	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	GLY	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	GLY	-	expression tag	UNP Q12146
C	-17	GLY	-	expression tag	UNP Q12146
C	-16	GLY	-	expression tag	UNP Q12146
C	-15	SER	-	expression tag	UNP Q12146
C	-14	TRP	-	expression tag	UNP Q12146
C	-13	SER	-	expression tag	UNP Q12146
C	-12	HIS	-	expression tag	UNP Q12146
C	-11	PRO	-	expression tag	UNP Q12146
C	-10	GLN	-	expression tag	UNP Q12146
C	-9	PHE	-	expression tag	UNP Q12146
C	-8	GLU	-	expression tag	UNP Q12146
C	-7	LYS	-	expression tag	UNP Q12146
C	-6	GLU	-	expression tag	UNP Q12146
C	-5	ASN	-	expression tag	UNP Q12146
C	-4	LEU	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP Q12146
C	-2	PHE	-	expression tag	UNP Q12146
C	-1	GLN	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 9 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	242	Total	C	N	O	S	0	0
			1990	1267	328	381	14		

- Molecule 10 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	566	Total	C	N	O	S	0	0
			4599	2937	778	870	14		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167G	TYR	GLU	conflict	UNP Q08032
E	167H	LYS	GLU	conflict	UNP Q08032
E	167J	ASP	GLU	conflict	UNP Q08032
E	167L	GLY	-	insertion	UNP Q08032
E	167M	ASP	-	insertion	UNP Q08032
E	167N	TYR	-	insertion	UNP Q08032
E	167O	LYS	-	insertion	UNP Q08032
E	167P	ASP	-	insertion	UNP Q08032
E	167Q	ASP	-	insertion	UNP Q08032
E	167R	ASP	-	insertion	UNP Q08032

- Molecule 11 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	551	Total	C	N	O	S	0	0
			4396	2819	755	804	18		

- Molecule 12 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	756	Total	C	N	O	S	0	0
			6113	3956	1006	1114	37		

- Molecule 13 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	26	Total	C	N	O	P	0	0
			546	260	130	130	26		

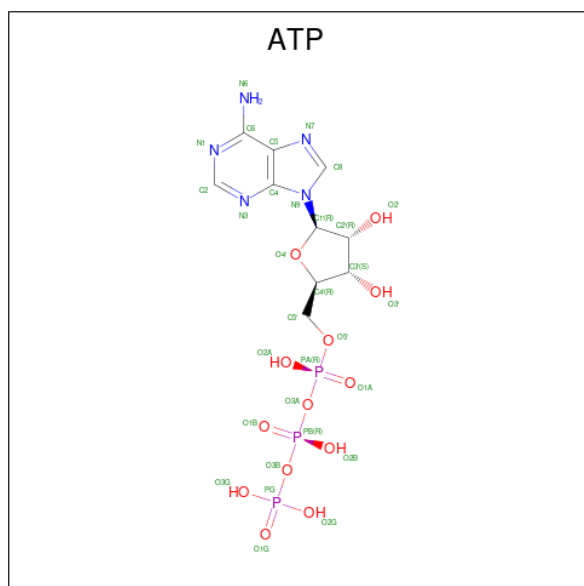
- Molecule 14 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	26	Total	C	N	O	P	0	0
			520	260	52	182	26		

- Molecule 15 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		

- Molecule 16 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
16	2	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
16	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	7	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

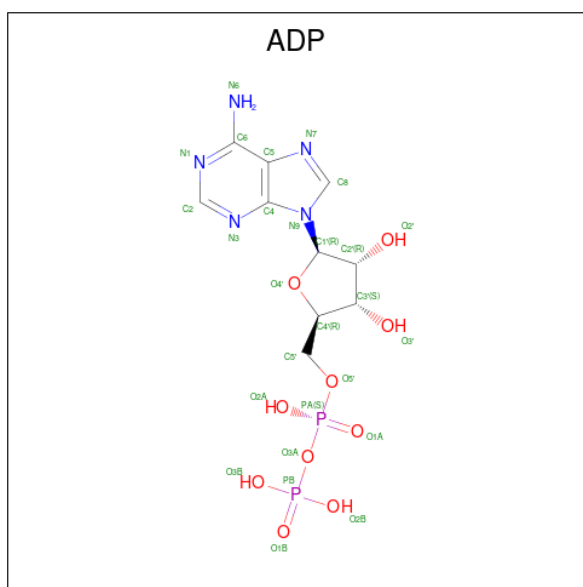
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	
17	G	2	Total	Zn	0
			2	2	
17	5	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	3	1	Total	Mg	0
			1	1	
18	7	1	Total	Mg	0
			1	1	
18	5	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

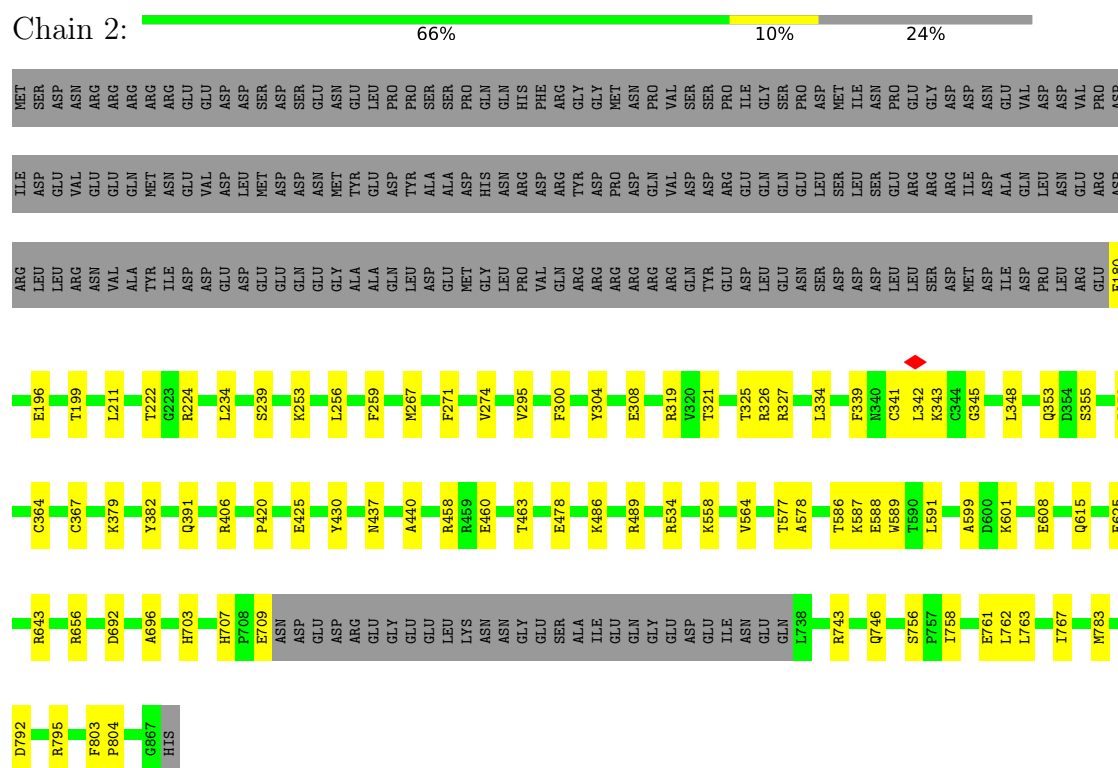


Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 27	C 10	N 5	O 10	P 2	0
19	6	1	Total 27	C 10	N 5	O 10	P 2	0

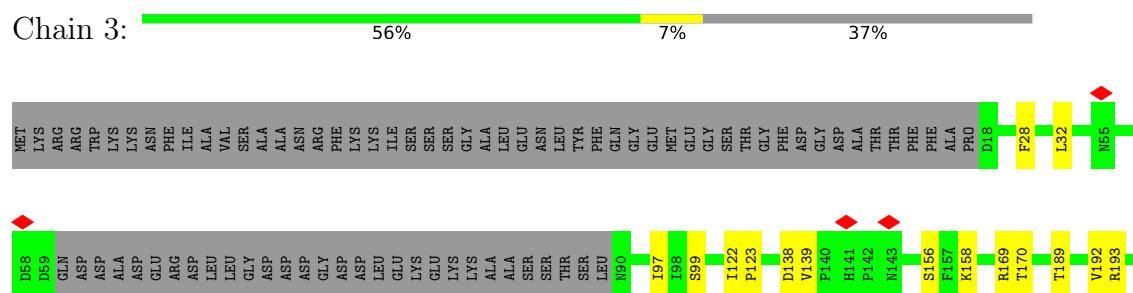
3 Residue-property plots

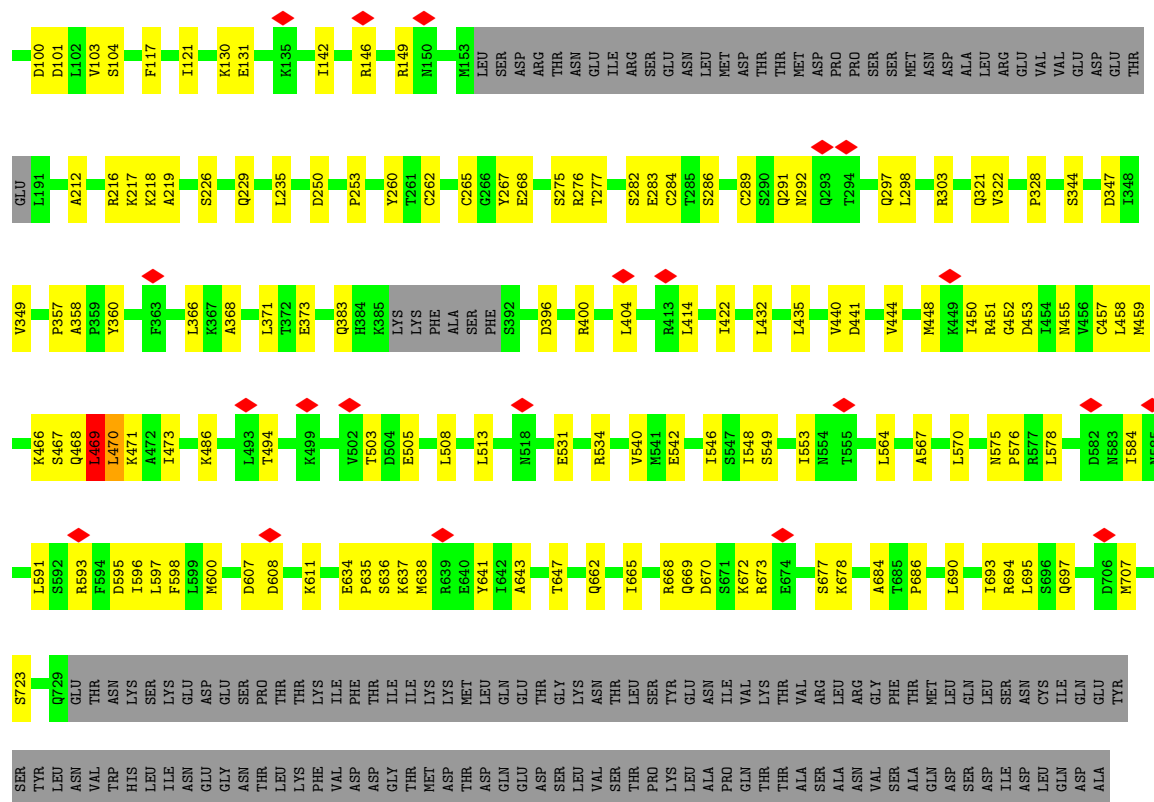
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA replication licensing factor MCM2

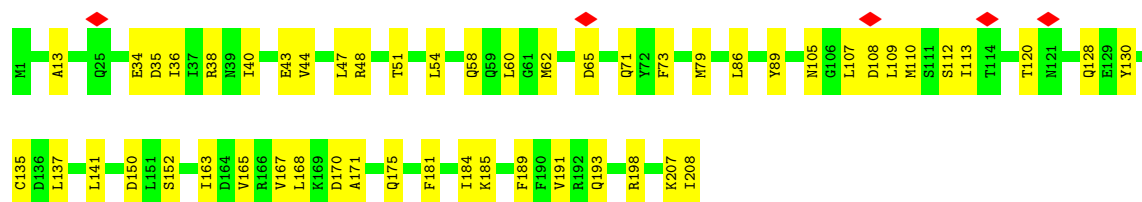
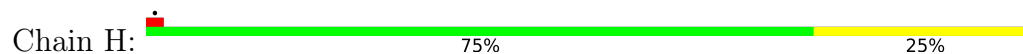


- Molecule 2: DNA replication licensing factor MCM3

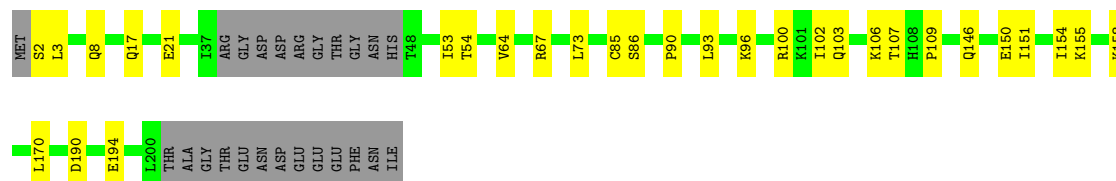




• Molecule 6: DNA replication complex GINS protein PSF1

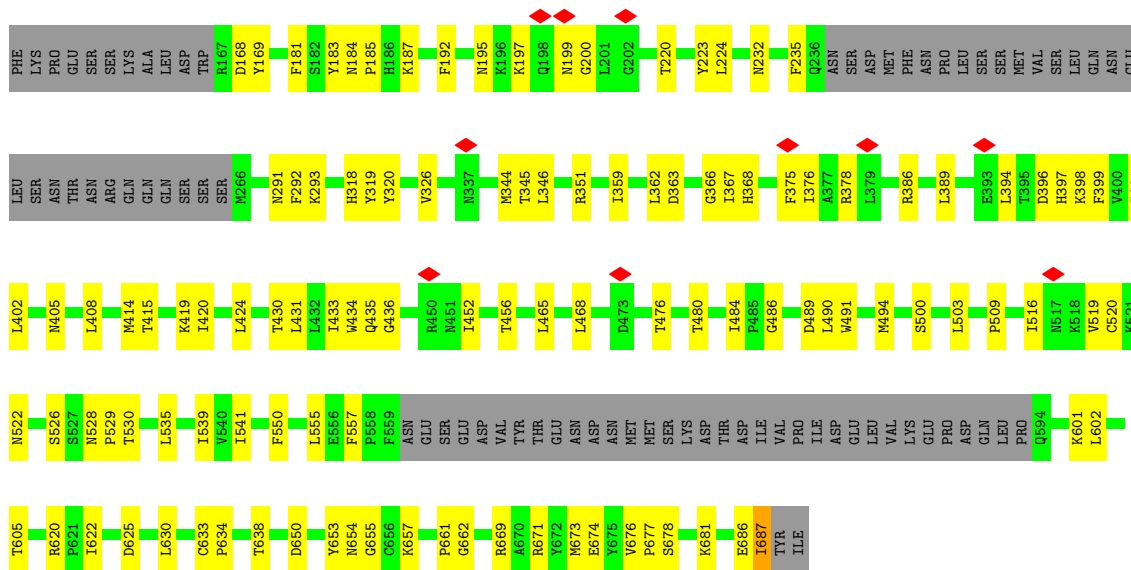


• Molecule 7: DNA replication complex GINS protein PSF2



• Molecule 8: DNA replication complex GINS protein PSF3





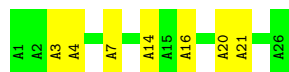
- Molecule 12: DNA polymerase epsilon catalytic subunit A



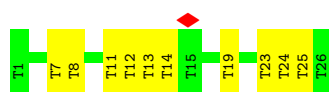
F1944	M1794	K1681	GLY	ALA	L1424	T1321	GLU	SER	ILE	ILE	MET	SER	GLY	GLU	VAL	SER	VAL	GLY	LEU	TRP	ARG	THR	LEU
E1952	L1795	L1687	LEU	SER	G1425	K1328	PRO	THR	ASP	ASP	VAL	LYS	THR	THR	CYS	GLU	VAL	GLY	TYR	TYR	TYR	THR	THR
M1956	E1797	E1691	GLN	SER	V1426	D1329	LEU	LEU	GLY	GLY	LYS	ASN	ASN	GLY	ASN	GLY	ASN	LEU	GLY	GLY	GLY	GLY	GLY
M1957	E1801	K1692	ILE	GLN	H1434	G1330	ASP	VAL	TYR	TYR	GLY	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
I1960	L1816	P1696	TYR	TYR	I1438	F1332	ASP	GLU	ARG	GLU	LEU	GLN	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
M1964	M1819	T1709	LYS	LYS	K1450	L1336	TYR	GLY	ARG	ARG	CYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
T1967	M1820	I1712	GLN	GLN	A1451	E1337	VAL	GLY	GLY	GLY	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
M1975	K1826	I1718	PHE	PHE	M1452	V1338	ILE	ILE	SER	SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
SER	L1827	F1718	LYS	LYS	E1464	F1339	ASN	ASN	ILE	ILE	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	F1828	I1721	LYS	LYS	M1465	V1346	TYR	GLY	GLN	GLN	SER	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
THR	V1836	V1726	GLY	GLY	K1466	H1352	ILE	ILE	ILE	ILE	PHE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLN	L1844	V1730	ILE	ILE	S1469	I1357	TRP	GLU	TRP	TRP	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ARG	E1850	V1731	THR	THR	R1475	Y1358	LYS	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
PRO	S1856	I1744	GLU	GLU	Y1476	M1359	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	GLN	I1744	SER	SER	F1480	K1360	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ILE	VAL	I1744	LEU	LEU	F1480	F1361	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ASN	Y1860	S1747	VAL	VAL	Y1486	K1362	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ASN	R1863	ALA	ASP	ASP	F1491	T1365	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
VAL	L1863	LEU	ILE	ILE	THR	M1366	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
LYS	K1869	ILE	ILE	ILE	THR	P1367	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
GLN	T1870	ASN	GLU	GLU	SER	L1368	ASP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
ASP	GLN	ALA	ASP	ASP	ILE	F1369	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LYS	ASP	ALA	ILE	ILE	GLY	K1370	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLU	GLY	GLY	ASN	ASN	TYR	I1371	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLU	P1875	SER	SER	SER	GLU	M1372	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
ASP	E1876	ASP	GLU	GLU	PHE	K1372	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LEU	K1887	LEU	PHE	PHE	PHE	C1374	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	VAL	VAL	VAL	VAL	SER	L1375	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	T1891	ASN	ASN	ASN	LEU	I1376	ASN	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
ASN	F1895	ASN	ASN	ASN	PHE	M1385	SER	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
F2002	L1898	MET	GLY	GLY	THR	S1390	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
S2004	D1899	ILE	ILE	ILE	TRP	N1391	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
F2007	Y1905	ASP	ASP	ASP	ASP	A1393	SER	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
S2008	M1906	ASP	ASP	ASP	THR	G1394	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
P2010	Y1933	LYS	LYS	LYS	ILE	G1395	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
R2014	M1946	ALA	ALA	ALA	ILE	Q1396	LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
L1920	VAL	VAL	VAL	VAL	LEU	L1397	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
V2039	L1920	ILE	ILE	ILE	VAL	I1400	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L2040	A1921	ASN	ASN	ASN	LEU	T1401	GLU	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
C1922	SER	SER	SER	SER	LYS	L1402	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S2043	K1928	SER	SER	SER	THR	P1403	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K2048	Y1933	LYS	LYS	LYS	ASN	G1404	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
N2049	VAL	VAL	VAL	VAL	GLN	S1405	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S2057	M1939	GLY	GLY	GLY	ALA	V1406	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	Q1940	ILE	ILE	ILE	GLN	E1409	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	L1941	ARG	ARG	ARG	ILE		SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER



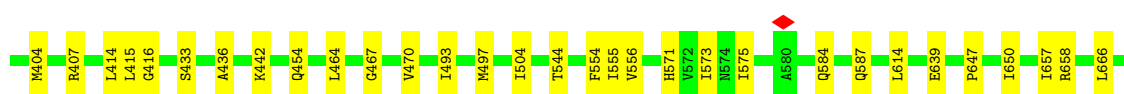
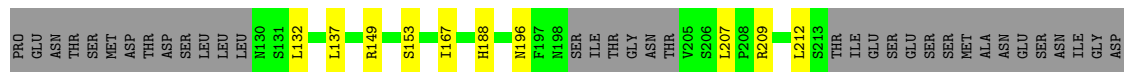
• Molecule 13: DNA (26-MER)



• Molecule 14: DNA (26-MER)



• Molecule 15: DNA replication licensing factor MCM5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.913	Depositor
Minimum map value	-0.926	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	221.40001, 209.52, 179.28001	wwPDB
Map dimensions	166, 194, 205	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: ZN, ATP, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.13	0/5319	0.36	0/7182
2	3	0.13	0/5044	0.35	0/6842
3	4	0.14	0/4921	0.40	0/6651
4	6	0.13	0/5051	0.37	0/6813
5	7	0.20	1/5261 (0.0%)	0.43	2/7110 (0.0%)
6	H	0.16	0/1719	0.41	0/2314
7	I	0.14	0/1613	0.37	0/2182
8	C	0.13	0/1431	0.32	0/1933
9	D	0.16	0/2032	0.38	0/2750
10	E	0.13	0/4685	0.34	0/6341
11	F	0.18	0/4492	0.45	0/6078
12	G	0.15	0/6250	0.41	0/8458
13	A	0.18	0/623	0.28	0/958
14	B	0.20	0/571	0.50	0/880
15	5	0.14	0/5530	0.37	0/7471
All	All	0.15	1/54542 (0.0%)	0.39	2/73963 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7	467	SER	CA-CB	-5.68	1.45	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	7	468	GLN	N-CA-C	-10.61	100.83	113.88
5	7	469	LEU	N-CA-C	-5.49	105.30	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5231	0	5280	60	0
2	3	4958	0	5005	43	0
3	4	4850	0	4926	119	0
4	6	4972	0	5007	70	0
5	7	5181	0	5258	107	0
6	H	1697	0	1698	39	0
7	I	1581	0	1635	21	0
8	C	1398	0	1418	13	0
9	D	1990	0	1985	27	0
10	E	4599	0	4603	56	0
11	F	4396	0	4442	105	0
12	G	6113	0	6177	101	0
13	A	546	0	287	5	0
14	B	520	0	313	8	0
15	5	5450	0	5510	61	0
16	2	31	0	12	0	0
16	3	31	0	12	0	0
16	5	31	0	12	0	0
16	7	31	0	12	1	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
17	G	2	0	0	0	0
18	3	1	0	0	0	0
18	5	1	0	0	0	0
18	7	1	0	0	0	0
19	4	27	0	12	0	0
19	6	27	0	12	4	0
All	All	53670	0	53616	770	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 (770) 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)
11:F:526:SER:HB2	11:F:530:THR:HG21	1.48	0.91
12:G:1438:ILE:HD11	12:G:1658:ILE:HG23	1.56	0.87
2:3:652:THR:HG22	2:3:654:PRO:HD2	1.59	0.85
12:G:1649:LEU:HB3	12:G:1660:ILE:HD11	1.65	0.79
12:G:1726:VAL:HG11	12:G:1964:MET:HE1	1.68	0.75
11:F:169:TYR:OH	11:F:368:HIS:ND1	2.20	0.75
3:4:333:LEU:HD12	3:4:398:LYS:HZ2	1.53	0.74
12:G:1357:ILE:HD12	12:G:1359:MET:HE3	1.70	0.73
6:H:60:LEU:HB3	6:H:62:MET:HE2	1.70	0.73
3:4:637:MET:HE3	3:4:642:ARG:HG2	1.71	0.73
9:D:98:ILE:HG23	9:D:126:LEU:HD11	1.70	0.72
1:2:339:PHE:HB2	1:2:348:LEU:HD12	1.72	0.71
10:E:615:GLU:HG3	10:E:616:THR:HG23	1.71	0.71
6:H:35:ASP:HA	6:H:38:ARG:HE	1.56	0.71
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.74	0.70
11:F:662:GLY:O	11:F:671:ARG:NH2	2.24	0.70
5:7:368:ALA:HB1	5:7:371:LEU:HB2	1.73	0.70
11:F:351:ARG:HG2	11:F:654:ASN:HB3	1.74	0.69
12:G:2166:ARG:NH1	12:G:2182:ALA:O	2.25	0.69
1:2:577:THR:HG22	1:2:578:ALA:H	1.57	0.69
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.58	0.69
3:4:407:PRO:HG2	3:4:410:GLN:HG3	1.73	0.69
3:4:234:ARG:O	3:4:234:ARG:NH1	2.24	0.69
10:E:1:MET:HE2	10:E:149:ASP:HA	1.75	0.68
11:F:401:ILE:HG13	11:F:433:ILE:HD12	1.75	0.68
12:G:2180:PRO:O	15:5:685:GLN:NE2	2.27	0.68
15:5:400:LEU:HD12	15:5:404:MET:HB3	1.73	0.68
11:F:528:ASN:HB3	11:F:529:PRO:HD3	1.74	0.68
4:6:151:ILE:HD11	4:6:265:ILE:HG12	1.75	0.68
12:G:1676:TYR:HA	12:G:1794:MET:HE1	1.74	0.68
4:6:318:VAL:HG21	4:6:330:PRO:HG3	1.76	0.67
3:4:210:ASP:OD1	3:4:211:GLU:N	2.28	0.66
5:7:494:THR:HG21	5:7:546:ILE:HG21	1.78	0.66
3:4:522:LEU:HD12	3:4:811:MET:HE1	1.77	0.66
5:7:457:CYS:HB3	5:7:597:LEU:HD13	1.76	0.66
4:6:270:LEU:HD12	4:6:289:SER:HB3	1.76	0.66
12:G:1362:LYS:O	12:G:1396:GLN:NE2	2.28	0.66
13:A:7:DA:N6	14:B:19:DT:O4	2.29	0.66
12:G:1385:ASN:ND2	12:G:1782:ALA:O	2.28	0.66
15:5:188:HIS:NE2	15:5:212:LEU:O	2.28	0.66
4:6:689:TYR:HA	4:6:698:ASN:HD21	1.61	0.66
5:7:358:ALA:HB3	5:7:373:GLU:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:493:ILE:HG22	15:5:497:MET:HG3	1.78	0.65
3:4:207:LYS:HE3	3:4:215:PHE:HB2	1.79	0.64
10:E:148:VAL:HG22	10:E:152:LEU:HD12	1.77	0.64
7:I:2:SER:OG	7:I:3:LEU:N	2.29	0.64
5:7:262:CYS:O	5:7:265:CYS:N	2.24	0.64
10:E:422:SER:O	10:E:426:GLU:HG2	1.97	0.64
11:F:183:TYR:HD1	11:F:224:LEU:HD22	1.62	0.64
2:3:698:THR:HG22	2:3:699:ALA:H	1.61	0.64
11:F:345:THR:HG22	11:F:346:LEU:H	1.61	0.64
2:3:169:ARG:NH1	2:3:269:GLN:OE1	2.30	0.64
1:2:353:GLN:HA	1:2:359:ILE:HD11	1.80	0.64
6:H:175:GLN:HE21	11:F:35:SER:HA	1.63	0.64
10:E:244:GLY:HA3	10:E:602:LEU:HB3	1.79	0.63
11:F:539:ILE:HG12	11:F:638:THR:HB	1.78	0.63
5:7:262:CYS:SG	5:7:284:CYS:HB3	2.37	0.63
12:G:2164:CYS:HB3	12:G:2167:CYS:O	1.99	0.63
11:F:386:ARG:HD3	11:F:389:LEU:HD12	1.81	0.63
11:F:480:THR:HG23	11:F:522:ASN:HB3	1.78	0.63
3:4:246:ARG:HH21	3:4:249:LEU:HD22	1.63	0.63
3:4:797:GLN:O	3:4:801:MET:HG3	1.99	0.63
3:4:583:LYS:HE3	3:4:583:LYS:HA	1.79	0.63
5:7:212:ALA:O	5:7:216:ARG:N	2.32	0.62
7:I:190:ASP:O	7:I:194:GLU:HG3	1.99	0.62
11:F:633:CYS:HB3	11:F:634:PRO:HD3	1.81	0.62
6:H:113:ILE:HG21	11:F:77:LEU:HD11	1.81	0.62
3:4:284:ILE:HG13	3:4:285:VAL:HG13	1.81	0.62
2:3:700:ARG:NH2	16:7:901:ATP:O3G	2.32	0.62
8:C:181:HIS:O	8:C:185:LYS:HG3	1.99	0.62
5:7:284:CYS:SG	5:7:289:CYS:HB3	2.39	0.62
3:4:607:ARG:NH1	4:6:616:GLU:OE2	2.33	0.61
10:E:503:GLN:OE1	10:E:547:ARG:NH1	2.33	0.61
3:4:812:LYS:O	3:4:814:LYS:HG3	2.00	0.61
2:3:308:GLN:OE1	15:5:209:ARG:NH1	2.29	0.61
5:7:82:LEU:HD23	5:7:103:VAL:HG23	1.82	0.61
6:H:58:GLN:NE2	6:H:65:ASP:OD1	2.34	0.61
1:2:587:LYS:NZ	14:B:12:DT:O3'	2.33	0.61
12:G:1333:PRO:HB2	12:G:1404:GLU:HB3	1.82	0.61
5:7:578:LEU:HD22	5:7:678:LYS:HB3	1.82	0.61
2:3:236:THR:OG1	2:3:237:GLU:OE2	2.19	0.61
6:H:163:ILE:HD13	6:H:193:GLN:HG3	1.83	0.61
3:4:454:LYS:HA	5:7:277:THR:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1345:LYS:HG2	12:G:1346:VAL:H	1.65	0.61
11:F:82:SER:O	11:F:85:LYS:N	2.33	0.60
3:4:796:ARG:NH1	19:6:1201:ADP:O3'	2.34	0.60
5:7:670:ASP:OD1	5:7:673:ARG:NH1	2.34	0.60
11:F:326:VAL:HG11	11:F:344:MET:HE2	1.83	0.60
2:3:384:MET:HE1	2:3:513:ILE:HB	1.82	0.60
11:F:500:SER:OG	11:F:620:ARG:NH1	2.29	0.60
1:2:319:ARG:NE	1:2:425:GLU:OE1	2.30	0.60
11:F:405:ASN:H	11:F:436:GLY:HA3	1.65	0.60
3:4:569:ASP:OD2	3:4:710:ASP:N	2.34	0.60
2:3:189:THR:O	2:3:456:ARG:NH1	2.35	0.60
11:F:431:LEU:HD23	11:F:480:THR:HB	1.84	0.60
3:4:711:LYS:HD3	3:4:712:VAL:H	1.66	0.59
4:6:134:LYS:HG2	4:6:137:ARG:HD3	1.84	0.59
10:E:106:ASP:HB2	10:E:115:SER:HB3	1.83	0.59
11:F:168:ASP:OD1	11:F:169:TYR:N	2.34	0.59
12:G:2205:ALA:HB2	12:G:2213:LEU:HD23	1.84	0.59
3:4:370:ARG:HE	3:4:379:PRO:HG3	1.67	0.59
5:7:92:LYS:HD2	5:7:97:THR:HB	1.85	0.59
8:C:38:ILE:HD11	8:C:42:THR:HG21	1.84	0.59
11:F:486:GLY:N	11:F:489:ASP:OD2	2.34	0.59
4:6:143:MET:HG2	4:6:148:LEU:HB2	1.84	0.59
6:H:73:PHE:HE2	8:C:57:VAL:HG11	1.68	0.59
15:5:704:SER:HB2	15:5:707:SER:HB2	1.84	0.59
4:6:608:LEU:HD23	4:6:652:ILE:HD11	1.85	0.58
10:E:124:ASP:OD1	10:E:125:ALA:N	2.36	0.58
5:7:584:ILE:HD11	5:7:591:LEU:HD11	1.85	0.58
7:I:53:ILE:HB	9:D:90:ARG:HD3	1.84	0.58
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.36	0.58
11:F:676:VAL:HG12	11:F:678:SER:H	1.67	0.58
3:4:510:ARG:NH2	3:4:753:TYR:OH	2.37	0.58
12:G:1465:MET:O	12:G:1469:SER:OG	2.22	0.58
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.86	0.58
11:F:291:ASN:OD1	11:F:292:PHE:N	2.35	0.58
3:4:281:VAL:HA	3:4:284:ILE:HG12	1.86	0.58
3:4:370:ARG:NH1	3:4:377:ASN:OD1	2.37	0.58
3:4:382:MET:HA	3:4:382:MET:HE2	1.86	0.58
3:4:762:ILE:HA	3:4:817:VAL:HG22	1.86	0.58
12:G:1352:HIS:HB2	12:G:1464:GLU:HA	1.84	0.58
3:4:194:PHE:CE1	3:4:272:MET:HE1	2.39	0.57
5:7:451:ARG:HG2	5:7:453:ASP:H	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:458:LEU:HB3	5:7:600:MET:HE1	1.86	0.57
11:F:46:GLY:HA2	11:F:49:ILE:HB	1.84	0.57
11:F:359:ILE:HG12	11:F:362:LEU:HD12	1.86	0.57
1:2:325:THR:HG22	1:2:326:ARG:HG3	1.86	0.57
5:7:459:MET:HE2	5:7:597:LEU:HD12	1.86	0.57
12:G:1336:LEU:HD11	12:G:1434:HIS:HA	1.86	0.57
10:E:89:VAL:HG23	10:E:90:ILE:HG23	1.86	0.57
4:6:134:LYS:HB3	4:6:137:ARG:HB2	1.87	0.57
4:6:644:MET:HE1	4:6:652:ILE:HD12	1.87	0.57
4:6:581:LYS:NZ	4:6:682:ALA:O	2.37	0.57
12:G:2117:ILE:HD11	12:G:2127:ILE:HA	1.86	0.57
5:7:68:GLN:O	5:7:72:ASN:ND2	2.38	0.57
5:7:597:LEU:O	5:7:723:SER:OG	2.23	0.57
12:G:1376:ILE:HG22	12:G:1400:ILE:HG23	1.87	0.57
15:5:167:ILE:HD11	15:5:257:LYS:HE3	1.87	0.56
6:H:36:ILE:O	6:H:40:ILE:HD12	2.05	0.56
12:G:1374:CYS:HB3	12:G:1402:LEU:HD12	1.87	0.56
2:3:665:GLU:HG3	2:3:666:ARG:HG2	1.87	0.56
6:H:86:LEU:HB3	9:D:198:ILE:HD13	1.88	0.56
8:C:126:GLU:OE2	8:C:130:GLN:NE2	2.29	0.56
11:F:31:LEU:HD11	11:F:77:LEU:HD23	1.87	0.56
11:F:601:LYS:O	11:F:605:THR:HG23	2.05	0.56
7:I:151:ILE:HG23	15:5:104:LEU:HD21	1.86	0.56
11:F:319:TYR:HB2	11:F:605:THR:HG21	1.88	0.56
7:I:90:PRO:HD2	7:I:93:LEU:HD12	1.86	0.56
11:F:398:LYS:O	11:F:430:THR:N	2.32	0.56
10:E:2:TYR:OH	10:E:138:GLN:OE1	2.24	0.56
3:4:767:LYS:HE2	4:6:732:VAL:HG13	1.88	0.56
12:G:1435:GLN:HA	12:G:1438:ILE:HG22	1.87	0.55
2:3:570:ARG:NH1	15:5:614:LEU:O	2.39	0.55
10:E:21:SER:O	10:E:55:GLN:NE2	2.39	0.55
10:E:267:LEU:HD13	10:E:316:LEU:HD22	1.88	0.55
11:F:399:PHE:HE1	11:F:677:PRO:HG3	1.70	0.55
15:5:718:LEU:HD21	15:5:761:ILE:HD11	1.88	0.55
1:2:379:LYS:HD2	1:2:379:LYS:O	2.07	0.55
1:2:792:ASP:OD1	1:2:795:ARG:NH2	2.39	0.55
2:3:233:THR:HG23	2:3:234:GLU:HG2	1.89	0.55
11:F:491:TRP:HZ3	12:G:2147:ILE:HG21	1.71	0.55
5:7:101:ASP:OD2	5:7:104:SER:OG	2.25	0.55
12:G:1637:ASN:OD1	12:G:1638:HIS:N	2.40	0.55
12:G:1797:GLU:O	12:G:1801:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1967:THR:HG21	12:G:2003:PHE:HB3	1.89	0.54
7:I:150:GLU:O	7:I:154:ILE:HG13	2.07	0.54
1:2:222:THR:HG23	1:2:224:ARG:HG3	1.89	0.54
1:2:743:ARG:HA	1:2:746:GLN:HG2	1.89	0.54
3:4:525:SER:HA	3:4:742:LEU:HD22	1.89	0.54
3:4:193:ASN:HB3	3:4:254:THR:HG22	1.89	0.54
4:6:608:LEU:HD12	4:6:627:ALA:HB3	1.89	0.54
5:7:451:ARG:O	5:7:694:ARG:NH1	2.39	0.54
6:H:40:ILE:HA	6:H:43:GLU:HG2	1.89	0.54
1:2:300:PHE:O	1:2:319:ARG:NH1	2.41	0.54
7:I:21:GLU:HA	7:I:73:LEU:HD23	1.90	0.54
2:3:201:HIS:CE1	2:3:232:PRO:HD2	2.43	0.54
9:D:125:PRO:O	9:D:129:MET:HG2	2.07	0.54
2:3:99:SER:HB3	2:3:158:LYS:HE2	1.89	0.54
11:F:293:LYS:HB3	15:5:734:ARG:HH12	1.72	0.54
2:3:499:LYS:HE2	13:A:14:DA:H5'	1.90	0.54
5:7:513:LEU:HD13	5:7:540:VAL:HG21	1.90	0.54
10:E:598:LYS:HG2	10:E:599:LYS:H	1.71	0.54
6:H:120:THR:HG21	11:F:375:PHE:HA	1.88	0.53
12:G:1365:THR:HG22	12:G:1366:MET:H	1.72	0.53
12:G:1679:LYS:HD3	12:G:1794:MET:HE2	1.89	0.53
12:G:1850:GLU:HG3	12:G:1895:PHE:HE2	1.73	0.53
1:2:391:GLN:NE2	4:6:620:ASP:OD2	2.40	0.53
1:2:586:THR:HG22	1:2:588:GLU:HG3	1.91	0.53
3:4:265:PRO:HB3	3:4:325:LEU:HG	1.89	0.53
3:4:587:ARG:NH1	3:4:623:LEU:O	2.42	0.53
11:F:195:ASN:HD21	11:F:197:LYS:HB3	1.73	0.53
3:4:207:LYS:NZ	3:4:210:ASP:OD2	2.39	0.53
3:4:319:PRO:HB3	5:7:253:PRO:HB3	1.91	0.53
8:C:20:PHE:HE2	8:C:44:LEU:HD12	1.73	0.53
10:E:161:LYS:O	10:E:165:LEU:HB2	2.09	0.53
1:2:608:GLU:OE2	4:6:653:HIS:ND1	2.41	0.53
6:H:107:LEU:HD23	6:H:109:LEU:H	1.73	0.53
1:2:321:THR:HG22	1:2:425:GLU:HG3	1.91	0.53
4:6:140:ILE:HD11	4:6:189:VAL:HG22	1.90	0.53
4:6:582:SER:OG	19:6:1201:ADP:O2B	2.23	0.53
5:7:18:PHE:HA	5:7:21:ILE:HD12	1.90	0.53
5:7:444:VAL:HB	5:7:448:MET:HB3	1.90	0.53
11:F:516:ILE:HA	11:F:519:VAL:HG22	1.91	0.53
2:3:698:THR:HG22	2:3:699:ALA:N	2.24	0.53
5:7:441:ASP:OD1	5:7:452:GLY:N	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:141:LEU:HD11	9:D:182:TYR:CD1	2.43	0.53
3:4:525:SER:O	3:4:528:PRO:HD3	2.09	0.52
11:F:686:GLU:O	11:F:687:ILE:C	2.52	0.52
12:G:1361:PHE:HD2	12:G:1362:LYS:HG3	1.73	0.52
4:6:550:GLN:HB2	4:6:571:ILE:HD11	1.90	0.52
15:5:31:PHE:CG	15:5:90:PHE:HD1	2.27	0.52
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.42	0.52
12:G:1475:ARG:HG3	12:G:1476:TYR:HD1	1.74	0.52
4:6:262:VAL:HG21	4:6:354:LEU:HD21	1.91	0.52
4:6:314:CYS:SG	4:6:338:CYS:HB2	2.50	0.52
4:6:777:TYR:HB2	4:6:800:LEU:HD13	1.91	0.52
10:E:82:LEU:HD23	10:E:121:TYR:HB2	1.92	0.52
10:E:248:VAL:O	10:E:290:ARG:NH2	2.43	0.52
1:2:478:GLU:OE1	10:E:357:LYS:NZ	2.29	0.52
3:4:698:LEU:HD12	3:4:701:ARG:HD2	1.91	0.52
5:7:435:LEU:HD13	5:7:564:LEU:HD13	1.92	0.52
12:G:1744:ILE:HD11	12:G:1836:VAL:HG22	1.91	0.52
3:4:506:LEU:O	3:4:510:ARG:HG2	2.10	0.52
5:7:458:LEU:HD23	5:7:598:PHE:HB2	1.91	0.52
5:7:548:ILE:HG13	5:7:549:SER:H	1.75	0.52
7:I:17:GLN:O	7:I:21:GLU:HG3	2.09	0.52
10:E:401:LEU:HB3	10:E:404:ILE:HD12	1.92	0.52
12:G:1709:THR:HA	12:G:1712:ILE:HG12	1.90	0.52
5:7:400:ARG:HD2	5:7:637:LYS:HE2	1.91	0.52
9:D:97:LEU:O	9:D:101:ILE:HD12	2.10	0.52
10:E:144:ASP:OD1	10:E:145:ASP:N	2.42	0.52
10:E:345:ASN:HA	10:E:350:LEU:HD13	1.92	0.52
4:6:816:VAL:HG12	4:6:818:GLU:H	1.75	0.52
11:F:415:THR:O	11:F:419:LYS:HG3	2.10	0.52
12:G:1664:ARG:HH12	12:G:1666:ASP:HB2	1.74	0.52
3:4:559:ARG:NH1	3:4:649:MET:O	2.43	0.52
5:7:596:ILE:HD11	5:7:695:LEU:HD11	1.91	0.52
12:G:1952:GLU:OE2	12:G:2014:ARG:NH2	2.40	0.52
1:2:196:GLU:HA	1:2:199:THR:HG22	1.92	0.51
12:G:1670:TYR:O	12:G:1674:VAL:HG23	2.10	0.51
15:5:614:LEU:HD11	15:5:657:ILE:HG23	1.92	0.51
1:2:341:CYS:O	1:2:345:GLY:HA2	2.11	0.51
8:C:105:PHE:O	8:C:109:ILE:HD12	2.09	0.51
1:2:271:PHE:HA	1:2:274:VAL:HG12	1.92	0.51
1:2:440:ALA:HB1	4:6:408:THR:HG22	1.93	0.51
6:H:207:LYS:HG2	6:H:208:ILE:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:84:VAL:O	11:F:88:ILE:HG13	2.10	0.51
11:F:550:PHE:HE2	11:F:602:LEU:HG	1.75	0.51
5:7:142:ILE:O	5:7:146:ARG:HG2	2.09	0.51
6:H:107:LEU:HD21	6:H:112:SER:HB3	1.93	0.51
11:F:394:LEU:HD22	11:F:397:HIS:HE1	1.76	0.51
11:F:669:ARG:NH1	11:F:687:ILE:HG12	2.26	0.51
2:3:170:THR:HG21	2:3:588:LEU:HD11	1.92	0.51
2:3:293:ASN:ND2	2:3:594:GLU:OE2	2.33	0.51
3:4:316:GLU:HG2	3:4:316:GLU:O	2.11	0.51
4:6:152:TYR:HB3	4:6:268:PHE:HE1	1.76	0.51
11:F:414:MET:HE3	11:F:468:LEU:HD22	1.92	0.51
3:4:196:ASN:O	3:4:200:SER:HB2	2.11	0.51
3:4:209:LEU:HD13	3:4:250:ALA:HA	1.92	0.51
6:H:128:GLN:OE1	11:F:378:ARG:NH1	2.44	0.51
9:D:94:GLN:O	9:D:98:ILE:HD12	2.11	0.51
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.93	0.51
3:4:445:ARG:HA	3:4:453:LEU:HD23	1.92	0.51
3:4:748:THR:HB	3:4:749:MET:HE2	1.92	0.51
3:4:826:VAL:HA	3:4:829:ILE:HG22	1.93	0.51
6:H:35:ASP:OD1	6:H:36:ILE:HD12	2.10	0.51
3:4:728:TYR:HE1	5:7:450:ILE:HG21	1.76	0.50
4:6:137:ARG:O	4:6:140:ILE:HG22	2.10	0.50
6:H:141:LEU:HD11	9:D:182:TYR:HD1	1.77	0.50
11:F:398:LYS:NZ	11:F:674:GLU:OE2	2.38	0.50
5:7:69:LYS:HD2	5:7:75:LEU:HB2	1.93	0.50
12:G:1369:GLN:HG2	12:G:1371:ILE:H	1.76	0.50
5:7:216:ARG:HG2	5:7:217:LYS:H	1.76	0.50
5:7:432:LEU:HD13	5:7:473:ILE:HD11	1.93	0.50
5:7:575:ASN:OD1	5:7:576:PRO:HD2	2.11	0.50
12:G:1731:VAL:HB	12:G:1906:TRP:HB2	1.93	0.50
12:G:1856:SER:HA	12:G:1869:LYS:O	2.11	0.50
4:6:652:ILE:HG22	4:6:656:MET:HG3	1.93	0.50
2:3:259:GLN:HG3	2:3:273:SER:HB3	1.94	0.50
10:E:328:LEU:HD23	10:E:423:GLU:HG2	1.92	0.50
7:I:109:PRO:HA	7:I:155:LYS:HE2	1.93	0.50
1:2:382:TYR:HB2	15:5:153:SER:HB2	1.92	0.50
1:2:589:TRP:HD1	15:5:454:GLN:HE22	1.60	0.50
4:6:690:ASN:HD22	4:6:693:LEU:HD23	1.77	0.50
2:3:552:ASP:O	2:3:557:ARG:NH1	2.45	0.50
1:2:341:CYS:O	1:2:345:GLY:CA	2.60	0.50
5:7:322:VAL:HG21	5:7:328:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:97:LEU:HD11	8:C:127:LEU:HD21	1.93	0.50
11:F:2:PHE:HE1	11:F:94:ARG:HG2	1.77	0.50
11:F:625:ASP:OD1	11:F:625:ASP:N	2.43	0.50
12:G:1816:LEU:O	12:G:1820:VAL:HG23	2.12	0.50
12:G:1895:PHE:HB3	12:G:1898:LEU:HD12	1.93	0.50
12:G:1960:ILE:HD11	12:G:2062:MET:HE2	1.93	0.50
3:4:720:LEU:HD12	3:4:723:HIS:NE2	2.27	0.49
5:7:260:TYR:HB3	5:7:298:LEU:HD12	1.94	0.49
3:4:605:ILE:HD12	3:4:658:LYS:HB2	1.95	0.49
5:7:283:GLU:N	5:7:298:LEU:HD23	2.27	0.49
5:7:291:GLN:NE2	5:7:292:ASN:OD1	2.45	0.49
9:D:126:LEU:HD23	10:E:22:HIS:NE2	2.27	0.49
11:F:529:PRO:HA	11:F:541:ILE:O	2.12	0.49
12:G:2155:GLU:O	12:G:2159:ILE:HG12	2.12	0.49
15:5:50:LEU:HG	15:5:61:LEU:HD13	1.94	0.49
1:2:259:PHE:HB3	1:2:267:MET:HE3	1.93	0.49
3:4:520:SER:O	3:4:524:ARG:HG2	2.11	0.49
4:6:538:PHE:HB2	4:6:730:HIS:ND1	2.27	0.49
10:E:572:ILE:HD13	10:E:579:TYR:CE1	2.47	0.49
12:G:1366:MET:HG2	12:G:1368:LEU:HG	1.93	0.49
5:7:226:SER:OG	5:7:229:GLN:HG3	2.13	0.49
7:I:146:GLN:O	7:I:150:GLU:HG3	2.13	0.49
11:F:41:LEU:HD11	11:F:66:PHE:CE2	2.47	0.49
12:G:1360:LYS:HG3	12:G:1424:LEU:HB2	1.94	0.49
15:5:196:ASN:ND2	15:5:279:ASP:OD2	2.45	0.49
15:5:414:LEU:HD23	15:5:554:PHE:HB2	1.93	0.49
15:5:433:SER:HB3	15:5:436:ALA:HB2	1.94	0.49
12:G:1403:PRO:HG2	12:G:1406:VAL:HG22	1.94	0.49
15:5:584:GLN:O	15:5:587:GLN:HG2	2.12	0.49
1:2:656:ARG:NH2	4:6:793:TYR:OH	2.46	0.49
2:3:723:LYS:HE2	2:3:727:LYS:HE2	1.94	0.49
3:4:251:TYR:CE2	3:4:253:GLN:HB3	2.47	0.49
6:H:168:LEU:O	6:H:185:LYS:NZ	2.45	0.49
10:E:638:SER:OG	10:E:639:PRO:HD3	2.13	0.49
13:A:3:DA:H2'	13:A:4:DA:C8	2.48	0.49
3:4:191:THR:O	3:4:195:ARG:HG2	2.12	0.49
5:7:643:ALA:O	5:7:647:THR:HG23	2.13	0.49
6:H:175:GLN:OE1	11:F:18:ARG:NE	2.44	0.49
11:F:53:TRP:N	11:F:55:GLN:OE1	2.46	0.49
11:F:232:ASN:HB3	11:F:235:PHE:HD2	1.77	0.49
12:G:1874:SER:OG	12:G:1876:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:690:ASN:ND2	4:6:693:LEU:HD23	2.28	0.49
5:7:235:LEU:HD22	5:7:357:PRO:HG3	1.95	0.49
6:H:110:MET:SD	6:H:120:THR:HG22	2.53	0.49
12:G:1486:TYR:OH	12:G:1642:SER:HB2	2.13	0.49
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.48	0.49
4:6:596:VAL:HG22	4:6:631:ALA:HB2	1.94	0.49
11:F:34:LYS:HB2	11:F:79:ILE:O	2.12	0.49
1:2:334:LEU:HD13	15:5:322:ALA:HB1	1.93	0.48
6:H:198:ARG:HD3	11:F:31:LEU:HD22	1.95	0.48
11:F:386:ARG:CD	11:F:389:LEU:HD12	2.43	0.48
3:4:403:PRO:HD2	3:4:432:ARG:HH22	1.78	0.48
3:4:443:PRO:HB3	3:4:457:TYR:CE1	2.48	0.48
5:7:455:ASN:HB2	5:7:595:ASP:H	1.78	0.48
12:G:1593:GLN:OE1	12:G:1617:LEU:N	2.33	0.48
14:B:13:DT:H3'	14:B:14:DT:H5''	1.95	0.48
5:7:262:CYS:HB2	5:7:298:LEU:HD11	1.95	0.48
6:H:34:GLU:OE1	6:H:38:ARG:NH2	2.46	0.48
15:5:26:GLU:N	15:5:26:GLU:OE1	2.46	0.48
3:4:768:THR:O	3:4:772:ARG:HG2	2.13	0.48
10:E:366:MET:HE2	10:E:391:ILE:HG22	1.95	0.48
1:2:364:CYS:CB	1:2:367:CYS:HB3	2.43	0.48
3:4:728:TYR:CE1	5:7:450:ILE:HG21	2.48	0.48
4:6:585:LEU:HD22	4:6:637:CYS:HB3	1.94	0.48
15:5:209:ARG:HG3	15:5:209:ARG:HH11	1.78	0.48
10:E:28:VAL:HG23	10:E:78:ILE:HD12	1.95	0.48
11:F:84:VAL:O	11:F:87:VAL:HG22	2.12	0.48
11:F:362:LEU:HD21	11:F:376:ILE:HD12	1.96	0.48
11:F:408:LEU:HD21	11:F:465:LEU:HD11	1.96	0.48
15:5:544:THR:HG23	15:5:647:PRO:HG3	1.95	0.48
11:F:20:LEU:HD22	11:F:23:ARG:HH21	1.77	0.48
5:7:282:SER:HA	5:7:298:LEU:H	1.78	0.48
9:D:203:PRO:O	9:D:207:GLN:HG3	2.14	0.48
11:F:490:LEU:HD23	11:F:509:PRO:HG3	1.96	0.48
14:B:7:DT:H2''	14:B:8:DT:H5'	1.96	0.48
15:5:276:MET:HE1	15:5:294:ILE:HG13	1.96	0.48
15:5:571:HIS:O	15:5:575:ILE:HG12	2.13	0.48
1:2:463:THR:HG22	1:2:558:LYS:HG3	1.95	0.48
3:4:203:TYR:O	3:4:207:LYS:HG2	2.14	0.48
5:7:26:VAL:HG12	5:7:64:MET:HE3	1.95	0.48
5:7:349:VAL:HG12	5:7:383:GLN:HG2	1.96	0.48
3:4:233:MET:HE3	3:4:240:ASN:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:527:ALA:HB3	3:4:537:LYS:HD3	1.95	0.47
4:6:644:MET:HE2	4:6:649:GLN:HG2	1.96	0.47
5:7:396:ASP:O	5:7:400:ARG:HG2	2.13	0.47
6:H:170:ASP:OD1	6:H:171:ALA:N	2.46	0.47
11:F:17:LEU:HD13	11:F:53:TRP:HZ2	1.78	0.47
11:F:293:LYS:HG2	15:5:730:TYR:HE2	1.79	0.47
11:F:555:LEU:HD23	11:F:557:PHE:CZ	2.49	0.47
12:G:1998:ASN:HA	12:G:2001:ASN:OD1	2.13	0.47
6:H:105:ASN:HA	6:H:152:SER:HB2	1.95	0.47
9:D:206:LEU:HD12	9:D:206:LEU:O	2.15	0.47
12:G:1597:ILE:HG21	12:G:1614:LYS:HD2	1.96	0.47
15:5:738:VAL:HG22	15:5:743:PHE:HB2	1.95	0.47
3:4:272:MET:O	3:4:276:ILE:HG12	2.14	0.47
5:7:86:LEU:HD21	5:7:103:VAL:HG11	1.95	0.47
6:H:54:LEU:HD21	6:H:71:GLN:HB2	1.95	0.47
15:5:467:GLY:H	15:5:470:VAL:HB	1.78	0.47
3:4:329:LYS:HG2	3:4:434:GLU:HB3	1.96	0.47
4:6:751:LEU:O	4:6:755:ILE:HG12	2.14	0.47
10:E:246:THR:HG23	10:E:602:LEU:HD23	1.95	0.47
15:5:236:CYS:HB3	15:5:240:PRO:HG2	1.95	0.47
2:3:484:VAL:HG11	5:7:486:LYS:HE2	1.96	0.47
3:4:367:GLU:OE1	4:6:441:ARG:N	2.48	0.47
4:6:451:LYS:NZ	4:6:453:SER:OG	2.47	0.47
10:E:502:LEU:O	10:E:506:ILE:HG12	2.14	0.47
15:5:90:PHE:CD2	15:5:137:LEU:HD22	2.49	0.47
12:G:1944:PHE:HE1	12:G:2043:SER:HB3	1.80	0.47
1:2:589:TRP:CD1	15:5:454:GLN:HE22	2.32	0.47
1:2:615:GLN:O	15:5:442:LYS:NZ	2.48	0.47
2:3:469:VAL:HG12	2:3:511:SER:HB2	1.96	0.47
5:7:404:LEU:HD23	5:7:641:TYR:CD1	2.50	0.47
9:D:72:CYS:HB3	9:D:293:LEU:HD23	1.97	0.47
15:5:681:ILE:O	15:5:685:GLN:HG3	2.14	0.47
4:6:430:THR:HA	4:6:433:LEU:HB2	1.96	0.47
11:F:669:ARG:NH1	11:F:687:ILE:HG23	2.30	0.47
12:G:1365:THR:HG22	12:G:1366:MET:N	2.30	0.47
12:G:1450:LYS:HG3	12:G:1451:ALA:H	1.80	0.47
15:5:393:MET:HE3	15:5:666:LEU:HD23	1.97	0.47
1:2:696:ALA:HB3	4:6:774:VAL:HG23	1.97	0.47
3:4:714:GLU:OE1	3:4:715:LYS:HD3	2.14	0.47
5:7:707:MET:SD	5:7:707:MET:N	2.87	0.47
9:D:136:LEU:O	9:D:140:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:281:VAL:HG23	9:D:282:ILE:HG23	1.96	0.47
13:A:16:DA:H61	14:B:11:DT:H3	1.61	0.47
3:4:220:THR:HA	3:4:223:GLU:HG3	1.97	0.47
5:7:67:LEU:HD21	5:7:121:ILE:HD12	1.97	0.47
10:E:14:LYS:HG2	10:E:17:ARG:HH12	1.80	0.47
11:F:49:ILE:HG13	11:F:53:TRP:CZ3	2.49	0.47
11:F:435:GLN:HA	11:F:484:ILE:HB	1.97	0.46
12:G:1956:TRP:O	12:G:1960:ILE:HG13	2.15	0.46
14:B:24:DT:H2''	14:B:25:DT:O5'	2.15	0.46
9:D:109:GLN:NE2	9:D:114:ALA:O	2.48	0.46
12:G:1920:LEU:HG	12:G:1933:TYR:HB3	1.97	0.46
15:5:759:GLU:O	15:5:774:GLY:N	2.47	0.46
12:G:1616:SER:OG	12:G:1664:ARG:NH2	2.48	0.46
12:G:1795:LEU:HD13	12:G:1816:LEU:HD22	1.97	0.46
1:2:578:ALA:HB1	1:2:591:LEU:HD22	1.97	0.46
3:4:269:ILE:O	3:4:272:MET:HB2	2.14	0.46
7:I:54:THR:OG1	9:D:132:GLU:OE2	2.27	0.46
11:F:28:LYS:HE3	11:F:29:TYR:CE1	2.51	0.46
11:F:420:ILE:O	11:F:424:LEU:HD13	2.15	0.46
12:G:2039:VAL:O	12:G:2040:LEU:HD23	2.16	0.46
3:4:545:PHE:O	3:4:810:LYS:NZ	2.42	0.46
4:6:645:ASP:OD2	4:6:647:SER:OG	2.24	0.46
12:G:1339:PHE:HD1	12:G:1611:PRO:HB3	1.80	0.46
15:5:266:PRO:HG2	15:5:269:GLU:HG3	1.97	0.46
3:4:197:PHE:HB2	3:4:254:THR:HG21	1.97	0.46
10:E:286:GLN:H	10:E:286:GLN:CD	2.24	0.46
11:F:661:PRO:HG3	11:F:673:MET:SD	2.56	0.46
12:G:1595:PRO:HA	12:G:1618:ASN:OD1	2.16	0.46
15:5:87:ILE:O	15:5:91:GLU:HG2	2.16	0.46
3:4:209:LEU:HD22	3:4:250:ALA:HB2	1.98	0.46
12:G:1655:TYR:OH	12:G:1801:GLU:OE2	2.28	0.46
2:3:97:ILE:HG12	2:3:156:SER:HB2	1.97	0.46
3:4:251:TYR:HE2	3:4:253:GLN:HB3	1.81	0.46
3:4:778:ARG:HD3	3:4:793:ALA:O	2.16	0.46
4:6:796:THR:H	4:6:799:GLN:HG2	1.80	0.46
5:7:63:TYR:HA	5:7:66:MET:HG2	1.98	0.46
5:7:459:MET:HG2	5:7:567:ALA:HB3	1.96	0.46
12:G:1721:ILE:O	12:G:1860:TYR:HA	2.16	0.46
12:G:1941:LEU:HD21	12:G:2057:SER:HB2	1.97	0.46
5:7:668:ARG:HD2	5:7:684:ALA:HB3	1.98	0.46
11:F:669:ARG:HH11	11:F:687:ILE:HG12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1664:ARG:NH1	12:G:1666:ASP:HB2	2.30	0.46
3:4:336:THR:HG22	3:4:396:VAL:H	1.81	0.45
3:4:607:ARG:HH21	3:4:612:LYS:HB3	1.80	0.45
5:7:70:VAL:HG22	5:7:75:LEU:HB3	1.98	0.45
5:7:360:TYR:HD1	5:7:373:GLU:HG3	1.81	0.45
15:5:416:GLY:HA3	15:5:556:VAL:HB	1.99	0.45
1:2:783:MET:HG2	15:5:573:ILE:HG21	1.99	0.45
5:7:275:SER:OG	5:7:276:ARG:N	2.46	0.45
6:H:109:LEU:HD23	6:H:135:CYS:SG	2.56	0.45
12:G:1691:GLU:OE2	12:G:1692:LYS:HG2	2.17	0.45
2:3:730:ALA:O	2:3:734:ARG:HG3	2.16	0.45
3:4:245:ALA:HB1	3:4:258:TYR:HE1	1.82	0.45
7:I:102:ILE:O	7:I:106:LYS:HG2	2.17	0.45
11:F:476:THR:HG23	11:F:520:CYS:HA	1.98	0.45
11:F:650:ASP:OD1	11:F:650:ASP:N	2.48	0.45
12:G:2048:LYS:HG3	12:G:2049:ASN:N	2.31	0.45
4:6:728:ALA:O	4:6:732:VAL:HG12	2.16	0.45
6:H:44:VAL:HG23	6:H:79:MET:HG2	1.99	0.45
9:D:131:THR:O	9:D:135:ARG:HG3	2.16	0.45
12:G:2213:LEU:O	12:G:2217:ILE:HG12	2.16	0.45
4:6:516:LEU:HD21	4:6:757:TYR:CG	2.52	0.45
6:H:167:VAL:HG21	6:H:184:ILE:O	2.17	0.45
3:4:508:LYS:HA	3:4:511:GLU:HG2	1.99	0.45
3:4:522:LEU:HA	3:4:525:SER:OG	2.17	0.45
5:7:149:ARG:NH1	5:7:267:TYR:HB3	2.32	0.45
5:7:503:THR:HG23	5:7:505:GLU:HG2	1.99	0.45
7:I:158:LYS:NZ	15:5:104:LEU:HD12	2.31	0.45
8:C:162:THR:O	8:C:166:LEU:HG	2.17	0.45
11:F:181:PHE:CD1	11:F:192:PHE:HA	2.52	0.45
15:5:254:GLN:HB3	15:5:278:CYS:SG	2.56	0.45
1:2:253:LYS:HB3	1:2:256:LEU:HD12	1.98	0.45
3:4:632:ASP:OD2	3:4:633:GLU:N	2.50	0.45
3:4:704:LEU:HD11	3:4:804:LEU:HD21	1.99	0.45
5:7:662:GLN:HA	5:7:665:ILE:HG12	1.98	0.45
5:7:686:PRO:O	5:7:690:LEU:HG	2.17	0.45
10:E:553:ILE:HD11	10:E:584:LEU:HB3	1.99	0.45
11:F:184:ASN:HD22	11:F:187:LYS:HE2	1.80	0.45
15:5:92:THR:HA	15:5:95:THR:HG22	1.98	0.45
1:2:763:LEU:O	1:2:767:ILE:HG13	2.17	0.45
12:G:1887:LYS:O	12:G:1891:THR:OG1	2.26	0.45
10:E:539:TYR:HB3	10:E:545:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:203:TYR:HB2	3:4:220:THR:O	2.17	0.45
3:4:608:ASP:HB2	3:4:615:VAL:HG23	1.99	0.45
7:I:151:ILE:HA	7:I:154:ILE:HD12	1.99	0.45
9:D:54:VAL:HG12	9:D:54:VAL:O	2.16	0.45
11:F:435:GLN:HG2	11:F:436:GLY:N	2.32	0.45
11:F:452:ILE:HG13	11:F:456:THR:OG1	2.17	0.45
5:7:693:ILE:O	5:7:697:GLN:HG2	2.17	0.44
1:2:656:ARG:NH2	4:6:793:TYR:CZ	2.85	0.44
4:6:109:GLU:O	4:6:113:GLU:HG2	2.16	0.44
5:7:217:LYS:HE2	5:7:217:LYS:HA	1.99	0.44
5:7:260:TYR:O	5:7:268:GLU:HA	2.17	0.44
5:7:531:GLU:HA	5:7:534:ARG:HB2	1.99	0.44
7:I:96:LYS:O	7:I:100:ARG:HG3	2.17	0.44
15:5:407:ARG:HH21	15:5:658:ARG:NH1	2.14	0.44
6:H:150:ASP:O	9:D:141:ARG:HD3	2.17	0.44
10:E:103:TYR:O	10:E:117:ARG:N	2.50	0.44
10:E:231:HIS:HA	10:E:234:GLU:HG2	1.99	0.44
11:F:363:ASP:HB3	11:F:366:GLY:HA2	1.98	0.44
11:F:503:LEU:HD12	11:F:622:ILE:HG12	1.99	0.44
15:5:707:SER:HA	15:5:710:GLU:HB2	1.99	0.44
1:2:234:LEU:HG	1:2:239:SER:HB3	1.99	0.44
2:3:413:THR:O	2:3:413:THR:HG22	2.16	0.44
3:4:417:LEU:HD23	3:4:463:VAL:HG11	1.98	0.44
4:6:367:GLU:N	4:6:367:GLU:OE2	2.50	0.44
5:7:282:SER:HB3	5:7:297:GLN:HB2	2.00	0.44
5:7:635:PRO:O	5:7:638:MET:HB2	2.18	0.44
2:3:459:ALA:HB1	2:3:463:VAL:HG23	2.00	0.44
3:4:234:ARG:HH21	3:4:291:TYR:HB3	1.83	0.44
3:4:505:ASP:HA	3:4:508:LYS:HG2	1.99	0.44
1:2:437:ASN:OD1	4:6:416:LYS:HB3	2.18	0.44
3:4:280:MET:HE2	3:4:280:MET:HA	2.00	0.44
3:4:776:GLY:HA2	3:4:779:LYS:HG2	1.98	0.44
11:F:14:PRO:N	11:F:15:PRO:HD2	2.33	0.44
11:F:345:THR:HG22	11:F:346:LEU:N	2.32	0.44
11:F:503:LEU:HD13	11:F:630:LEU:HD13	1.99	0.44
14:B:23:DT:H2''	14:B:24:DT:O5'	2.18	0.44
3:4:227:ILE:HD11	3:4:283:LEU:HD21	1.99	0.44
3:4:413:HIS:CE1	5:7:250:ASP:HB3	2.52	0.44
3:4:775:VAL:HG21	4:6:725:THR:HG22	2.00	0.44
4:6:112:ARG:NH1	4:6:187:ARG:HH12	2.16	0.44
12:G:1656:SER:HB3	12:G:1658:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:733:LEU:HD21	2:3:737:LEU:HD12	1.99	0.44
4:6:269:ASN:HD22	4:6:269:ASN:C	2.24	0.44
10:E:50:LYS:HB2	10:E:50:LYS:HE3	1.78	0.44
10:E:326:LEU:HB3	10:E:337:SER:HB3	2.00	0.44
10:E:431:LEU:HD23	10:E:431:LEU:HA	1.86	0.44
2:3:735:PHE:CD2	2:3:741:ASP:HB3	2.53	0.44
3:4:264:TYR:HA	5:7:303:ARG:HH22	1.83	0.44
3:4:451:ARG:HH22	5:7:282:SER:HB2	1.83	0.44
19:6:1201:ADP:H8	19:6:1201:ADP:H2'	1.76	0.44
8:C:194:LYS:HD3	8:C:194:LYS:HA	1.80	0.44
2:3:276:VAL:HG11	2:3:294:VAL:HG11	1.99	0.43
5:7:360:TYR:CD1	5:7:373:GLU:HG3	2.53	0.43
5:7:634:GLU:OE1	5:7:636:SER:HB2	2.18	0.43
11:F:396:ASP:OD1	11:F:397:HIS:N	2.51	0.43
12:G:1371:ILE:HG13	12:G:1372:LYS:HG3	2.00	0.43
15:5:760:THR:HG22	15:5:761:ILE:HG12	2.00	0.43
1:2:458:ARG:HE	1:2:460:GLU:HB3	1.83	0.43
3:4:819:LEU:HD12	3:4:819:LEU:H	1.82	0.43
4:6:821:PRO:HA	4:6:824:ILE:HD13	2.00	0.43
10:E:129:TRP:CD2	10:E:134:ILE:HD11	2.53	0.43
11:F:402:LEU:HD13	11:F:434:TRP:HD1	1.81	0.43
15:5:650:ILE:HD12	15:5:650:ILE:H	1.83	0.43
4:6:722:LYS:O	4:6:725:THR:OG1	2.29	0.43
5:7:117:PHE:O	5:7:121:ILE:HG12	2.18	0.43
5:7:451:ARG:HD2	5:7:453:ASP:HB2	2.01	0.43
9:D:82:GLN:O	9:D:86:ARG:HG3	2.18	0.43
10:E:434:VAL:HG23	10:E:498:LEU:HD13	2.00	0.43
12:G:2009:LYS:HB3	12:G:2010:PRO:HD3	1.99	0.43
3:4:418:CYS:O	3:4:463:VAL:HG22	2.18	0.43
4:6:122:PHE:O	4:6:124:VAL:HG23	2.18	0.43
10:E:27:LEU:HD12	10:E:80:SER:HB2	2.00	0.43
11:F:181:PHE:HD1	11:F:192:PHE:HA	1.84	0.43
11:F:220:THR:O	11:F:224:LEU:HD23	2.18	0.43
15:5:207:LEU:HD23	15:5:241:TYR:HB3	2.01	0.43
1:2:707:HIS:CE1	1:2:709:GLU:HB2	2.53	0.43
4:6:538:PHE:H	19:6:1201:ADP:N6	2.16	0.43
7:I:170:LEU:O	9:D:274:ILE:HB	2.18	0.43
11:F:49:ILE:HG13	11:F:53:TRP:HZ3	1.83	0.43
12:G:1905:TYR:HB2	12:G:1922:CYS:SG	2.59	0.43
3:4:224:LEU:HB3	3:4:227:ILE:HG22	1.99	0.43
4:6:594:ARG:HG3	4:6:594:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:126:LEU:HA	9:D:129:MET:HG2	2.00	0.43
12:G:1656:SER:HB3	12:G:1658:ILE:CD1	2.49	0.43
1:2:534:ARG:NH2	1:2:625:GLU:OE1	2.51	0.43
1:2:577:THR:HG22	1:2:578:ALA:N	2.31	0.43
5:7:608:ASP:O	5:7:611:LYS:HG2	2.18	0.43
10:E:132:ASP:OD1	10:E:159:TYR:OH	2.24	0.43
12:G:1368:LEU:HB3	12:G:1370:LYS:NZ	2.34	0.43
12:G:1779:VAL:HG13	15:5:726:TRP:HB3	2.00	0.43
15:5:99:LYS:HG2	15:5:132:LEU:HD12	2.01	0.43
1:2:304:TYR:HD2	1:2:308:GLU:HG3	1.84	0.43
3:4:403:PRO:O	3:4:406:VAL:HG12	2.18	0.43
7:I:103:GLN:O	7:I:107:THR:HG23	2.19	0.43
11:F:318:HIS:NE2	11:F:320:TYR:OH	2.49	0.43
2:3:674:GLU:OE1	2:3:723:LYS:HB2	2.18	0.43
3:4:280:MET:O	3:4:284:ILE:HG23	2.18	0.43
3:4:644:VAL:O	3:4:647:GLU:HG2	2.19	0.43
3:4:728:TYR:OH	5:7:690:LEU:HD22	2.19	0.43
4:6:720:ASN:OD1	4:6:723:ILE:HB	2.19	0.43
5:7:440:VAL:HG12	5:7:697:GLN:HG3	2.01	0.43
6:H:47:LEU:O	6:H:51:THR:HG23	2.18	0.43
12:G:1328:LYS:O	12:G:1337:GLU:N	2.51	0.43
12:G:1696:PRO:HG3	12:G:1828:PHE:O	2.18	0.43
12:G:1863:ARG:HE	12:G:1863:ARG:HB3	1.63	0.43
1:2:342:LEU:HD12	1:2:343:LYS:N	2.33	0.43
6:H:107:LEU:HD23	6:H:108:ASP:N	2.33	0.43
10:E:351:TRP:CD1	10:E:351:TRP:H	2.35	0.43
1:2:353:GLN:HG2	1:2:355:SER:H	1.84	0.42
3:4:602:THR:HB	3:4:654:ILE:HG21	2.01	0.42
11:F:494:MET:HE2	11:F:494:MET:HB2	1.98	0.42
12:G:1669:ASP:HB2	12:G:1819:TRP:HD1	1.84	0.42
15:5:415:LEU:O	15:5:555:ILE:HA	2.19	0.42
4:6:752:ARG:HG3	4:6:752:ARG:HH11	1.83	0.42
5:7:216:ARG:C	5:7:218:LYS:H	2.28	0.42
5:7:494:THR:HB	5:7:548:ILE:HD12	2.01	0.42
10:E:29:ILE:HG12	10:E:82:LEU:HD12	2.01	0.42
11:F:86:GLU:O	11:F:90:GLU:HG3	2.18	0.42
12:G:1681:LYS:HE2	12:G:1687:LEU:HD11	2.01	0.42
15:5:40:LEU:HD23	15:5:40:LEU:HA	1.89	0.42
1:2:486:LYS:HA	1:2:489:ARG:NH1	2.34	0.42
1:2:564:VAL:HG23	1:2:599:ALA:HB2	2.01	0.42
1:2:803:PHE:HD1	1:2:804:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:3:LEU:HA	7:I:8:GLN:OE1	2.19	0.42
11:F:28:LYS:HE3	11:F:29:TYR:HE1	1.84	0.42
12:G:1402:LEU:HD21	12:G:1406:VAL:HG23	2.00	0.42
15:5:276:MET:HA	15:5:328:ILE:O	2.19	0.42
3:4:779:LYS:HB3	3:4:779:LYS:HE3	1.75	0.42
5:7:422:ILE:HD13	5:7:469:LEU:HD22	2.01	0.42
8:C:174:LYS:HE2	8:C:174:LYS:HB3	1.78	0.42
15:5:72:ASN:HB3	15:5:75:ILE:HD12	2.01	0.42
1:2:300:PHE:HB3	1:2:319:ARG:HD2	2.02	0.42
5:7:130:LYS:NZ	5:7:131:GLU:OE1	2.34	0.42
5:7:414:LEU:HD23	5:7:638:MET:SD	2.59	0.42
11:F:657:LYS:HZ1	11:F:681:LYS:HE2	1.84	0.42
5:7:64:MET:HA	5:7:67:LEU:HD12	2.01	0.42
5:7:286:SER:HB2	5:7:289:CYS:SG	2.58	0.42
5:7:508:LEU:HD11	5:7:548:ILE:HG12	2.01	0.42
6:H:130:TYR:CD2	9:D:189:ILE:HG22	2.54	0.42
11:F:199:ASN:OD1	11:F:200:GLY:N	2.53	0.42
1:2:327:ARG:NH1	1:2:420:PRO:HD3	2.35	0.42
1:2:692:ASP:OD1	4:6:781:ARG:NH2	2.52	0.42
5:7:469:LEU:HD13	5:7:469:LEU:HA	1.77	0.42
5:7:542:GLU:OE2	5:7:593:ARG:NH2	2.52	0.42
6:H:13:ALA:HB2	6:H:89:TYR:HD1	1.85	0.42
10:E:431:LEU:HD11	10:E:491:LEU:HG	2.00	0.42
11:F:7:VAL:HG23	11:F:8:LEU:N	2.35	0.42
11:F:399:PHE:CE1	11:F:677:PRO:HG3	2.53	0.42
12:G:2004:SER:HA	12:G:2007:PHE:CE1	2.54	0.42
12:G:2193:SER:O	12:G:2197:LYS:HG3	2.19	0.42
15:5:442:LYS:HD2	15:5:442:LYS:HA	1.80	0.42
2:3:28:PHE:O	2:3:32:LEU:HD23	2.20	0.42
3:4:258:TYR:O	3:4:262:LEU:HD13	2.19	0.42
3:4:341:ASP:OD2	4:6:435:SER:OG	2.29	0.42
3:4:365:ILE:HD11	4:6:437:VAL:HB	2.02	0.42
11:F:399:PHE:HB2	11:F:431:LEU:HB2	2.02	0.42
1:2:756:SER:OG	1:2:758:ILE:O	2.35	0.42
3:4:196:ASN:O	3:4:200:SER:CB	2.67	0.42
4:6:143:MET:HE1	4:6:151:ILE:HG22	2.01	0.42
7:I:64:VAL:HG21	7:I:67:ARG:HE	1.83	0.42
9:D:260:ILE:O	9:D:264:LYS:N	2.53	0.42
10:E:394:LYS:HG3	10:E:395:ASN:OD1	2.20	0.42
2:3:678:VAL:O	2:3:681:LYS:HG2	2.20	0.42
3:4:824:GLU:OE1	3:4:827:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:350:ARG:HE	4:6:350:ARG:HB2	1.67	0.42
15:5:639:GLU:HG2	15:5:746:LEU:HD11	2.01	0.42
3:4:293:LEU:HA	3:4:296:ILE:HD12	2.02	0.41
3:4:581:VAL:HG11	3:4:672:LEU:HD23	2.01	0.41
5:7:282:SER:HA	5:7:298:LEU:HB2	2.02	0.41
6:H:105:ASN:OD1	6:H:152:SER:OG	2.25	0.41
12:G:1330:SER:OG	12:G:1331:GLY:N	2.53	0.41
12:G:1616:SER:H	12:G:1664:ARG:HH21	1.68	0.41
14:B:14:DT:H5"	14:B:14:DT:O2	2.19	0.41
15:5:149:ARG:NH2	15:5:260:GLU:OE2	2.52	0.41
1:2:761:GLU:HG2	1:2:762:LEU:N	2.35	0.41
2:3:138:ASP:OD1	2:3:139:VAL:N	2.53	0.41
3:4:435:VAL:HG12	3:4:466:VAL:HG13	2.01	0.41
5:7:344:SER:OG	5:7:347:ASP:OD2	2.29	0.41
6:H:48:ARG:HG2	9:D:203:PRO:HG3	2.01	0.41
10:E:128:PRO:HD2	10:E:245:THR:HG22	2.02	0.41
11:F:169:TYR:CE1	11:F:367:ILE:HG22	2.55	0.41
2:3:448:THR:HG22	2:3:455:ARG:HG2	2.02	0.41
3:4:767:LYS:O	3:4:771:VAL:HG23	2.19	0.41
5:7:146:ARG:CZ	5:7:149:ARG:HD3	2.50	0.41
12:G:1916:ASN:HB3	12:G:1939:TRP:CZ3	2.55	0.41
13:A:20:DA:H2"	13:A:21:DA:C8	2.56	0.41
11:F:386:ARG:HE	11:F:535:LEU:HD22	1.86	0.41
12:G:2124:PRO:C	12:G:2126:SER:H	2.29	0.41
3:4:195:ARG:HB2	3:4:199:MET:HE1	2.02	0.41
4:6:438:THR:HB	4:6:447:ASP:OD1	2.20	0.41
5:7:607:ASP:O	5:7:611:LYS:HE3	2.20	0.41
10:E:421:ALA:O	10:E:425:VAL:HG13	2.21	0.41
11:F:83:GLY:O	11:F:87:VAL:HG13	2.21	0.41
12:G:1391:ASN:HA	12:G:1392:PRO:HD3	1.96	0.41
15:5:385:LYS:O	15:5:389:VAL:HG23	2.21	0.41
1:2:180:GLU:N	1:2:180:GLU:OE2	2.54	0.41
4:6:586:LYS:HA	4:6:589:VAL:HG12	2.02	0.41
5:7:20:GLU:OE1	5:7:100:ASP:HB2	2.20	0.41
5:7:366:LEU:HD23	5:7:366:LEU:HA	1.92	0.41
5:7:669:GLN:O	5:7:672:LYS:HG2	2.21	0.41
8:C:193:LYS:C	8:C:193:LYS:HD3	2.46	0.41
10:E:161:LYS:HE3	10:E:161:LYS:HB3	1.68	0.41
12:G:1358:TYR:CD2	12:G:1397:LEU:HD21	2.56	0.41
12:G:1794:MET:O	12:G:1797:GLU:HG2	2.21	0.41
12:G:2130:CYS:SG	12:G:2131:VAL:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:364:CYS:HB3	1:2:367:CYS:H	1.85	0.41
2:3:192:VAL:O	2:3:193:ARG:HD2	2.20	0.41
8:C:133:GLN:H	8:C:133:GLN:HG2	1.71	0.41
9:D:79:TYR:CZ	9:D:84:MET:HG3	2.55	0.41
10:E:598:LYS:HG2	10:E:599:LYS:N	2.35	0.41
3:4:572:THR:OG1	3:4:573:SER:N	2.54	0.41
5:7:470:LEU:O	5:7:471:LYS:C	2.63	0.41
10:E:318:LEU:HD23	10:E:318:LEU:HA	1.91	0.41
12:G:1634:LYS:HD2	12:G:1634:LYS:HA	1.77	0.41
15:5:464:LEU:HD21	15:5:504:ILE:HG21	2.02	0.41
2:3:122:ILE:HB	2:3:123:PRO:HD3	2.02	0.41
2:3:698:THR:CG2	2:3:699:ALA:H	2.33	0.41
3:4:565:LEU:HB2	3:4:702:PHE:CD2	2.56	0.41
3:4:601:LEU:HA	3:4:620:ALA:H	1.86	0.41
4:6:440:LEU:HD12	4:6:440:LEU:HA	1.88	0.41
5:7:531:GLU:HG3	5:7:534:ARG:HD2	2.03	0.41
5:7:578:LEU:HD13	5:7:677:SER:HB2	2.03	0.41
6:H:137:LEU:O	6:H:141:LEU:HG	2.21	0.41
6:H:165:VAL:HG23	6:H:189:PHE:HB2	2.03	0.41
6:H:181:PHE:CZ	6:H:191:VAL:HG21	2.56	0.41
11:F:37:GLY:O	11:F:41:LEU:HD23	2.21	0.41
11:F:293:LYS:HG2	15:5:730:TYR:CE2	2.56	0.41
12:G:1691:GLU:HA	12:G:1826:LYS:HE3	2.03	0.41
12:G:1730:VAL:HG23	12:G:1870:THR:HB	2.03	0.41
12:G:1957:MET:HE2	12:G:1957:MET:HB2	1.86	0.41
15:5:263:GLU:HG3	15:5:264:LEU:HD12	2.01	0.41
3:4:333:LEU:HD11	3:4:400:GLN:OE1	2.21	0.41
3:4:711:LYS:HD3	3:4:712:VAL:N	2.33	0.41
11:F:57:PRO:O	11:F:61:LYS:HG2	2.21	0.41
11:F:185:PRO:HG3	11:F:223:TYR:CE2	2.56	0.41
12:G:1336:LEU:HD23	12:G:1336:LEU:HA	1.92	0.41
1:2:601:LYS:HE3	1:2:643:ARG:HH21	1.87	0.40
2:3:212:ARG:NH1	2:3:232:PRO:HG3	2.36	0.40
3:4:545:PHE:HE1	3:4:751:ILE:HG12	1.85	0.40
3:4:761:ILE:HG13	3:4:816:VAL:HG23	2.03	0.40
4:6:629:MET:SD	4:6:672:LEU:HD13	2.62	0.40
8:C:115:PHE:O	8:C:117:GLU:HG3	2.21	0.40
12:G:1679:LYS:HD3	12:G:1794:MET:CE	2.49	0.40
2:3:524:ASP:OD2	2:3:527:ARG:NH2	2.34	0.40
2:3:653:ILE:HD12	2:3:653:ILE:H	1.86	0.40
3:4:206:ARG:HH12	3:4:246:ARG:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:337:PRO:HA	4:6:375:ARG:HH12	1.86	0.40
3:4:430:GLY:HA3	5:7:553:ILE:O	2.20	0.40
3:4:558:TYR:HD2	4:6:735:HIS:CE1	2.39	0.40
3:4:623:LEU:HD23	3:4:623:LEU:HA	1.91	0.40
7:I:54:THR:N	9:D:132:GLU:OE2	2.48	0.40
10:E:223:ARG:O	10:E:227:LYS:NZ	2.48	0.40
10:E:235:GLY:O	10:E:238:GLU:HG2	2.20	0.40
11:F:20:LEU:HD22	11:F:23:ARG:NH2	2.36	0.40
11:F:653:TYR:CG	11:F:654:ASN:N	2.88	0.40
11:F:653:TYR:O	11:F:655:GLY:N	2.54	0.40
1:2:703:HIS:CE1	4:6:565:LEU:HD13	2.56	0.40
3:4:566:LEU:HD23	3:4:706:TYR:HB2	2.04	0.40
4:6:178:LEU:HB3	4:6:179:PRO:HD3	2.03	0.40
5:7:226:SER:HB3	5:7:321:GLN:NE2	2.37	0.40
5:7:570:LEU:HG	5:7:584:ILE:HA	2.03	0.40
10:E:113:GLU:HB3	10:E:114:GLN:H	1.73	0.40
10:E:312:THR:OG1	10:E:315:THR:HG23	2.22	0.40
12:G:1359:MET:HE1	12:G:1426:VAL:HB	2.03	0.40
12:G:2081:LYS:HB2	12:G:2081:LYS:HE2	1.87	0.40
3:4:687:PRO:HG2	3:4:690:GLU:OE1	2.21	0.40
4:6:368:ILE:HG23	4:6:372:SER:HB3	2.04	0.40
12:G:1622:LEU:HA	12:G:1622:LEU:HD23	1.82	0.40
12:G:1665:LEU:HD23	12:G:1665:LEU:HA	1.83	0.40
3:4:257:LEU:HD23	3:4:257:LEU:HA	1.93	0.40
5:7:218:LYS:HG2	5:7:219:ALA:H	1.86	0.40
5:7:634:GLU:HA	5:7:635:PRO:HD3	2.00	0.40
7:I:85:CYS:SG	7:I:86:SER:N	2.95	0.40
10:E:357:LYS:HB3	10:E:357:LYS:HE2	1.86	0.40
10:E:388:LEU:HD12	10:E:388:LEU:HA	1.91	0.40
11:F:85:LYS:HA	11:F:88:ILE:HD12	2.03	0.40
12:G:1718:PHE:HE2	12:G:1844:LEU:HD23	1.87	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	2	656/868 (76%)	641 (98%)	15 (2%)	0	100	100
2	3	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
3	4	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
4	6	619/1017 (61%)	599 (97%)	20 (3%)	0	100	100
5	7	650/845 (77%)	615 (95%)	35 (5%)	0	100	100
6	H	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
7	I	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
8	C	167/229 (73%)	164 (98%)	3 (2%)	0	100	100
9	D	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
10	E	558/657 (85%)	546 (98%)	12 (2%)	0	100	100
11	F	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
12	G	748/2222 (34%)	716 (96%)	32 (4%)	0	100	100
15	5	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
All	All	6478/9956 (65%)	6232 (96%)	246 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	578/770 (75%)	578 (100%)	0	100	100
2	3	549/864 (64%)	549 (100%)	0	100	100
3	4	551/848 (65%)	551 (100%)	0	100	100
4	6	549/886 (62%)	548 (100%)	1 (0%)	87	88
5	7	580/753 (77%)	577 (100%)	3 (0%)	81	83
6	H	193/193 (100%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	179/198 (90%)	179 (100%)	0	100	100
8	C	157/199 (79%)	157 (100%)	0	100	100
9	D	232/279 (83%)	232 (100%)	0	100	100
10	E	512/592 (86%)	512 (100%)	0	100	100
11	F	494/629 (78%)	493 (100%)	1 (0%)	87	88
12	G	694/2014 (34%)	694 (100%)	0	100	100
15	5	618/688 (90%)	618 (100%)	0	100	100
All	All	5886/8913 (66%)	5881 (100%)	5 (0%)	87	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	6	269	ASN
5	7	466	LYS
5	7	469	LEU
5	7	470	LEU
11	F	687	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	238	ASN
1	2	333	GLN
1	2	376	ASN
1	2	442	ASN
1	2	465	ASN
1	2	627	GLN
1	2	665	GLN
1	2	703	HIS
2	3	201	HIS
2	3	210	HIS
2	3	253	HIS
2	3	340	GLN
2	3	351	ASN
2	3	587	ASN
3	4	193	ASN
3	4	217	ASN
3	4	287	ASN

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Mol	Chain	Res	Type
3	4	288	ASN
3	4	646	HIS
4	6	157	HIS
4	6	434	ASN
4	6	649	GLN
4	6	669	HIS
4	6	683	ASN
4	6	690	ASN
4	6	698	ASN
5	7	68	GLN
5	7	124	ASN
5	7	320	GLN
6	H	46	ASN
6	H	182	ASN
6	H	188	GLN
7	I	35	GLN
7	I	146	GLN
7	I	172	ASN
8	C	103	HIS
9	D	69	ASN
9	D	82	GLN
9	D	109	GLN
10	E	141	GLN
10	E	155	GLN
10	E	229	GLN
10	E	468	ASN
10	E	604	ASN
11	F	184	ASN
11	F	281	ASN
11	F	397	HIS
11	F	528	ASN
11	F	553	HIS
12	G	1391	ASN
12	G	1422	ASN
12	G	1626	ASN
12	G	1702	GLN
12	G	1722	ASN
12	G	1864	ASN
12	G	1950	GLN
12	G	1975	ASN
12	G	2022	GLN
12	G	2060	HIS

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Mol	Chain	Res	Type
15	5	43	GLN
15	5	155	HIS
15	5	284	ASN
15	5	302	ASN
15	5	424	GLN
15	5	454	GLN
15	5	499	GLN
15	5	574	ASN
15	5	768	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](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	ADP	6	1201	-	28,29,29	1.40	4 (14%)	43,45,45	1.81	10 (23%)
16	ATP	7	901	18	32,33,33	0.31	0	48,52,52	0.38	0
16	ATP	2	901	-	32,33,33	0.29	0	48,52,52	0.33	0
16	ATP	3	1101	18	32,33,33	0.34	0	48,52,52	0.31	0
16	ATP	5	1701	18	32,33,33	0.37	0	48,52,52	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	ADP	4	1001	-	28,29,29	1.42	5 (17%)	43,45,45	1.86	8 (18%)

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
19	ADP	6	1201	-	-	6/16/32/32	0/3/3/3
16	ATP	7	901	18	-	8/22/38/38	0/3/3/3
16	ATP	2	901	-	-	5/22/38/38	0/3/3/3
16	ATP	3	1101	18	-	1/22/38/38	0/3/3/3
16	ATP	5	1701	18	-	0/22/38/38	0/3/3/3
19	ADP	4	1001	-	-	4/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1001	ADP	C5-C4	4.74	1.47	1.39
19	6	1201	ADP	C5-C4	4.65	1.47	1.39
19	4	1001	ADP	C5-C6	2.70	1.48	1.41
19	6	1201	ADP	C5-C6	2.64	1.48	1.41
19	4	1001	ADP	C5-N7	-2.31	1.34	1.39
19	6	1201	ADP	C8-N7	2.31	1.36	1.31
19	6	1201	ADP	C5-N7	-2.24	1.35	1.39
19	4	1001	ADP	C8-N7	2.22	1.35	1.31
19	4	1001	ADP	PA-O3A	2.00	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1001	ADP	C5-C4-N3	-6.19	118.19	126.72
19	6	1201	ADP	C5-C4-N3	-5.67	118.92	126.72
19	4	1001	ADP	N3-C4-N9	4.92	135.53	127.17
19	6	1201	ADP	N3-C4-N9	4.57	134.93	127.17
19	4	1001	ADP	C2-N3-C4	3.81	121.14	111.83
19	6	1201	ADP	C2-N3-C4	3.66	120.77	111.83
19	6	1201	ADP	C4-C5-N7	-3.36	106.74	110.58
19	4	1001	ADP	C4-C5-N7	-3.35	106.75	110.58
19	6	1201	ADP	N3-C2-N1	-3.31	123.58	128.58
19	4	1001	ADP	N3-C2-N1	-3.17	123.78	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	1201	ADP	C4-N9-C8	2.81	108.69	105.74
19	4	1001	ADP	C3'-C2'-C1'	2.63	106.44	101.46
19	6	1201	ADP	C5-N7-C8	2.49	107.37	103.45
19	4	1001	ADP	C5-N7-C8	2.44	107.28	103.45
19	4	1001	ADP	C4-N9-C8	2.31	108.16	105.74
19	6	1201	ADP	C3'-C2'-C1'	2.22	105.67	101.46
19	6	1201	ADP	C6-C5-N7	2.10	136.13	132.09
19	6	1201	ADP	N9-C8-N7	-2.02	111.06	113.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

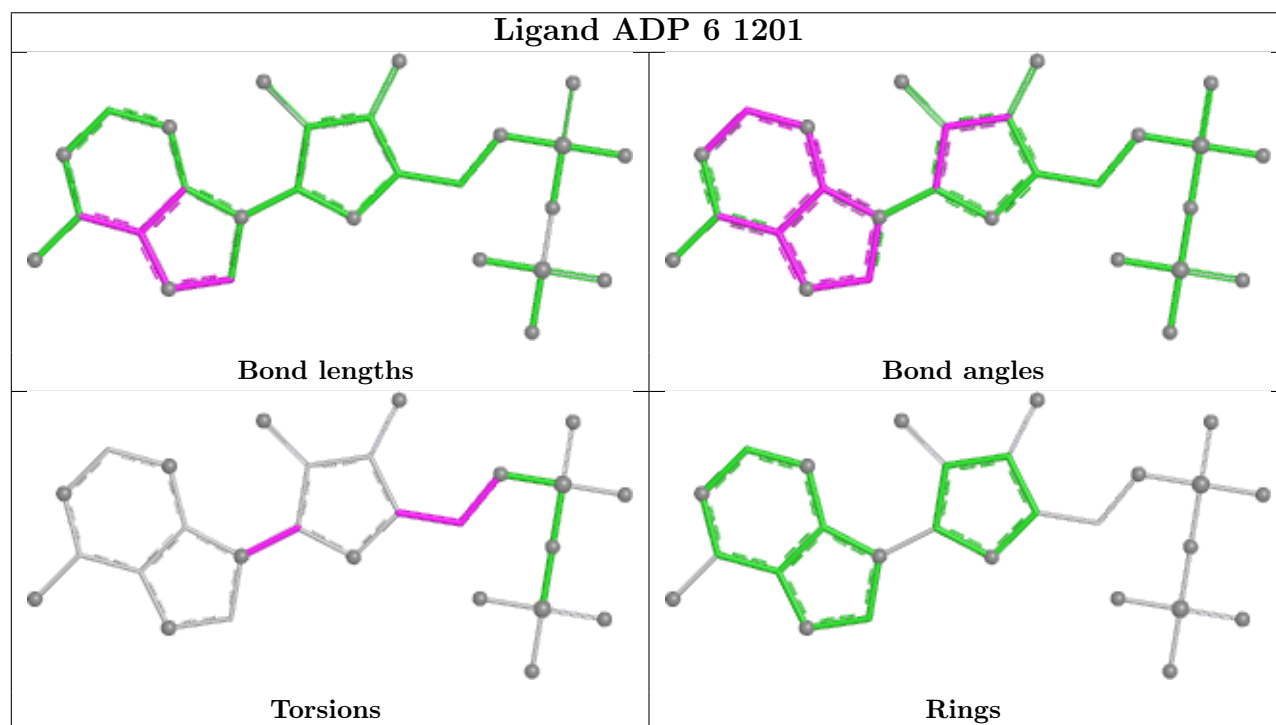
Mol	Chain	Res	Type	Atoms
16	7	901	ATP	PB-O3B-PG-O2G
16	7	901	ATP	C5'-O5'-PA-O3A
16	7	901	ATP	C4'-C5'-O5'-PA
19	4	1001	ADP	C5'-O5'-PA-O1A
19	4	1001	ADP	C5'-O5'-PA-O2A
19	4	1001	ADP	C5'-O5'-PA-O3A
19	6	1201	ADP	O4'-C4'-C5'-O5'
19	6	1201	ADP	C3'-C4'-C5'-O5'
16	2	901	ATP	O4'-C1'-N9-C8
16	2	901	ATP	O4'-C1'-N9-C4
19	6	1201	ADP	C2'-C1'-N9-C8
16	2	901	ATP	O4'-C4'-C5'-O5'
16	2	901	ATP	C3'-C4'-C5'-O5'
16	7	901	ATP	PB-O3B-PG-O3G
16	7	901	ATP	C2'-C1'-N9-C4
19	6	1201	ADP	C2'-C1'-N9-C4
19	6	1201	ADP	C4'-C5'-O5'-PA
16	7	901	ATP	C2'-C1'-N9-C8
16	7	901	ATP	C5'-O5'-PA-O1A
16	3	1101	ATP	PA-O3A-PB-O2B
19	4	1001	ADP	O4'-C4'-C5'-O5'
16	2	901	ATP	PA-O3A-PB-O1B
16	7	901	ATP	PB-O3B-PG-O1G
19	6	1201	ADP	O4'-C1'-N9-C8

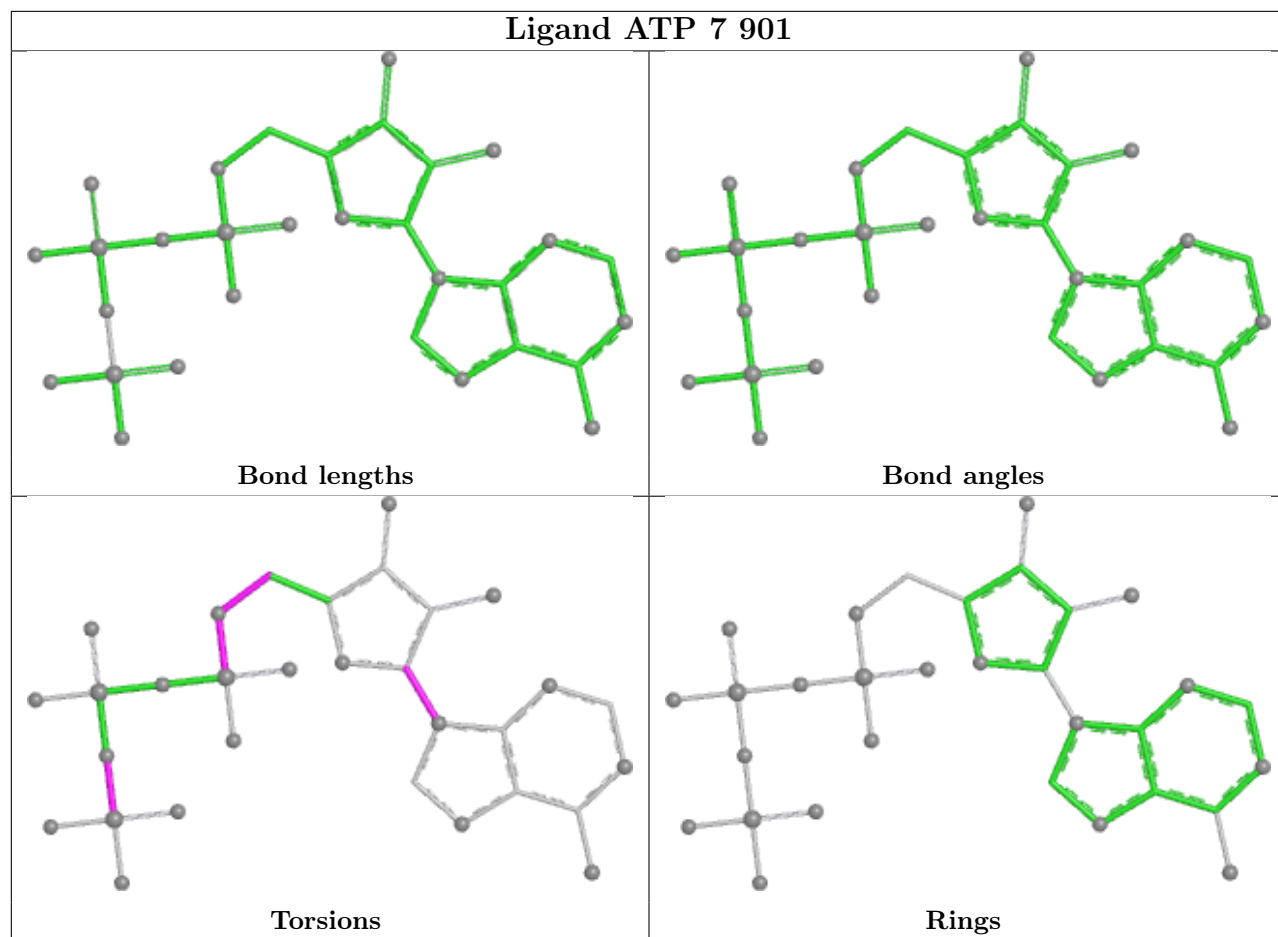
There are no ring outliers.

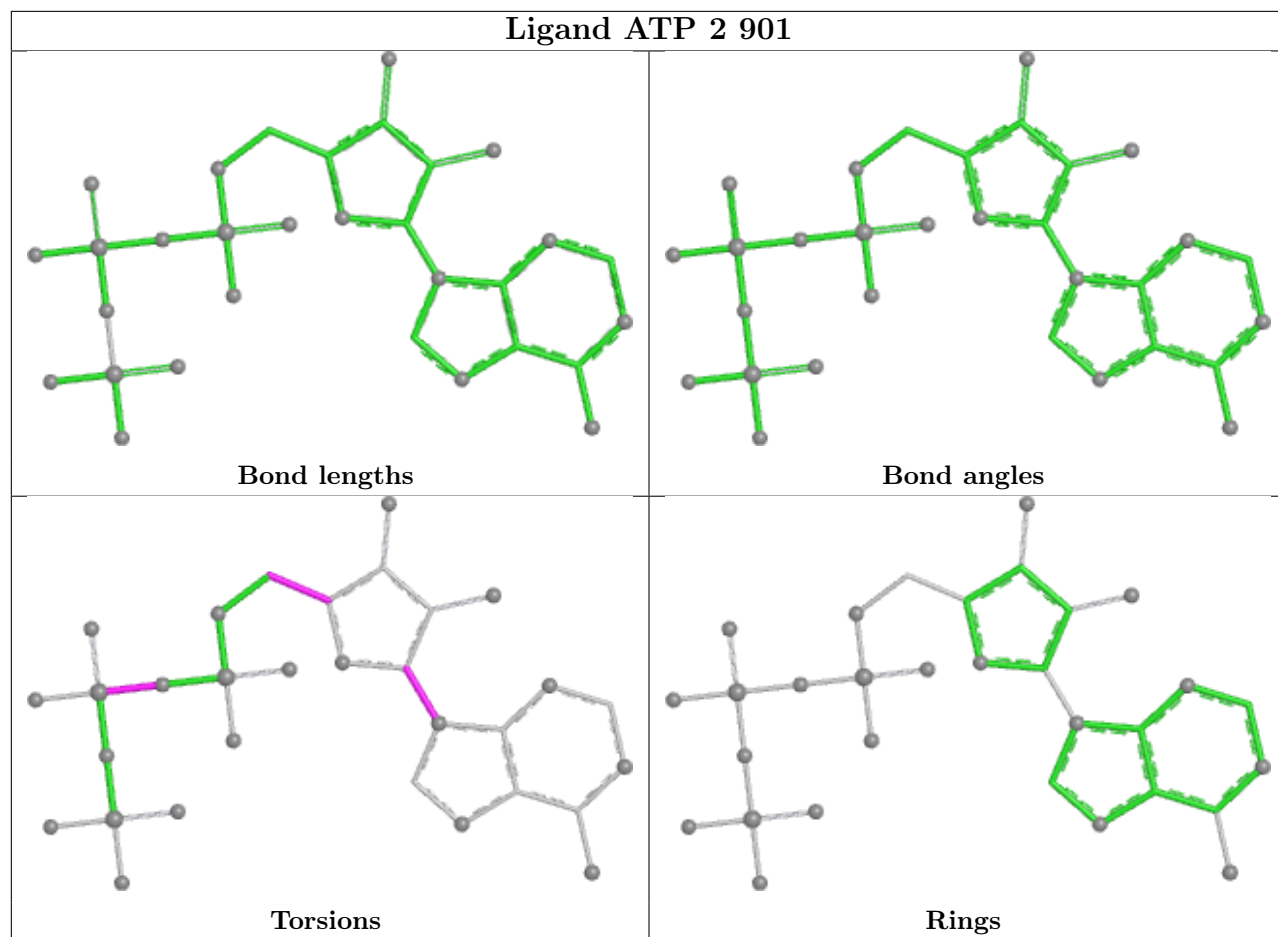
2 monomers are involved in 5 short contacts:

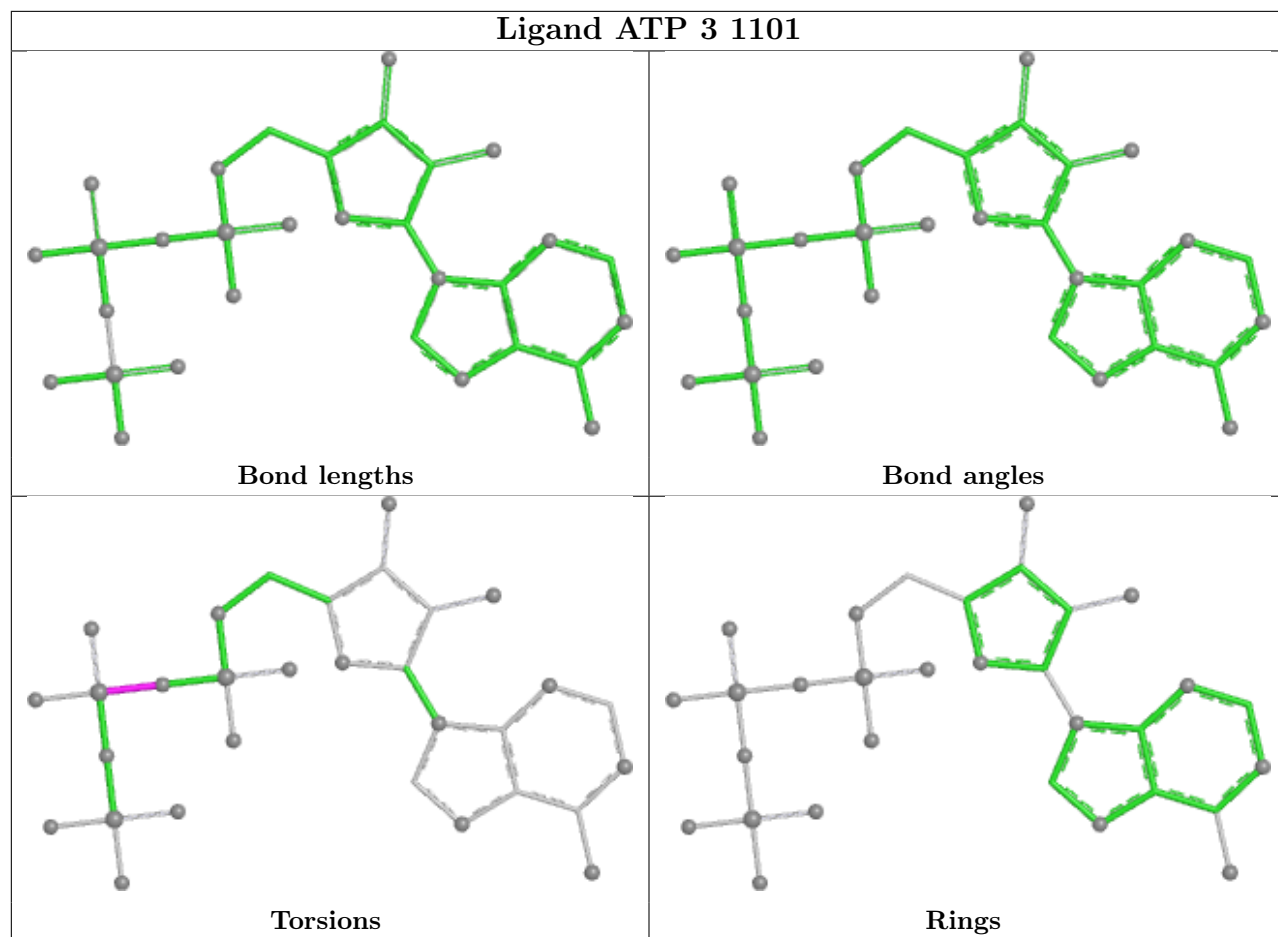
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	1201	ADP	4	0
16	7	901	ATP	1	0

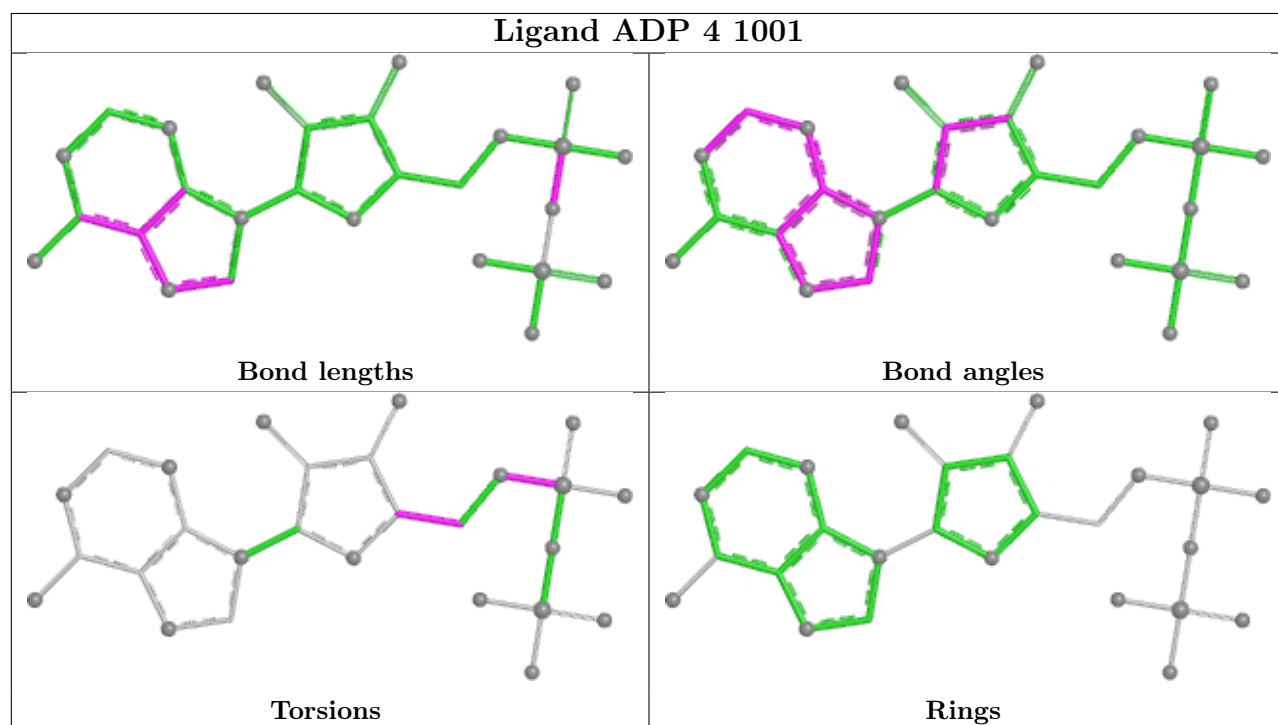
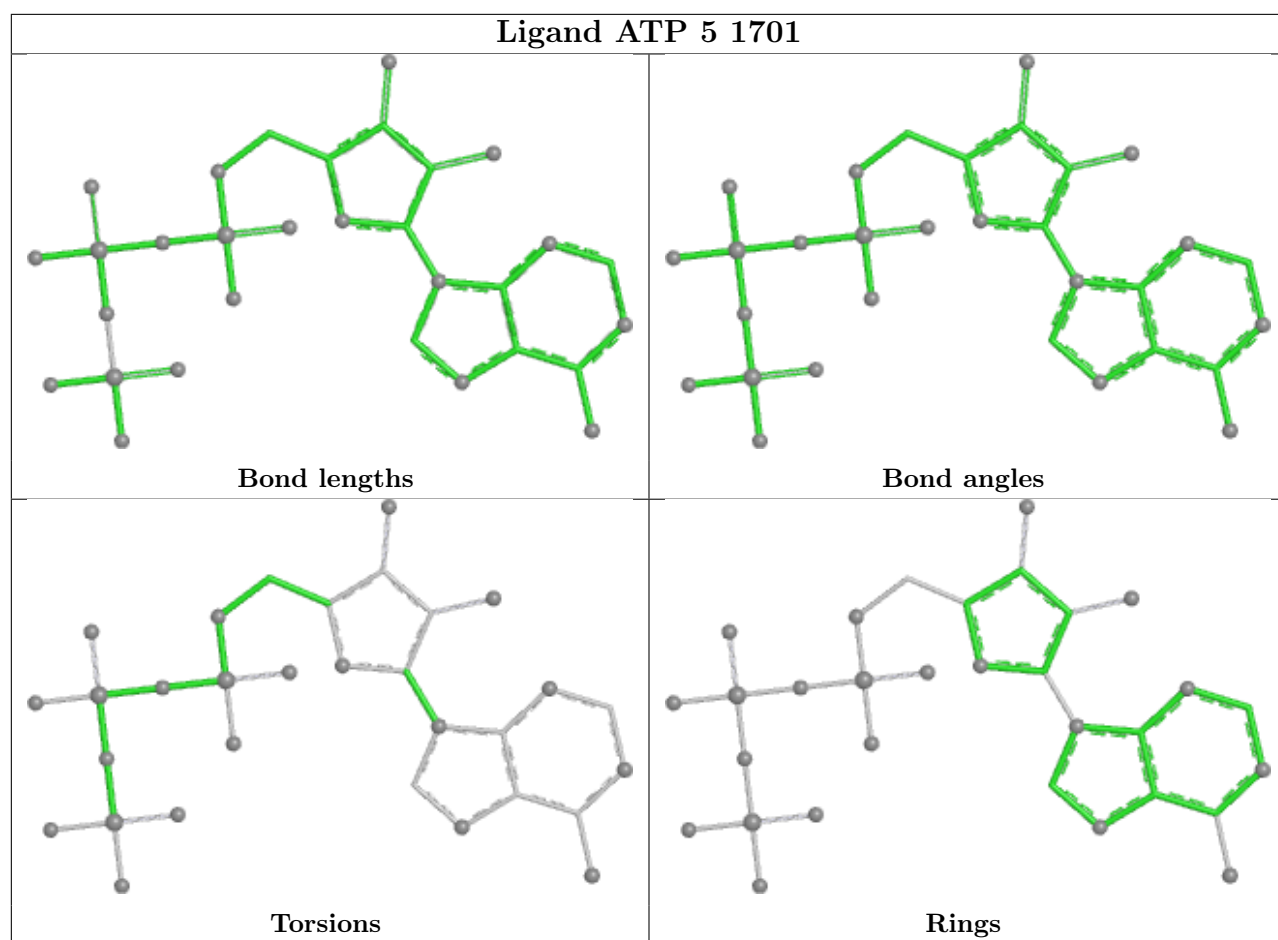
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

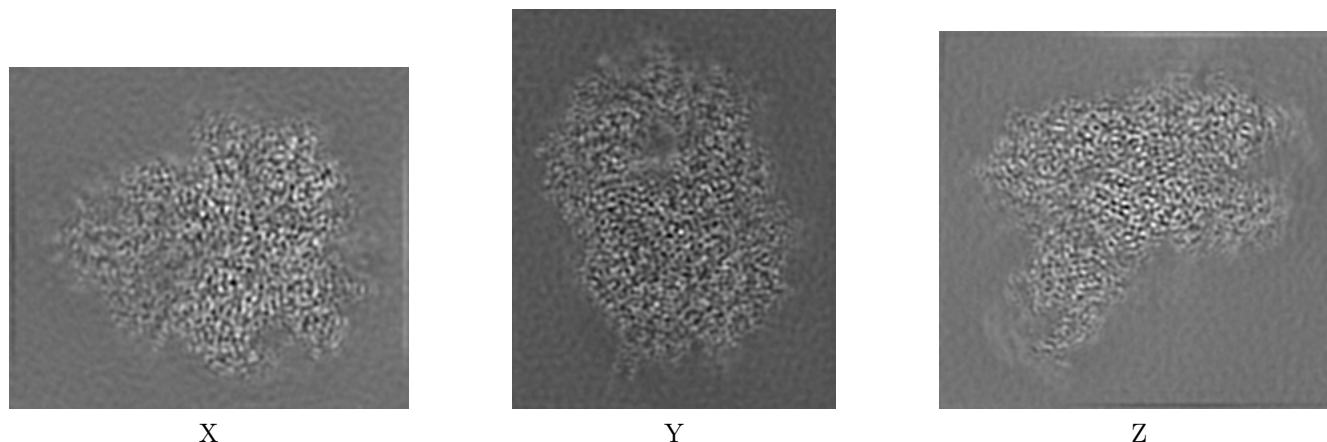
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13978. These allow visual inspection of the internal detail of the map and identification of artifacts.

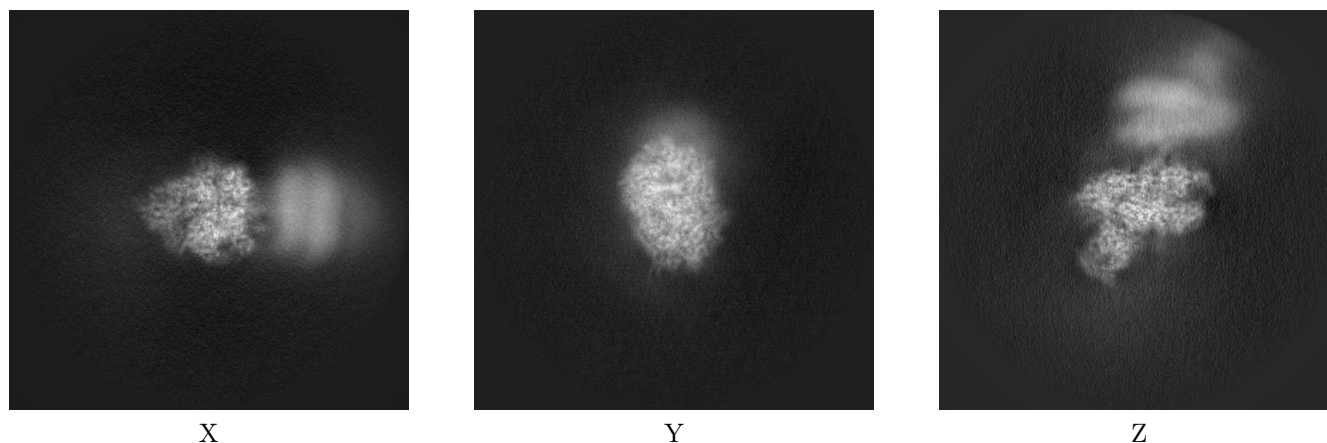
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



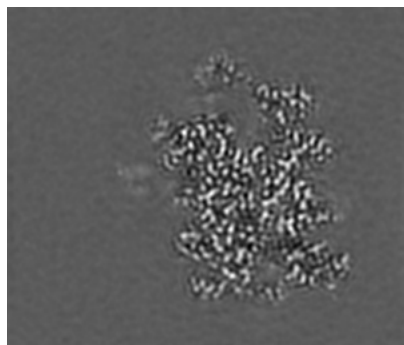
6.1.2 Raw map



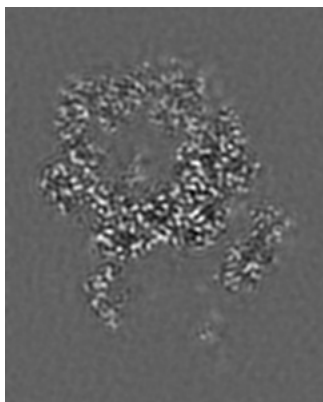
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

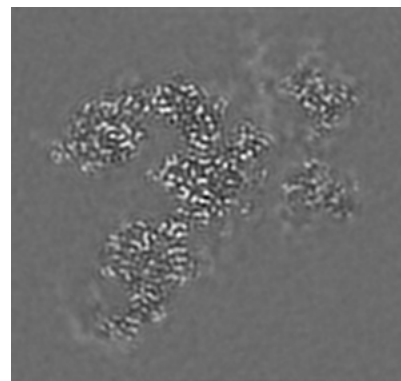
6.2.1 Primary map



X Index: 102

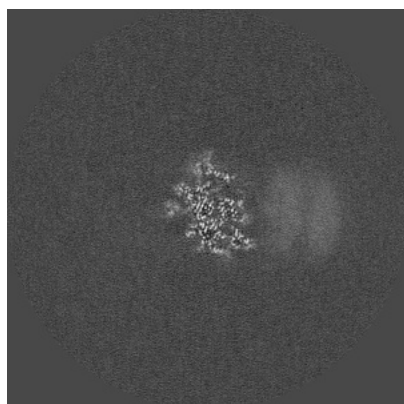


Y Index: 97

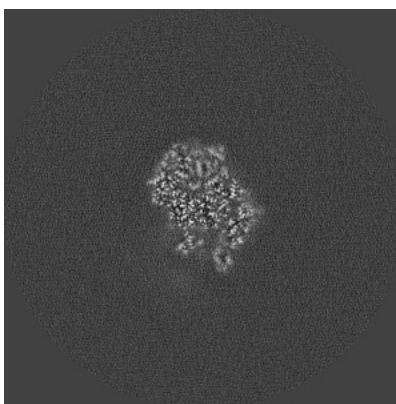


Z Index: 83

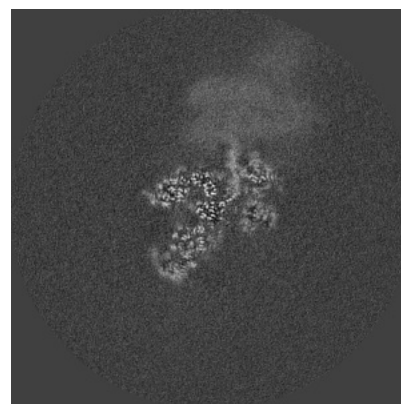
6.2.2 Raw map



X Index: 256



Y Index: 256

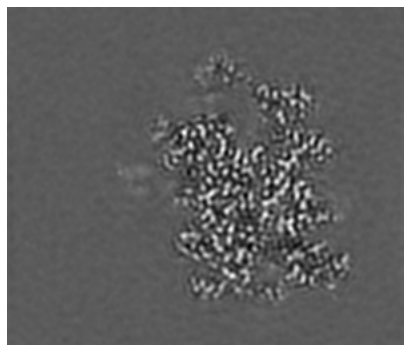


Z Index: 256

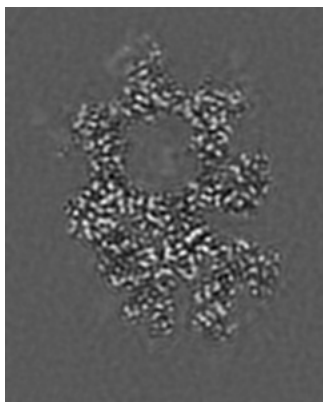
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

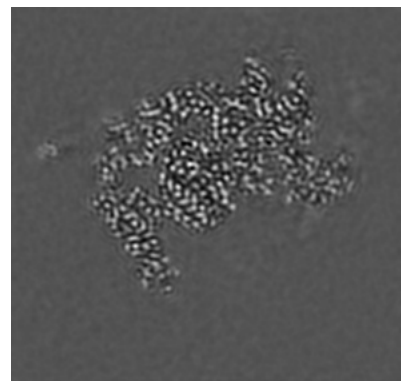
6.3.1 Primary map



X Index: 102

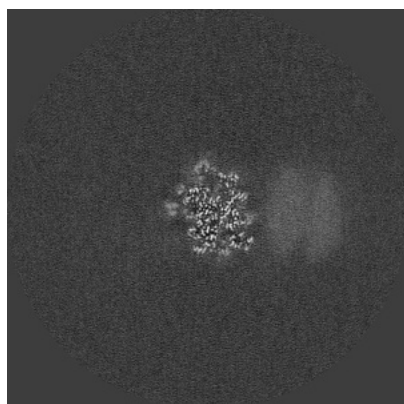


Y Index: 141

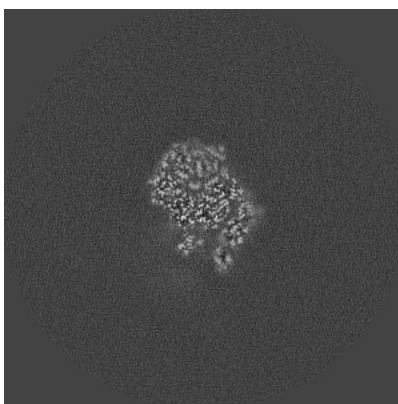


Z Index: 51

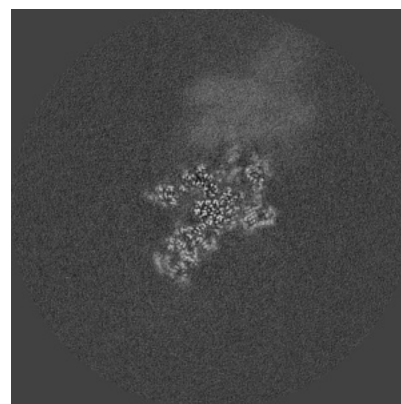
6.3.2 Raw map



X Index: 260



Y Index: 255

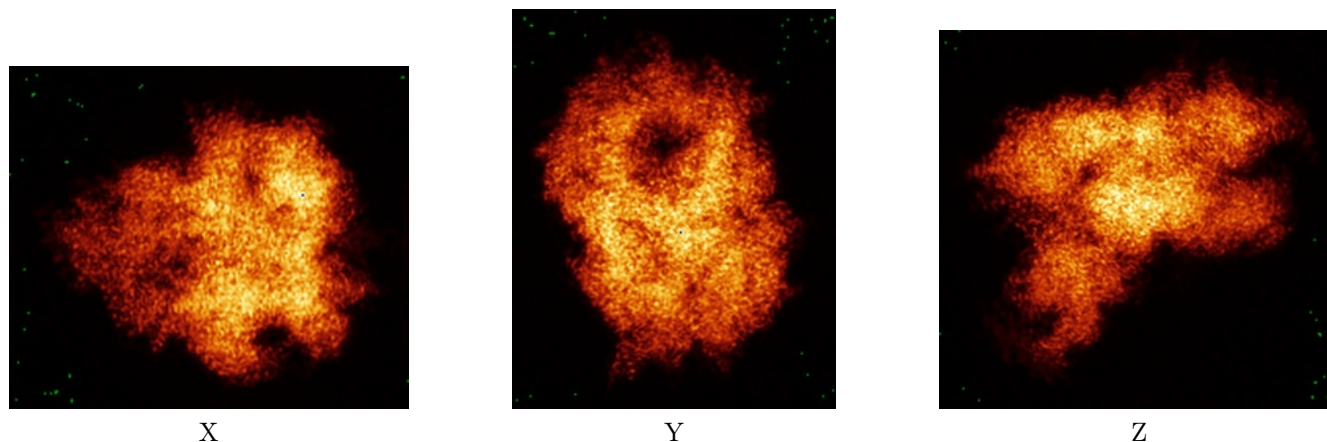


Z Index: 261

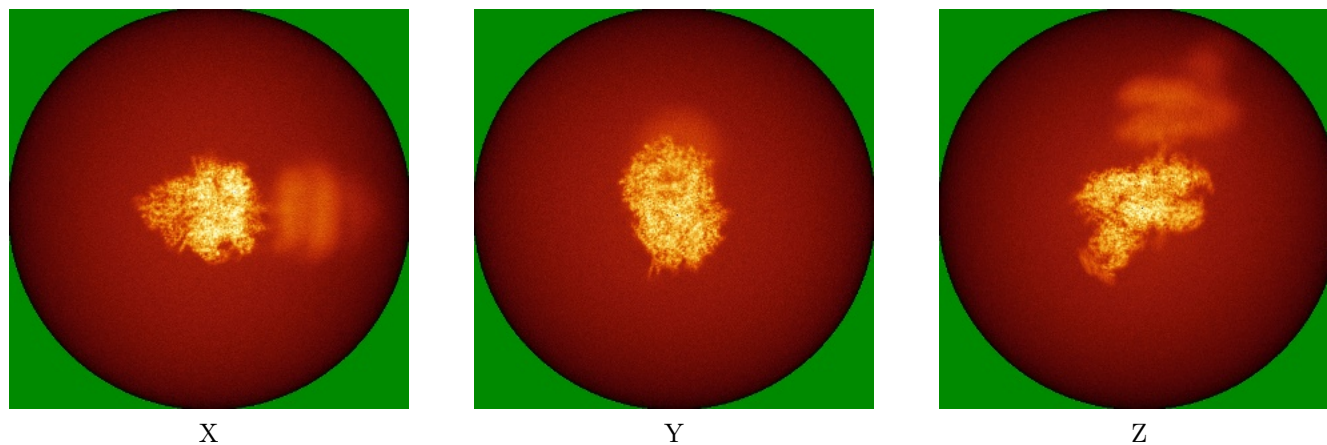
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



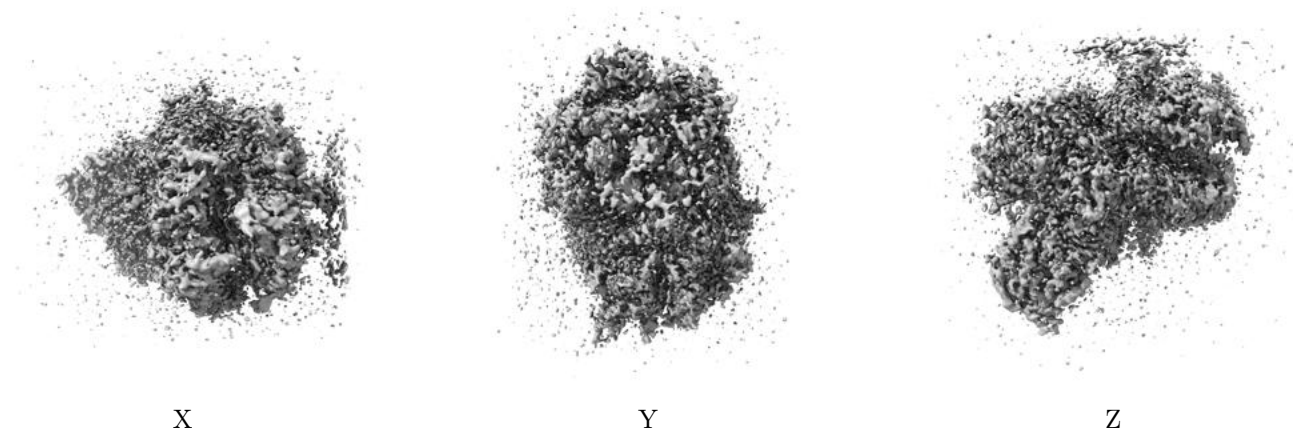
6.4.2 Raw map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

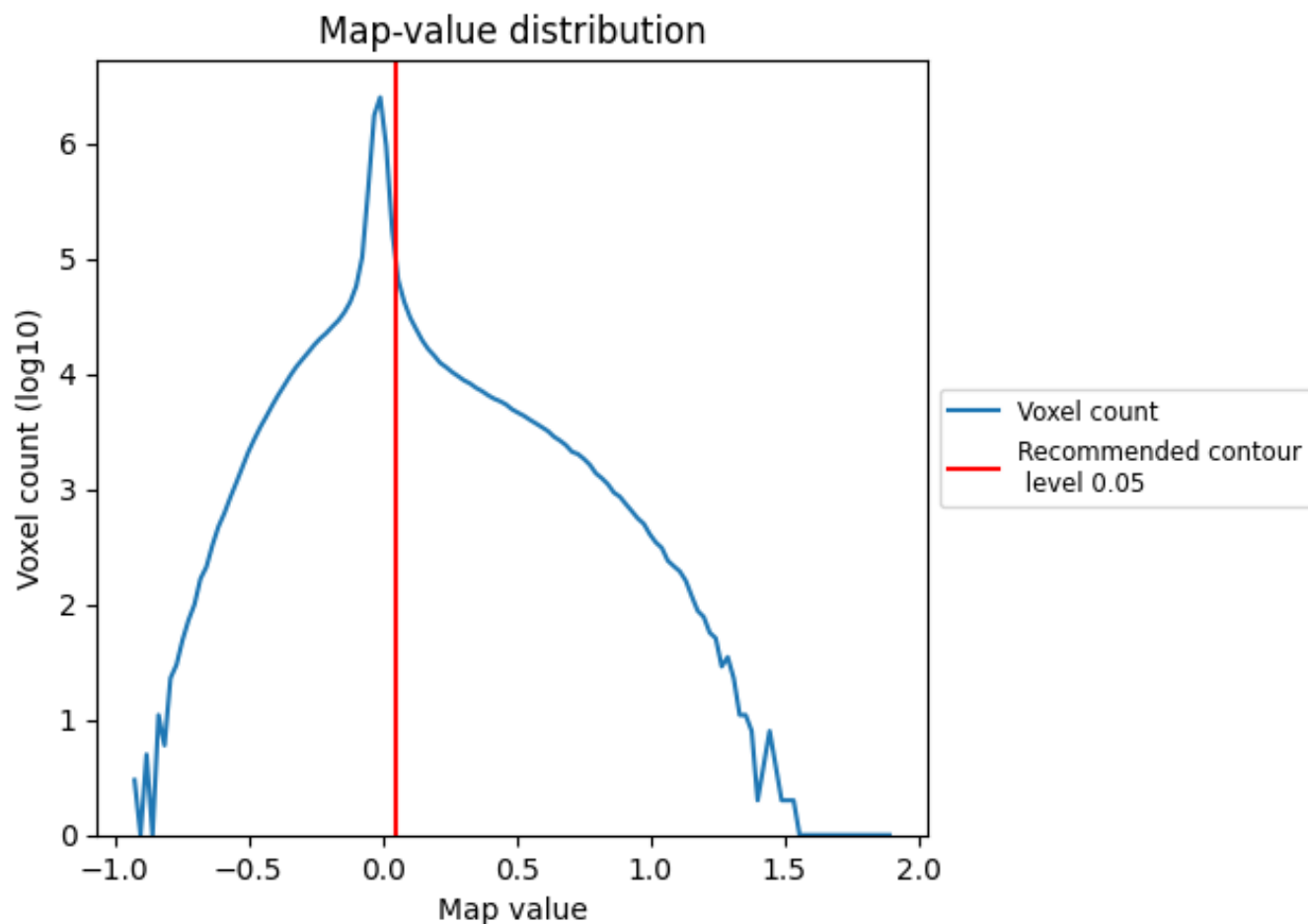
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

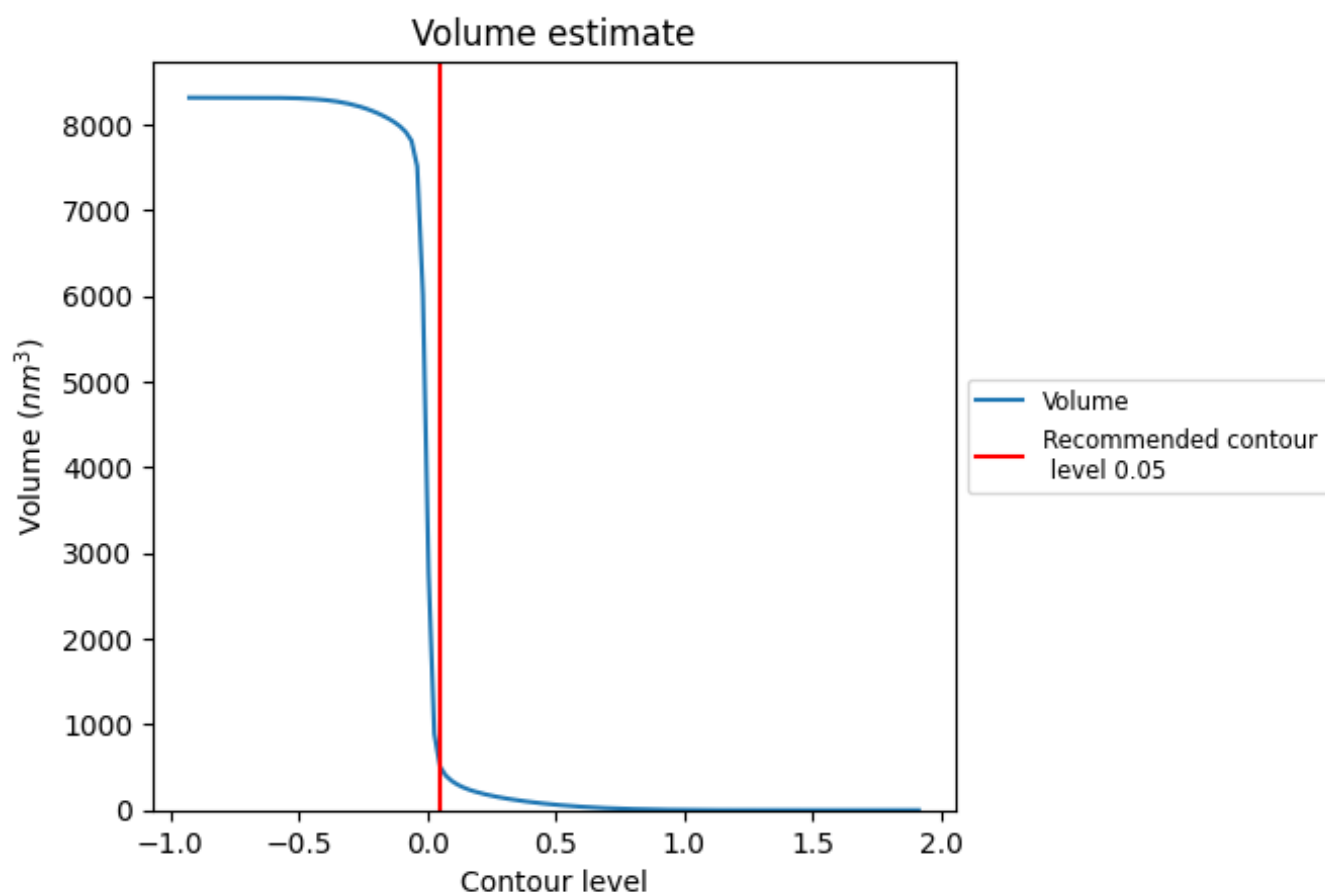
This section contains the results of statistical analysis of the map.

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 507 nm^3 ; this corresponds to an approximate mass of 458 kDa.

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

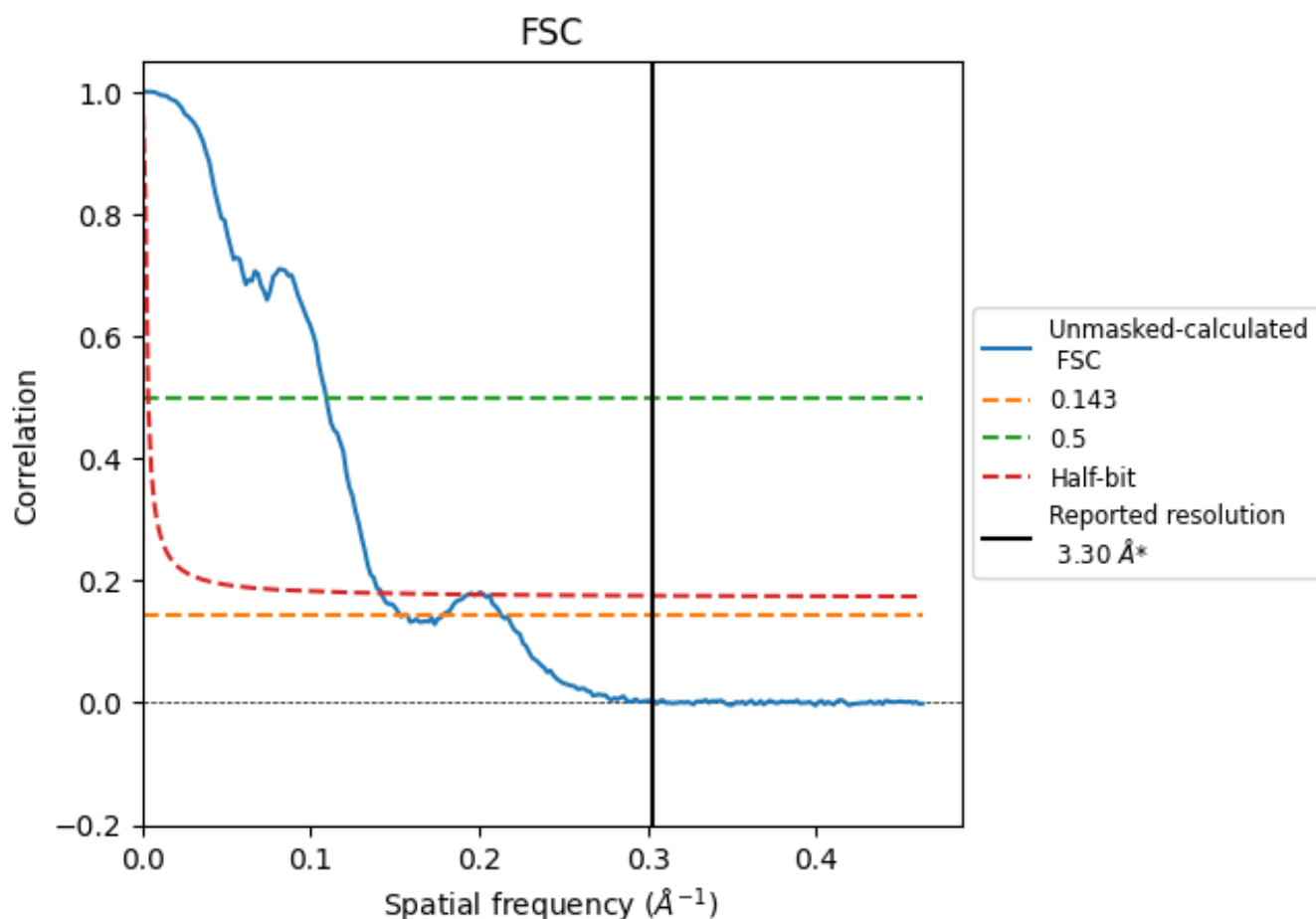
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	9.16	7.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.53 differs from the reported value 3.3 by more than 10 %

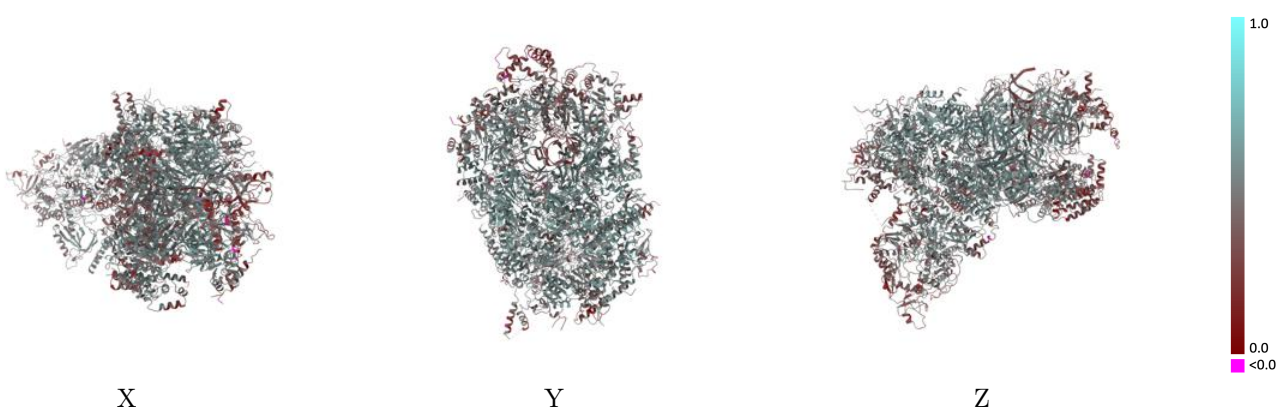
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13978 and PDB model 7QHS. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

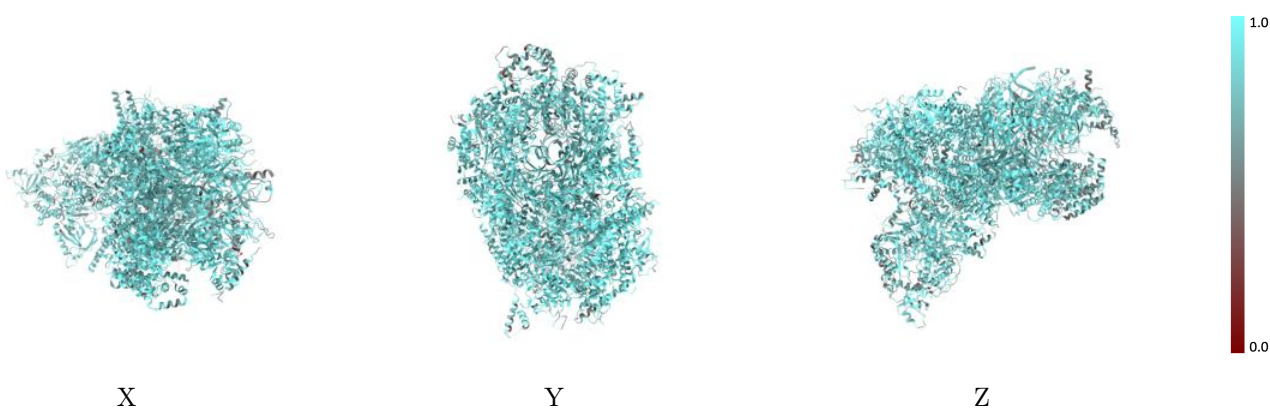
This section was not generated.

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



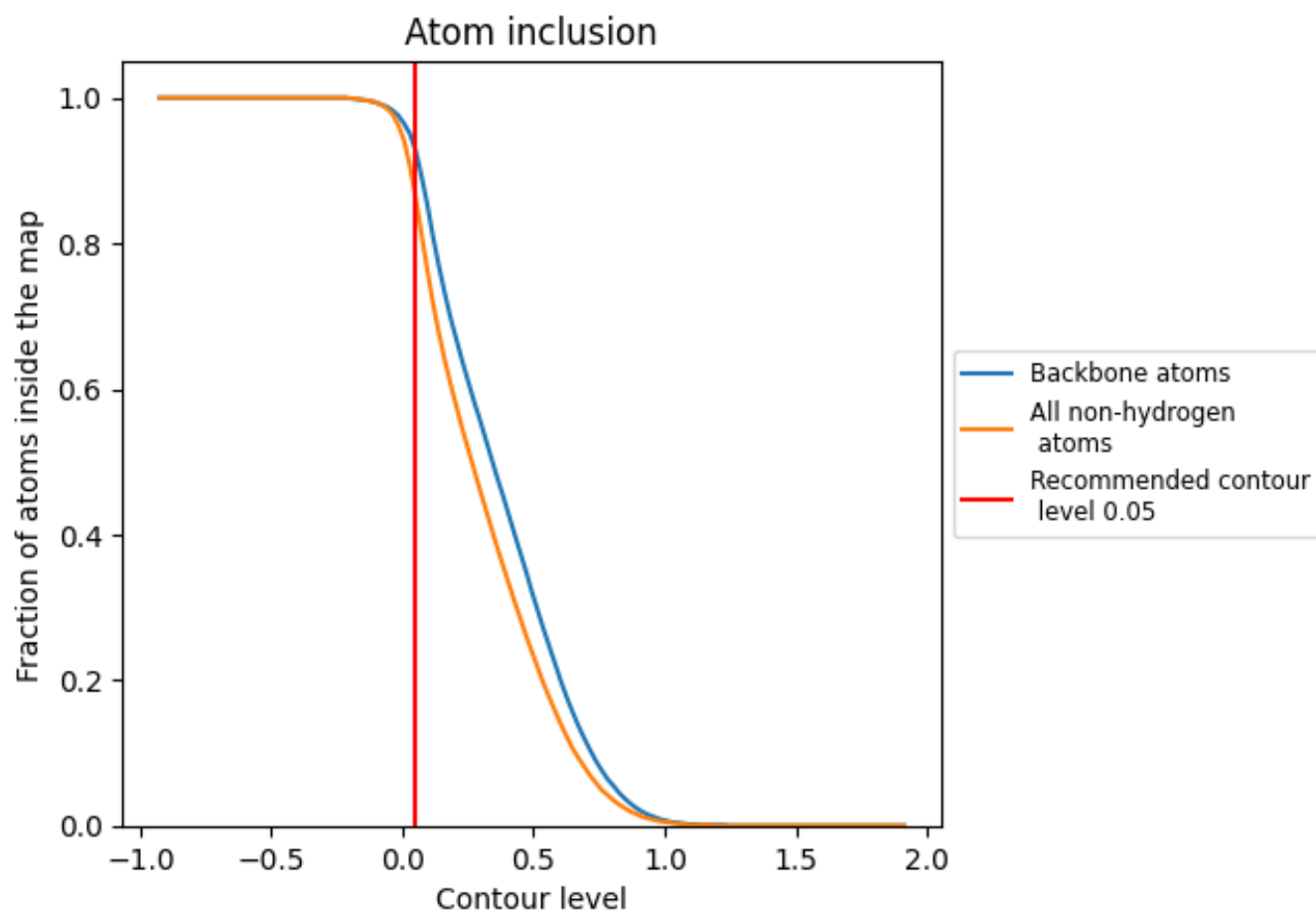
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.4730
2	0.9180	0.5340
3	0.9110	0.5200
4	0.8040	0.4010
5	0.9040	0.5270
6	0.8700	0.4810
7	0.7980	0.4020
A	0.8430	0.3860
B	0.7600	0.3370
C	0.8950	0.5100
D	0.8650	0.4760
E	0.8970	0.5040
F	0.8310	0.4380
G	0.8310	0.4480
H	0.8400	0.4550
I	0.9140	0.5240

