Full wwPDB EM Validation Report ⓘ

Aug 20, 2026 – 05:16 PM EDT

PDB ID	:	12JV / pdb_000012jv
EMDB ID	:	EMD-76497
Title	:	Structural determination of lipid-bound Factor VIII
Authors	:	Mohammed, B.M.
Deposited on	:	2026-04-08
Resolution	:	3.56 Å(reported)
Based on initial models	:	., 12JP, 3CDZ

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:

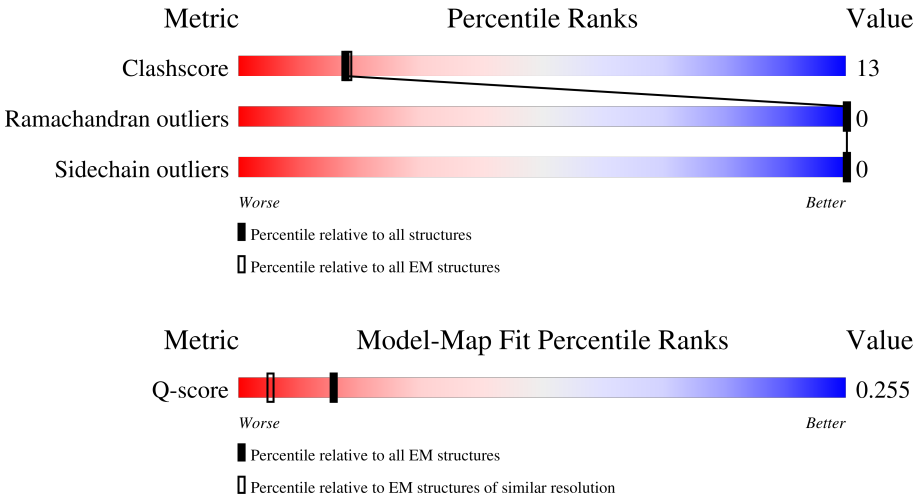
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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	12750 (3.06 - 4.06)

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

Mol	Chain	Length	Quality of chain
1	A	2332	37% 16% 47%

2 Entry composition

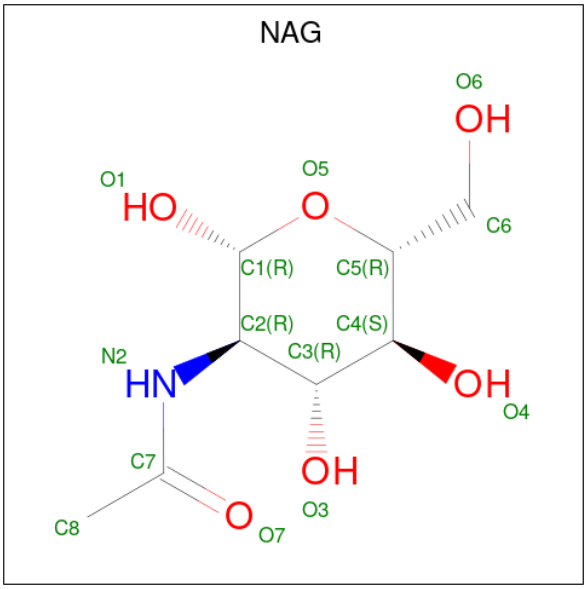
There are 4 unique types of molecules in this entry. The entry contains 10145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1247	10100	6499	1716	1829	56	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Ca 1 1	0

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Cu 2 2	0

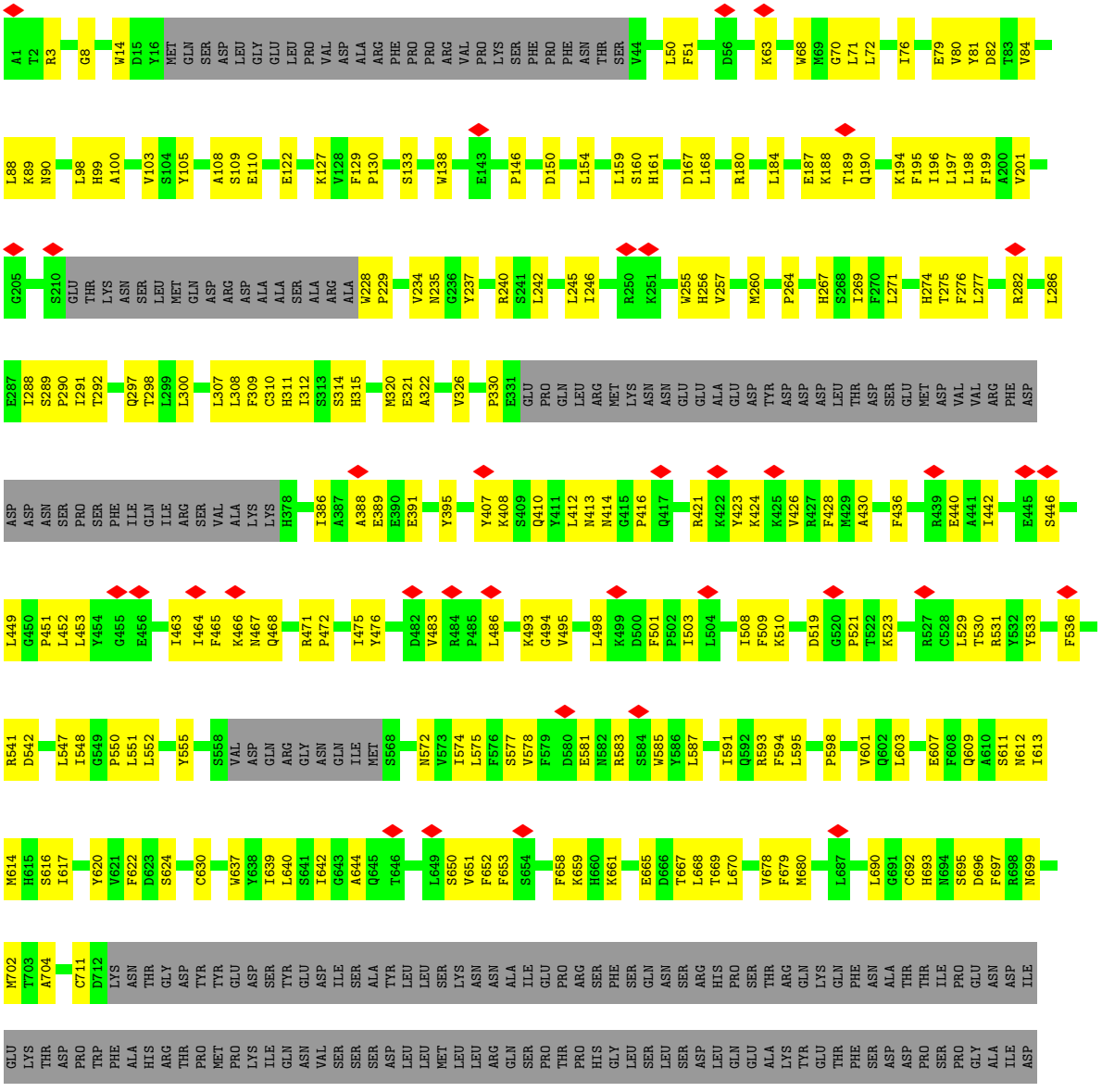
3 Residue-property plots (i)

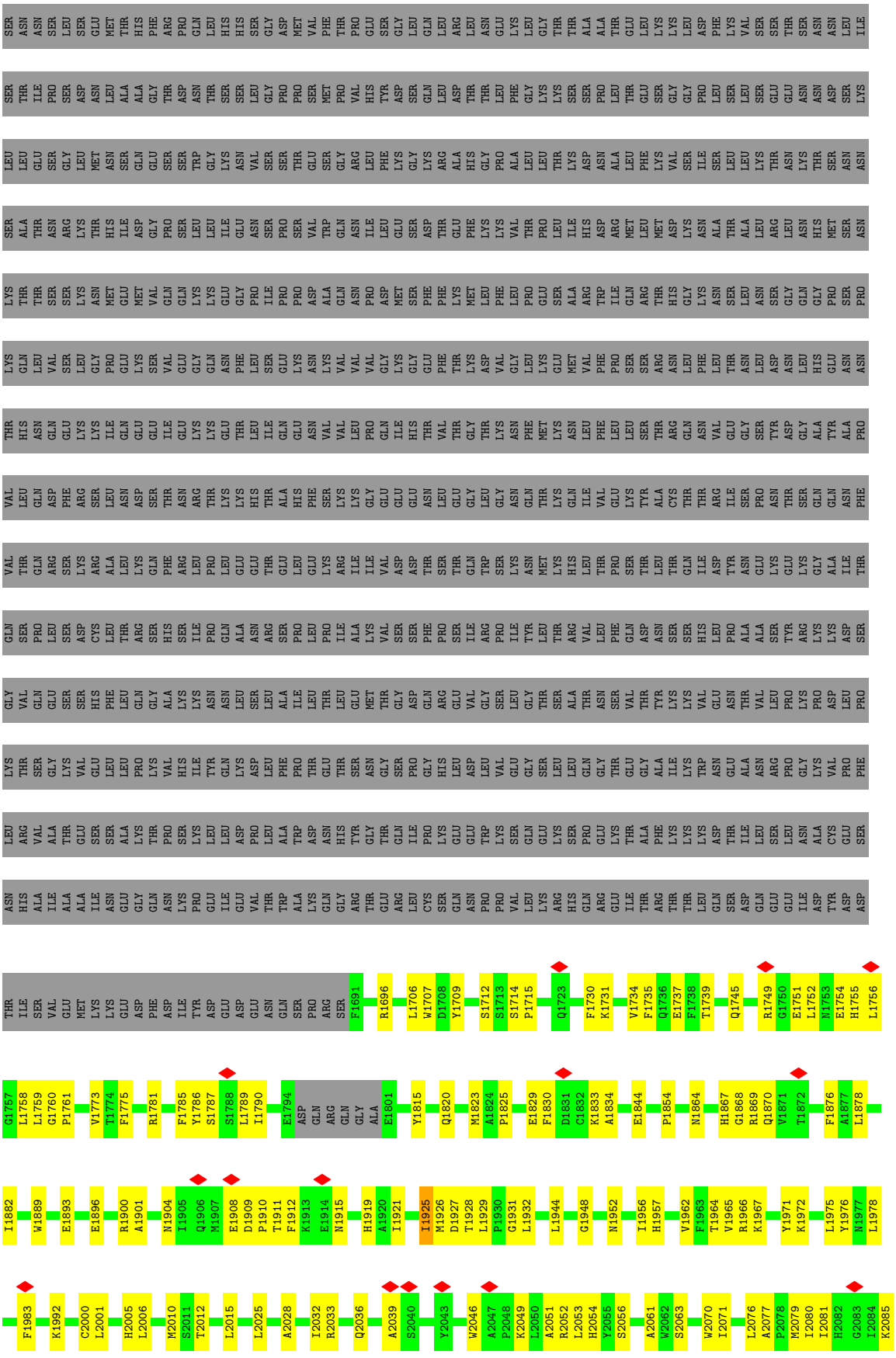
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

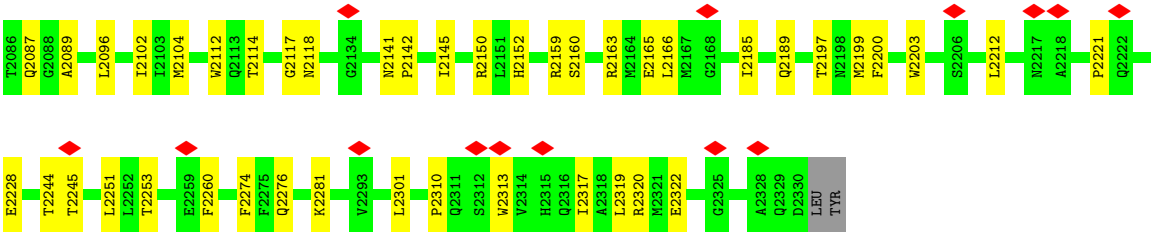
- Molecule 1: Coagulation factor VIII

Chain A:






SER ASN ASN SER LEU SER GLU MET THR HIS PHE ARG PRO GLN LEU HIS HIS SER GLY ASP MET VAL PHE THR PRO GLU SER GLY LEU GLN LEU ARG LEU ASN GLU GLU LYS LEU GLY THR THR ALA ALA THR GLU LEU LYS LEU ASP PHE LYS VAL SER SER THR SER GLU GLU ASN ASN ASP SER LYS
SER THR ILE PRO SER ASP ALA ALA GLY THR ASP ASN THR HIS SER SER LEU GLY PRO VAL HIS TYR ASP SER GLN LEU ASP THR THR LEU PHE GLY LYS LYS SER SER PRO LEU THR GLU SER GLY GLY PRO LEU SER LEU SER GLU GLU ASN ASN ASP SER
LEU LEU GLU SER GLY LEU MET ASN SER GLN GLU GLU SER SER TRP GLY LYS ASN VAL SER SER THR GLU SER GLY ARG LEU PHE LYS GLY LYS ARG ALA HIS GLY PRO ALA LEU LEU THR LYS ASP ASN ALA LEU PHE LYS VAL SER ILE SER LEU LEU LYS THR ASN LYS THR ASN ASN
SER ALA THR ASN ARG LYS THR HIS ILE ASP GLY PRO SER LEU LEU ILE GLU GLU ASN SER PRO SER VAL TRP GLN ASN ILE LEU GLU SER ASP THR GLU HIS ASP ARG MET LEU MET ASP LYS ASN ALA THR GLU ASN ARG LEU ASN SER ASP ASN HIS MET SER ASN
LYS THR THR SER SER LYS ASN MET GLU MET VAL GLN GLN LYS LYS LYS GLU GLY PRO ILE PRO PRO ASP MET SER SER PHE PHE LYS MET LEU PHE LEU PRO GLU SER ALA ARG TRP ILE GLN ARG THR HIS GLY LYS ASN SER LEU ASN SER GLY GLN LEU HIS GLU SER PRO
LYS GLN LEU VAL SER LEU GLY PRO GLU LYS GLY GLN ASN GLU SER VAL GLU GLY LYS ASN LYS LYS VAL GLU GLY PHE LEU SER GLU LYS SER VAL VAL LEU GLY LEU LYS LYS GLU MET VAL PHE PRO SER SER ARG THR ASN LEU PHE LEU ASP ASN SER LEU ASP ASN ASN ASN
THR HIS ASN GLN GLU LYS LYS ILE GLN GLU GLU ILE GLU LYS LYS GLU THR LEU ILE GLU GLN GLU ASN VAL VAL LEU PRO GLN ILE HIS THR VAL THR GLY THR LYS ASN PHE MET LYS ASN LEU PHE LEU SER THR ARG GLN ASN VAL GLU GLY SER TYR ASP GLY ALA TYR ALA PRO
VAL LEU GLN ASP PHE ARG SER LEU ASN ASP SER THR ASN ARG THR LYS LYS HIS THR ALA HIS PHE SER LYS LYS GLY GLU GLU GLU ASN LEU GLU GLU THR LYS GLN ILE LEU VAL GLU LYS TYR ALA CYS THR THR ARG ILE SER PRO ASN THR SER GLN GLN ASN PHE
VAL THR GLN ARG SER LYS ARG ALA LEU LYS GLN PHE ARG LEU PRO LEU GLU GLU GLU THR GLU LEU GLU LYS ARG ILE ILE VAL ASP ASP THR SER THR GLN TRP SER LYS ASN MET LYS HIS LEU LEU THR PRO SER THR LEU THR GLN ILE ASP TYR ASN GLU GLU LYS GLU LYS GLY ALA ILE THR
GLN SER PRO LEU SER ASP CYS LEU THR ARG SER HIS SER ILE PRO GLN ALA ASN ARG SER SER PRO LEU PRO ILE ALA LYS VAL SER SER PHE PRO SER ILE ARG PRO ILE TYR LEU THR ARG VAL LEU PHE GLN ASP ASN SER SER HIS LEU PRO ALA ALA SER TYR ARG LYS LYS ASP SER
GLY VAL GLN GLU SER ASP ASN LEU ASP SER GLU THR LEU GLU MET THR GLU GLN ASN SER VAL THR TYR LYS LYS VAL GLU GLU ASN VAL THR PRO LYS PRO ASP LEU PRO
LYS THR SER GLY LYS VAL GLU LEU LEU ASP ASP LEU ASP LEU VAL GLU GLY SER LEU GLY THR SER ALA THR ASN SER VAL THR TYR ALA ILE LYS LYS TRP THR GLU GLY ALA ILE LYS ASN ARG PRO GLY LYS VAL PRO PHE
LEU ARG VAL ALA THR GLU SER SER ALA LYS THR PRO ASP ASN HIS TYR GLY THR GLN ILE PRO LYS GLU GLU TRP LYS SER GLN GLU LYS GLU GLN ASN GLU ASP PRO VAL GLU LYS THR ALA PHE LYS LYS LYS ASP THR ILE ALA ASN ALA CYS GLU SER
ASN HIS ALA ILE ALA ALA ILE ASN GLU GLY GLN ASN LYS PRO GLU ILE ASP VAL THR TRP ALA LYS GLN GLY ARG THR GLU ARG LEU CYS SER GLN ASN PRO GLU LEU VAL ILE ASP PRO PRO VAL LEU LYS GLN ARG GLU ILE THR ARG THR THR LEU GLN SER ASP GLN GLU GLU ILE ASP TYR ASP ASP
THR ILE SER VAL GLU MET F1691 R1696 L1706 W1707 D1708 Y1709 S1712 S1713 S1714 P1715 Q1723 F1730 K1731 V1734 F1735 Q1736 E1737 F1738 T1739 Q1745 R1749 G1750 E1751 L1752 N1753 E1754 H1755 L1756
G1757 L1758 L1759 G1760 P1761 V1773 T1774 F1775 R1781 F1785 Y1786 S1787 S1788 L1789 I1790 E1794 ASP GLN ARG GLY ALA E1801 Y1815 Q1820 M1823 A1824 P1825 E1829 F1830 D1831 C1832 K1833 A1834 E1844 P1864 N1864 H1867 G1868 R1869 Q1870 V1871 T1872 F1876 A1877 L1878
I1882 W1889 E1893 E1896 R1900 A1901 N1904 I1905 Q1906 M1907 E1908 D1909 P1910 T1911 F1912 K1913 E1914 N1915 H1919 A1920 I1921 I1925 M1926 D1927 T1928 L1929 P1930 G1931 L1932 L1944 G1948 N1952 I1956 H1957 V1962 F1963 T1964 V1965 R1966 K1967 Y1971 K1972 L1975 Y1976 N1977 L1978
F1983 K1992 C2000 L2001 H2005 L2006 M2010 S2011 T2012 L2015 L2025 A2028 I2032 R2033 Q2036 A2039 S2040 Y2043 W2046 A2047 P2048 K2049 L2050 A2051 R2052 L2053 H2054 Y2055 S2056 A2061 W2062 S2063 W2070 I2071 L2076 A2077 P2078 M2079 I2080 I2081 H2082 G2083 I2084 K2085


T2086
Q2087
G2088
A2089
L2096
I2102
I2103
M2104
W2112
Q2113
T2114
G2117
N2118
G2134
N2141
P2142
I2145
R2150
L2151
H2152
R2159
S2160
R2163
M2164
E2165
L2166
M2167
G2168
I2185
Q2189
T2197
N2198
M2199
F2200
W2203
S2206
L2212
N2217
A2218
P2221
Q2222
E2228
T2244
T2245
L2251
L2262
T2253
E2259
F2260
F2274
F2275
Q2276
K2281
V2293
L2301
P2310
Q2311
S2312
W2313
V2314
H2315
Q2316
I2317
A2318
L2319
R2320
M2321
E2322
G2325
A2328
Q2329
D2330
LEU
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.350	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.162	Depositor
Map size (Å)	386.04797, 386.04797, 386.04797	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9279999, 0.9279999, 0.9279999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CU, 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	A	0.13	0/10388	0.35	0/14085

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1925	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10100	0	9849	270	0
2	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	2	0	0	0	0
All	All	10145	0	9888	270	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 13.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:ARG:HD3	1:A:1901:ALA:H	1.27	0.96
1:A:79:GLU:HB3	1:A:82:ASP:HB2	1.58	0.84
1:A:1904:ASN:HB2	1:A:1911:THR:HG21	1.56	0.84
1:A:639:ILE:HG22	1:A:670:LEU:HD11	1.64	0.78
1:A:1925:ILE:HD11	1:A:1929:LEU:HB3	1.67	0.76
1:A:277:LEU:HD12	1:A:282:ARG:HE	1.50	0.75
1:A:2244:THR:HB	1:A:2322:GLU:HB3	1.72	0.71
1:A:275:THR:HA	1:A:298:THR:HG22	1.73	0.70
1:A:1900:ARG:CD	1:A:1901:ALA:H	2.05	0.69
1:A:1864:ASN:H	1:A:1869:ARG:H	1.39	0.69
1:A:2005:HIS:HB3	1:A:2010:MET:HG2	1.74	0.68
1:A:541:ARG:HH11	1:A:585:TRP:HE1	1.42	0.68
1:A:2245:THR:HB	1:A:2319:LEU:HD11	1.76	0.67
1:A:1882:ILE:H	1:A:1952:ASN:HD21	1.43	0.67
1:A:591:ILE:HG21	1:A:601:VAL:HG12	1.78	0.66
1:A:1921:ILE:HB	1:A:1925:ILE:HB	1.76	0.66
1:A:1787:SER:H	1:A:1790:ILE:HD11	1.60	0.65
1:A:196:ILE:HG22	1:A:256:HIS:HB2	1.77	0.65
1:A:1715:PRO:HG2	1:A:1928:THR:HG21	1.77	0.65
1:A:2185:ILE:HG21	1:A:2189:GLN:HB3	1.79	0.65
1:A:617:ILE:HD11	1:A:704:ALA:HB2	1.79	0.64
1:A:242:LEU:HD12	1:A:322:ALA:HB1	1.80	0.64
1:A:1759:LEU:HD13	1:A:1854:PRO:HD3	1.79	0.64
1:A:277:LEU:HD22	1:A:297:GLN:HG2	1.80	0.64
1:A:2051:ALA:HB3	1:A:2056:SER:HB3	1.80	0.63
1:A:2102:ILE:HG13	1:A:2152:HIS:HB2	1.81	0.63
1:A:2096:LEU:HD22	1:A:2159:ARG:HG2	1.81	0.62
1:A:395:TYR:HE2	1:A:614:MET:HG3	1.65	0.62
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.81	0.62
1:A:575:LEU:HG	1:A:577:SER:HB2	1.80	0.62
1:A:620:TYR:HB3	1:A:624:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2260:PHE:HA	1:A:2310:PRO:HA	1.82	0.61
1:A:197:LEU:HB2	1:A:257:VAL:HG12	1.82	0.61
1:A:388:ALA:HB3	1:A:468:GLN:H	1.66	0.61
1:A:414:ASN:HB2	1:A:595:LEU:HD11	1.82	0.61
1:A:2085:LYS:HB2	1:A:2165:GLU:HB3	1.82	0.61
1:A:476:TYR:HE1	1:A:483:VAL:HG11	1.66	0.61
1:A:1707:TRP:HB2	1:A:1758:LEU:HD11	1.83	0.61
1:A:312:ILE:HG22	1:A:314:SER:H	1.65	0.60
1:A:495:VAL:HG11	1:A:501:PHE:HB2	1.84	0.59
1:A:199:PHE:HD2	1:A:320:MET:HE2	1.67	0.59
1:A:658:PHE:HB2	1:A:678:VAL:HB	1.84	0.59
1:A:483:VAL:HG22	1:A:498:LEU:HD22	1.84	0.59
1:A:1948:GLY:HA3	1:A:1952:ASN:HD22	1.67	0.59
1:A:413:ASN:HB2	1:A:416:PRO:HG3	1.85	0.59
1:A:1944:LEU:HB3	1:A:1978:LEU:HD11	1.84	0.59
1:A:2036:GLN:HG2	1:A:2076:LEU:HD21	1.84	0.59
1:A:452:LEU:HA	1:A:550:PRO:HG2	1.84	0.58
1:A:2028:ALA:HB1	1:A:2052:ARG:HA	1.85	0.58
1:A:2197:THR:HG1	1:A:2203:TRP:CD1	2.21	0.58
1:A:659:LYS:HB3	1:A:679:PHE:HB3	1.85	0.58
1:A:1900:ARG:HD3	1:A:1901:ALA:N	2.09	0.58
1:A:184:LEU:HD23	1:A:187:GLU:HB3	1.84	0.58
1:A:2104:MET:HE2	1:A:2114:THR:HG22	1.87	0.57
1:A:2141:ASN:H	2:A:2401:NAG:H82	1.69	0.57
1:A:105:TYR:CE1	1:A:110:GLU:HB2	2.40	0.57
1:A:264:PRO:HA	1:A:290:PRO:HB3	1.86	0.57
1:A:1786:TYR:HA	1:A:1790:ILE:HD11	1.87	0.57
1:A:1789:LEU:HB3	1:A:1823:MET:HE1	1.87	0.56
1:A:2221:PRO:HB3	1:A:2228:GLU:HG3	1.88	0.56
1:A:653:PHE:HA	1:A:690:LEU:HD12	1.86	0.56
1:A:2049:LYS:HD2	1:A:2051:ALA:H	1.71	0.56
1:A:2070:TRP:HB3	1:A:2152:HIS:HD2	1.69	0.56
1:A:2197:THR:HG23	1:A:2203:TRP:HE1	1.71	0.56
1:A:1908:GLU:OE1	1:A:1910:PRO:HD2	2.06	0.56
1:A:658:PHE:HB3	1:A:680:MET:HE3	1.88	0.56
1:A:2028:ALA:HB1	1:A:2052:ARG:HG3	1.87	0.56
1:A:421:ARG:HH21	1:A:595:LEU:HB2	1.71	0.56
1:A:2089:ALA:HB2	1:A:2163:ARG:HD2	1.88	0.55
1:A:1948:GLY:HA3	1:A:1952:ASN:ND2	2.21	0.55
1:A:160:SER:HB3	1:A:167:ASP:HB3	1.87	0.55
1:A:1929:LEU:HD21	1:A:1932:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1957:HIS:HB3	1:A:1975:LEU:HB3	1.88	0.55
1:A:1749:ARG:HE	1:A:1756:LEU:HD23	1.71	0.55
1:A:127:LYS:HE2	1:A:129:PHE:HE1	1.71	0.55
1:A:300:LEU:HD13	1:A:326:VAL:HG22	1.89	0.55
1:A:1929:LEU:HG	1:A:1931:GLY:H	1.72	0.54
1:A:407:TYR:HA	1:A:410:GLN:HG3	1.89	0.54
1:A:2080:ILE:HG12	1:A:2145:ILE:HG22	1.89	0.54
1:A:466:LYS:HB2	1:A:508:ILE:HG22	1.88	0.54
1:A:696:ASP:HA	1:A:699:ASN:HD21	1.73	0.54
1:A:312:ILE:HB	1:A:315:HIS:HB2	1.89	0.54
1:A:2104:MET:HB2	1:A:2152:HIS:HE1	1.73	0.54
1:A:88:LEU:HD13	1:A:98:LEU:HD12	1.90	0.54
1:A:541:ARG:HE	1:A:583:ARG:HE	1.54	0.54
1:A:240:ARG:HB3	1:A:321:GLU:HB3	1.91	0.53
1:A:1734:VAL:HG11	1:A:1758:LEU:HD12	1.89	0.53
1:A:271:LEU:HD13	1:A:308:LEU:HD23	1.89	0.53
1:A:476:TYR:HB3	1:A:536:PHE:CD1	2.43	0.53
1:A:1882:ILE:H	1:A:1952:ASN:ND2	2.05	0.53
1:A:1707:TRP:CG	1:A:1758:LEU:HD21	2.44	0.53
1:A:464:ILE:HG12	1:A:510:LYS:HG2	1.91	0.53
1:A:421:ARG:HH11	1:A:423:TYR:HE1	1.57	0.52
1:A:228:TRP:HB3	1:A:229:PRO:HD3	1.91	0.52
1:A:2199:MET:HG3	1:A:2200:PHE:H	1.74	0.52
1:A:591:ILE:HG23	1:A:595:LEU:HD23	1.91	0.52
1:A:235:ASN:HB2	1:A:237:TYR:CE2	2.44	0.52
1:A:1925:ILE:CD1	1:A:1929:LEU:HB3	2.39	0.52
1:A:291:ILE:HG21	1:A:2001:LEU:HB3	1.91	0.52
1:A:1925:ILE:HD11	1:A:1929:LEU:HD22	1.90	0.52
1:A:449:LEU:HD21	1:A:575:LEU:HD22	1.91	0.52
1:A:1785:PHE:HB3	1:A:1815:TYR:CZ	2.45	0.51
1:A:2070:TRP:HB3	1:A:2152:HIS:CD2	2.46	0.51
1:A:529:LEU:HD13	1:A:531:ARG:CZ	2.40	0.51
1:A:541:ARG:NE	1:A:583:ARG:HE	2.09	0.51
1:A:542:ASP:HB3	1:A:547:LEU:HD12	1.93	0.51
1:A:2006:LEU:HA	1:A:2010:MET:HB3	1.93	0.51
1:A:1956:ILE:HA	1:A:2000:CYS:HA	1.93	0.51
1:A:386:ILE:HG21	1:A:428:PHE:CD2	2.46	0.51
1:A:486:LEU:HD12	1:A:510:LYS:HB3	1.93	0.51
1:A:1706:LEU:HA	1:A:1730:PHE:O	2.10	0.51
1:A:530:THR:HG22	1:A:640:LEU:HD13	1.92	0.50
1:A:1909:ASP:HA	1:A:1912:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD22	1:A:198:LEU:HD13	1.92	0.50
1:A:274:HIS:HB3	1:A:276:PHE:CD2	2.46	0.50
1:A:108:ALA:HB2	1:A:122:GLU:HG2	1.94	0.50
1:A:541:ARG:HD3	1:A:585:TRP:HE1	1.76	0.50
1:A:1919:HIS:HB3	1:A:2010:MET:SD	2.52	0.50
1:A:1707:TRP:CD1	1:A:1758:LEU:HD21	2.47	0.50
1:A:2087:GLN:HB3	1:A:2163:ARG:HB2	1.94	0.50
1:A:1759:LEU:HD13	1:A:1854:PRO:CD	2.40	0.49
1:A:246:ILE:HD11	1:A:330:PRO:HD3	1.93	0.49
1:A:575:LEU:HD11	1:A:642:ILE:HG22	1.93	0.49
1:A:2015:LEU:HD21	1:A:2080:ILE:HD11	1.94	0.49
1:A:413:ASN:ND2	1:A:421:ARG:HD2	2.26	0.49
1:A:68:TRP:CH2	1:A:195:PHE:HA	2.47	0.49
1:A:260:MET:HA	1:A:291:ILE:HD13	1.94	0.49
1:A:587:LEU:HD21	1:A:603:LEU:HD21	1.94	0.49
1:A:424:LYS:HZ2	1:A:594:PHE:HD2	1.61	0.49
1:A:1751:GLU:HA	1:A:1754:GLU:HB2	1.94	0.49
1:A:1830:PHE:HZ	1:A:1964:THR:HG23	1.78	0.49
1:A:289:SER:HB2	1:A:292:THR:HB	1.95	0.49
1:A:3:ARG:HB2	1:A:84:VAL:HG12	1.94	0.49
1:A:1714:SER:OG	1:A:1715:PRO:HD3	2.13	0.49
1:A:1781:ARG:NH2	1:A:1889:TRP:HB3	2.28	0.49
1:A:503:ILE:HD13	1:A:509:PHE:HB3	1.95	0.48
1:A:267:HIS:HB2	1:A:288:ILE:HB	1.94	0.48
1:A:1731:LYS:HD3	1:A:1896:GLU:OE2	2.14	0.48
1:A:308:LEU:HB2	1:A:322:ALA:HB3	1.96	0.48
1:A:650:SER:HA	1:A:669:THR:HA	1.95	0.48
1:A:1921:ILE:HD11	1:A:2010:MET:HA	1.95	0.48
1:A:103:VAL:HG11	1:A:138:TRP:HB3	1.96	0.48
1:A:1965:VAL:HG11	1:A:1976:TYR:HE2	1.78	0.48
1:A:89:LYS:HB2	1:A:133:SER:HB2	1.95	0.48
1:A:2053:LEU:HD23	1:A:2054:HIS:N	2.28	0.48
1:A:188:LYS:HG3	1:A:189:THR:N	2.29	0.48
1:A:2077:ALA:HB3	1:A:2079:MET:HE2	1.95	0.48
1:A:8:GLY:HA2	1:A:88:LEU:HG	1.95	0.48
1:A:1775:PHE:HB3	1:A:1815:TYR:HE1	1.78	0.47
1:A:2032:ILE:HG23	1:A:2033:ARG:H	1.79	0.47
1:A:595:LEU:HD23	1:A:598:PRO:HA	1.95	0.47
1:A:421:ARG:NH2	1:A:595:LEU:HB2	2.28	0.47
1:A:2141:ASN:HB3	1:A:2142:PRO:HD3	1.95	0.47
1:A:1707:TRP:CZ2	1:A:1709:TYR:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ALA:HB2	1:A:451:PRO:HG3	1.95	0.47
1:A:146:PRO:HG2	1:A:180:ARG:HB2	1.96	0.47
1:A:2039:ALA:HA	1:A:2071:ILE:HA	1.96	0.47
1:A:63:LYS:H	1:A:63:LYS:HD2	1.80	0.47
1:A:234:VAL:HG23	1:A:320:MET:HB2	1.96	0.47
1:A:446:SER:HB2	1:A:449:LEU:HD12	1.96	0.47
1:A:1752:LEU:HD13	1:A:2142:PRO:HG3	1.96	0.47
1:A:2025:LEU:HD11	1:A:2081:ILE:HG22	1.97	0.47
1:A:2212:LEU:HD22	1:A:2320:ARG:HH21	1.80	0.47
1:A:467:ASN:ND2	1:A:472:PRO:HA	2.30	0.47
1:A:388:ALA:HB1	1:A:426:VAL:HG23	1.97	0.46
1:A:609:GLN:O	1:A:613:ILE:HG13	2.14	0.46
1:A:2102:ILE:CG1	1:A:2152:HIS:HB2	2.44	0.46
1:A:446:SER:HB2	1:A:449:LEU:HB2	1.97	0.46
1:A:493:LYS:HG3	1:A:494:GLY:N	2.31	0.46
1:A:548:ILE:HG12	1:A:642:ILE:HG21	1.96	0.46
1:A:471:ARG:HD3	1:A:472:PRO:HD2	1.98	0.46
1:A:2199:MET:HG3	1:A:2200:PHE:N	2.30	0.46
1:A:452:LEU:HD21	1:A:552:LEU:HD12	1.97	0.46
1:A:2274:PHE:CG	1:A:2301:LEU:HD11	2.51	0.46
1:A:386:ILE:HD12	1:A:463:ILE:HD11	1.98	0.46
1:A:412:LEU:H	1:A:611:SER:HB2	1.80	0.46
1:A:630:CYS:HB3	1:A:711:CYS:HB3	1.71	0.46
1:A:99:HIS:HB2	1:A:161:HIS:HB2	1.98	0.46
1:A:1829:GLU:HG2	1:A:1966:ARG:HB3	1.98	0.46
1:A:1912:PHE:HA	1:A:1915:ASN:HB3	1.97	0.46
1:A:105:TYR:C	1:A:1992:LYS:HE2	2.41	0.45
1:A:307:LEU:HD12	1:A:322:ALA:H	1.80	0.45
1:A:309:PHE:CE2	1:A:311:HIS:HB2	2.51	0.45
1:A:652:PHE:HD1	1:A:693:HIS:CD2	2.33	0.45
1:A:105:TYR:HE1	1:A:110:GLU:HB2	1.81	0.45
1:A:188:LYS:HG3	1:A:189:THR:H	1.81	0.45
1:A:530:THR:HG21	1:A:640:LEU:HD22	1.98	0.45
1:A:2063:SER:HA	1:A:2160:SER:O	2.17	0.45
1:A:105:TYR:CD1	1:A:109:SER:HB2	2.52	0.45
1:A:389:GLU:HG3	1:A:391:GLU:HG3	1.99	0.45
1:A:652:PHE:H	1:A:692:CYS:HA	1.82	0.45
1:A:50:LEU:HD11	1:A:72:LEU:C	2.42	0.45
1:A:1925:ILE:HG21	1:A:2012:THR:HB	1.98	0.45
1:A:1755:HIS:NE2	1:A:1876:PHE:HA	2.32	0.45
1:A:2025:LEU:HD12	1:A:2166:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:HB3	1:A:71:LEU:HD23	1.98	0.44
1:A:90:ASN:HB3	1:A:130:PRO:HA	1.99	0.44
1:A:159:LEU:HD13	1:A:168:LEU:HD21	1.99	0.44
1:A:199:PHE:HA	1:A:234:VAL:HG22	1.99	0.44
1:A:408:LYS:HG3	1:A:622:PHE:CD1	2.52	0.44
1:A:1834:ALA:HB3	1:A:1983:PHE:CZ	2.52	0.44
1:A:1925:ILE:O	1:A:1926:MET:HE2	2.17	0.44
1:A:2046:TRP:HB3	1:A:2061:ALA:O	2.17	0.44
1:A:665:GLU:HG3	1:A:667:THR:H	1.81	0.44
1:A:412:LEU:HD13	1:A:607:GLU:HB3	1.99	0.44
1:A:310:CYS:HB2	1:A:320:MET:SD	2.57	0.44
1:A:14:TRP:CZ2	1:A:70:GLY:HA2	2.52	0.44
1:A:697:PHE:HB3	1:A:702:MET:SD	2.58	0.44
1:A:1927:ASP:O	1:A:2012:THR:HA	2.17	0.44
1:A:1956:ILE:HG22	1:A:2000:CYS:HB2	2.00	0.44
1:A:76:ILE:HG13	1:A:76:ILE:O	2.17	0.43
1:A:276:PHE:HB3	1:A:282:ARG:HB3	2.00	0.43
1:A:1909:ASP:HB2	1:A:1910:PRO:HD3	2.00	0.43
1:A:637:TRP:CE2	1:A:653:PHE:HZ	2.36	0.43
1:A:146:PRO:HB3	1:A:154:LEU:HG	1.99	0.43
1:A:695:SER:OG	1:A:1844:GLU:HB2	2.18	0.43
1:A:197:LEU:HD11	1:A:255:TRP:CD2	2.53	0.43
1:A:453:LEU:HD13	1:A:533:TYR:CE2	2.53	0.43
1:A:1755:HIS:HE2	1:A:1876:PHE:HA	1.83	0.43
1:A:578:VAL:HB	1:A:644:ALA:HA	2.00	0.43
1:A:1707:TRP:HH2	1:A:1926:MET:HE3	1.84	0.43
1:A:2112:TRP:CH2	1:A:2150:ARG:HG3	2.54	0.43
1:A:2276:GLN:HG3	1:A:2281:LYS:HE2	2.01	0.43
1:A:150:ASP:OD1	1:A:1971:TYR:HB2	2.19	0.42
1:A:2313:TRP:CD2	1:A:2317:ILE:HG12	2.54	0.42
1:A:50:LEU:HG	1:A:51:PHE:O	2.19	0.42
1:A:80:VAL:HG13	1:A:81:TYR:CD2	2.54	0.42
1:A:436:PHE:HE2	1:A:466:LYS:HB2	1.84	0.42
1:A:465:PHE:HB2	1:A:475:ILE:HD12	2.00	0.42
1:A:651:VAL:HG12	1:A:668:LEU:HB3	2.01	0.42
1:A:1735:PHE:HB2	1:A:1760:GLY:HA3	2.01	0.42
1:A:71:LEU:HD12	1:A:71:LEU:O	2.18	0.42
1:A:1944:LEU:HD13	1:A:1956:ILE:HD11	2.01	0.42
1:A:245:LEU:HD23	1:A:246:ILE:N	2.34	0.42
1:A:269:ILE:HB	1:A:286:LEU:HD23	2.01	0.42
1:A:201:VAL:HG12	1:A:201:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2089:ALA:HA	1:A:2163:ARG:HH11	1.85	0.42
1:A:276:PHE:HE2	1:A:519:ASP:HA	1.85	0.42
1:A:1867:HIS:NE2	1:A:2118:ASN:HB3	2.35	0.42
1:A:449:LEU:HD21	1:A:575:LEU:CD2	2.50	0.42
1:A:1864:ASN:HB3	1:A:1868:GLY:H	1.85	0.42
1:A:245:LEU:HD11	1:A:255:TRP:HE1	1.85	0.42
1:A:1962:VAL:HG12	1:A:1972:LYS:HD2	2.02	0.42
1:A:661:LYS:HE2	1:A:1967:LYS:HE3	2.01	0.41
1:A:1749:ARG:NE	1:A:1756:LEU:HB3	2.35	0.41
1:A:1731:LYS:H	1:A:1893:GLU:HG2	1.85	0.41
1:A:2251:LEU:O	1:A:2253:THR:HG23	2.21	0.41
1:A:616:SER:HB2	1:A:620:TYR:O	2.21	0.41
1:A:1709:TYR:HB2	1:A:1712:SER:HB2	2.02	0.41
1:A:1773:VAL:HB	1:A:1815:TYR:HB2	2.02	0.41
1:A:1825:PRO:HB3	1:A:1833:LYS:HB2	2.02	0.41
1:A:190:GLN:OE1	1:A:194:LYS:HE2	2.20	0.41
1:A:523:LYS:O	1:A:523:LYS:HD3	2.21	0.41
1:A:1756:LEU:HD11	1:A:1760:GLY:O	2.21	0.41
1:A:1867:HIS:HB3	1:A:1870:GLN:HG3	2.03	0.41
1:A:2032:ILE:HG23	1:A:2033:ARG:N	2.36	0.41
1:A:100:ALA:HB3	1:A:105:TYR:CE2	2.56	0.40
1:A:1696:ARG:NH1	1:A:1696:ARG:HG3	2.36	0.40
1:A:1739:THR:OG1	1:A:1745:GLN:HB3	2.21	0.40
1:A:1820:GLN:HA	1:A:1820:GLN:OE1	2.20	0.40
1:A:424:LYS:NZ	1:A:593:ARG:HB3	2.36	0.40
1:A:541:ARG:HH11	1:A:585:TRP:NE1	2.13	0.40
1:A:572:ASN:O	1:A:574:ILE:HD12	2.21	0.40
1:A:1737:GLU:HB2	1:A:1761:PRO:HG3	2.03	0.40
1:A:453:LEU:HD22	1:A:551:LEU:HD12	2.03	0.40
1:A:521:PRO:HG2	1:A:555:TYR:HB2	2.02	0.40
1:A:440:GLU:O	1:A:442:ILE:HG23	2.21	0.40
1:A:2117:GLY:HA2	1:A:2142:PRO:HG2	2.03	0.40
1:A:100:ALA:HB2	1:A:138:TRP:CZ2	2.56	0.40
1:A:1878:LEU:HB2	1:A:1944:LEU:HD23	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	A	1233/2332 (53%)	1135 (92%)	98 (8%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1109/2093 (53%)	1109 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	590	ASN
1	A	699	ASN
1	A	1729	GLN
1	A	1770	ASN
1	A	1898	ASN
1	A	1952	ASN
1	A	1954	HIS
1	A	2087	GLN
1	A	2152	HIS
1	A	2213	GLN
1	A	2225	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	NAG	A	2401	1	14,14,15	0.73	0	17,19,21	0.81	0
2	NAG	A	2402	1	14,14,15	0.71	0	17,19,21	0.93	0
2	NAG	A	2403	1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)

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
2	NAG	A	2401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	1	-	2/6/23/26	0/1/1/1
2	NAG	A	2403	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2403	NAG	C2-N2-C7	3.37	127.42	122.90
2	A	2403	NAG	C1-O5-C5	2.27	115.23	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2402	NAG	C8-C7-N2-C2
2	A	2402	NAG	O7-C7-N2-C2
2	A	2403	NAG	C3-C2-N2-C7
2	A	2403	NAG	O5-C5-C6-O6
2	A	2403	NAG	C1-C2-N2-C7

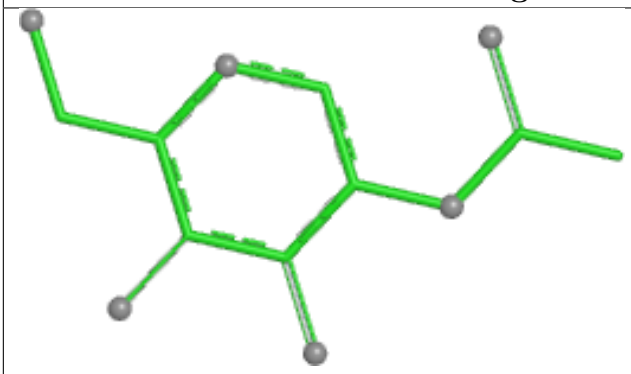
There are no ring outliers.

1 monomer is involved in 1 short contact:

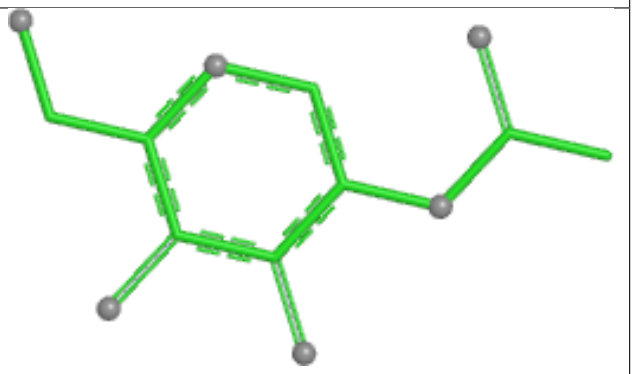
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAG	1	0

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

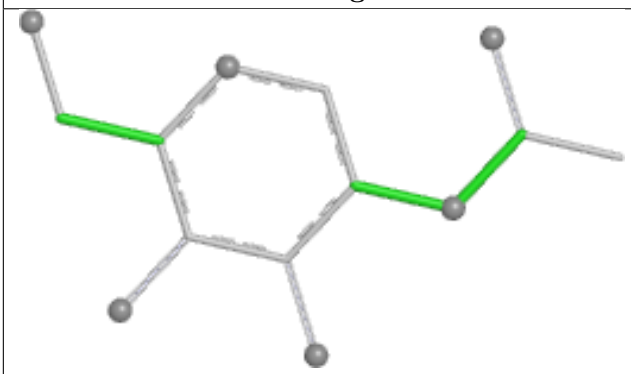
Ligand NAG A 2401



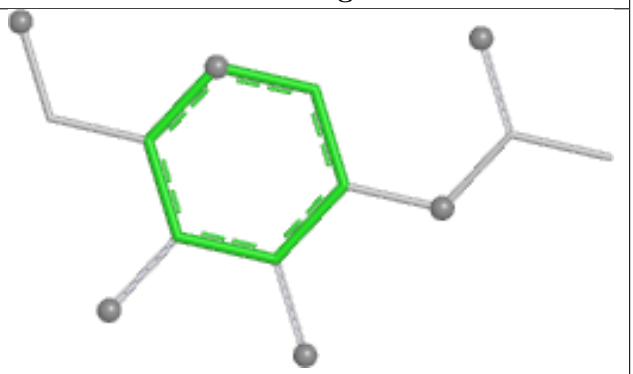
Bond lengths



Bond angles

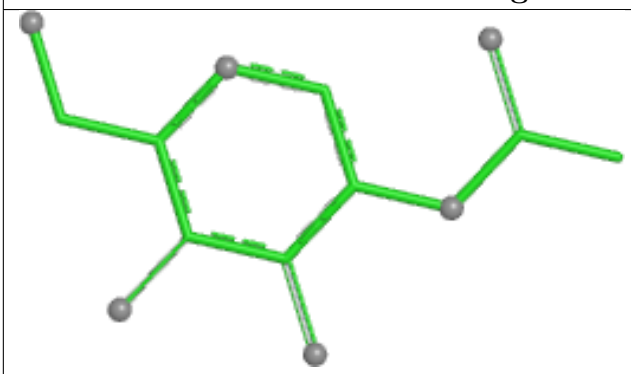


Torsions

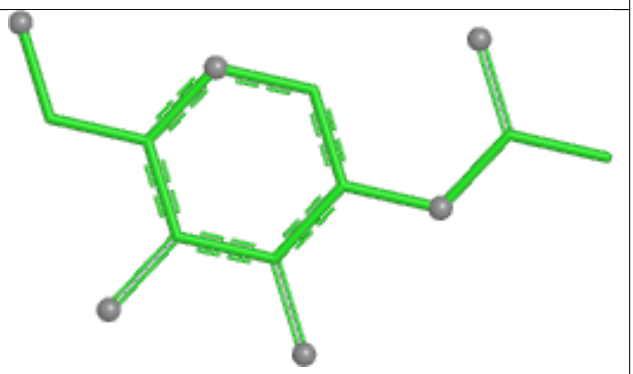


Rings

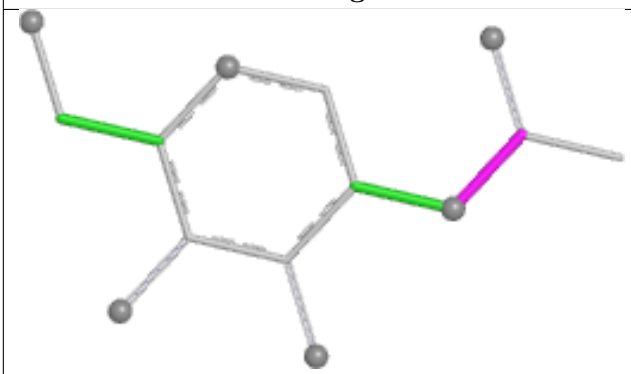
Ligand NAG A 2402



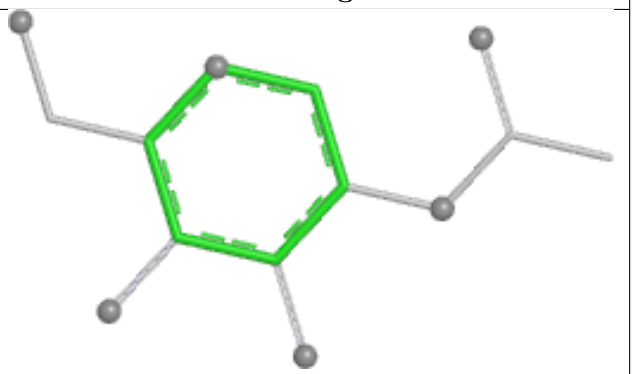
Bond lengths



Bond angles

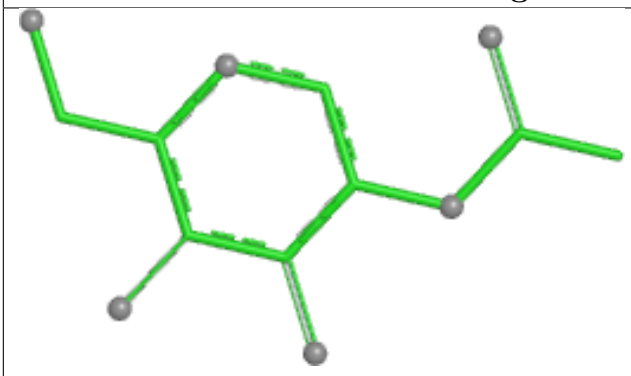


Torsions

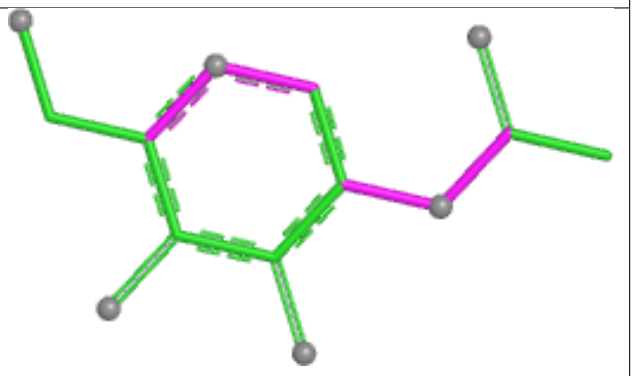


Rings

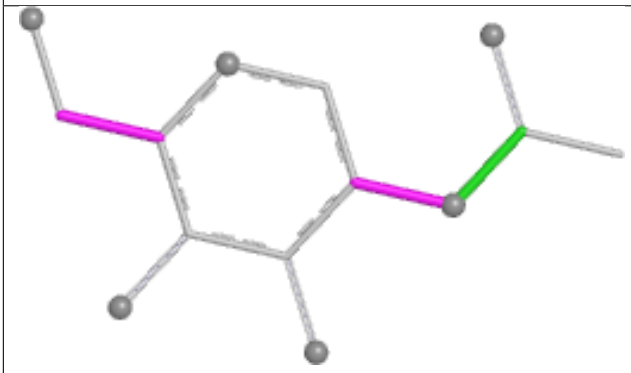
Ligand NAG A 2403



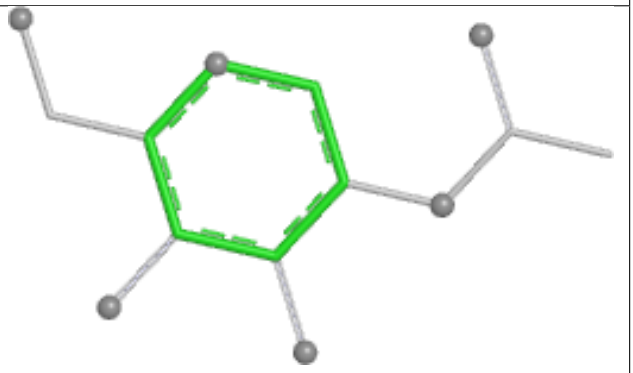
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76497. These allow visual inspection of the internal detail of the map and identification of artifacts.

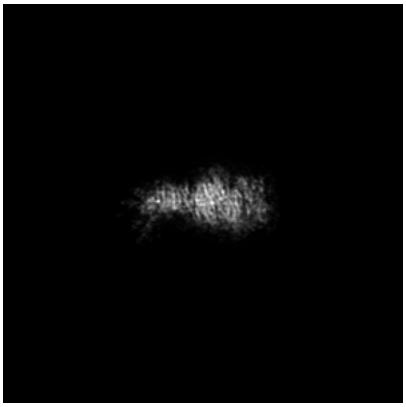
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

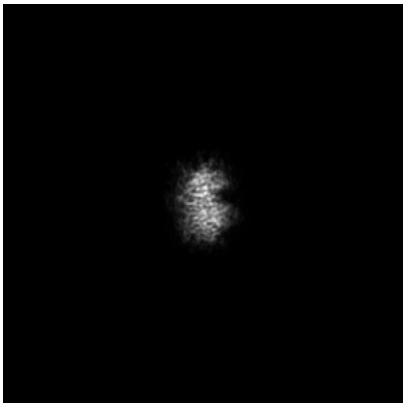
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

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

6.3 Largest variance slices (i)

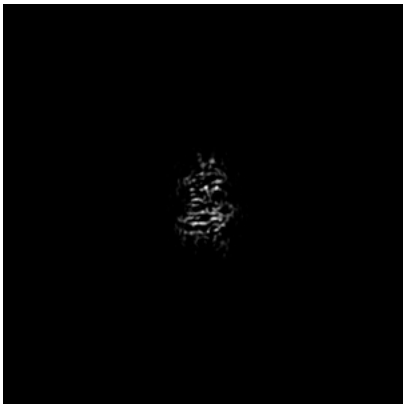
6.3.1 Primary map



X Index: 210



Y Index: 198

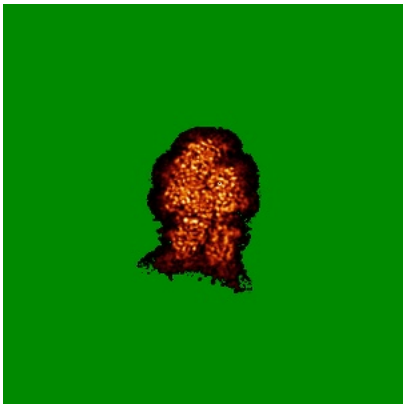


Z Index: 210

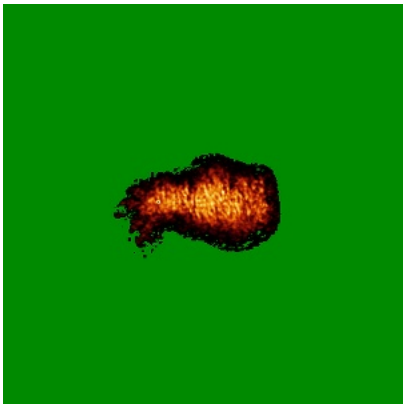
The images above show the largest variance slices of the map in three orthogonal directions.

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

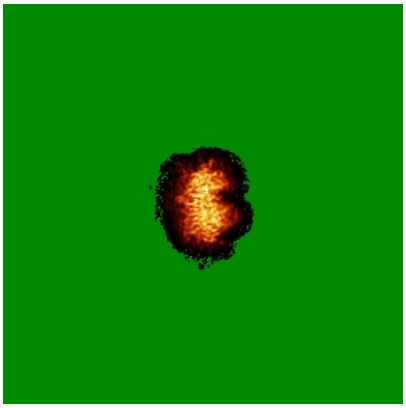
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.162. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

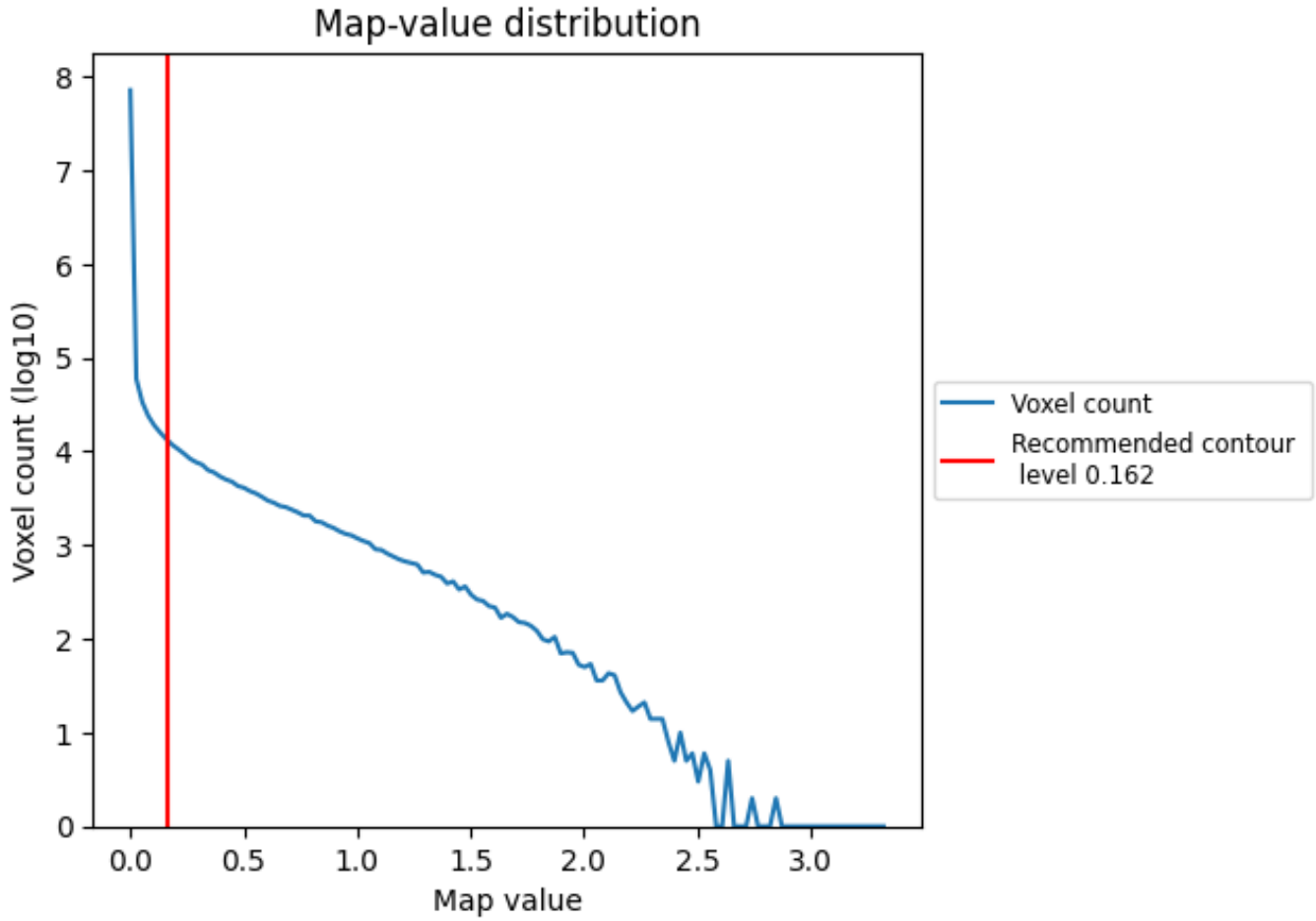
6.6 Mask visualisation (i)

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

7 Map analysis

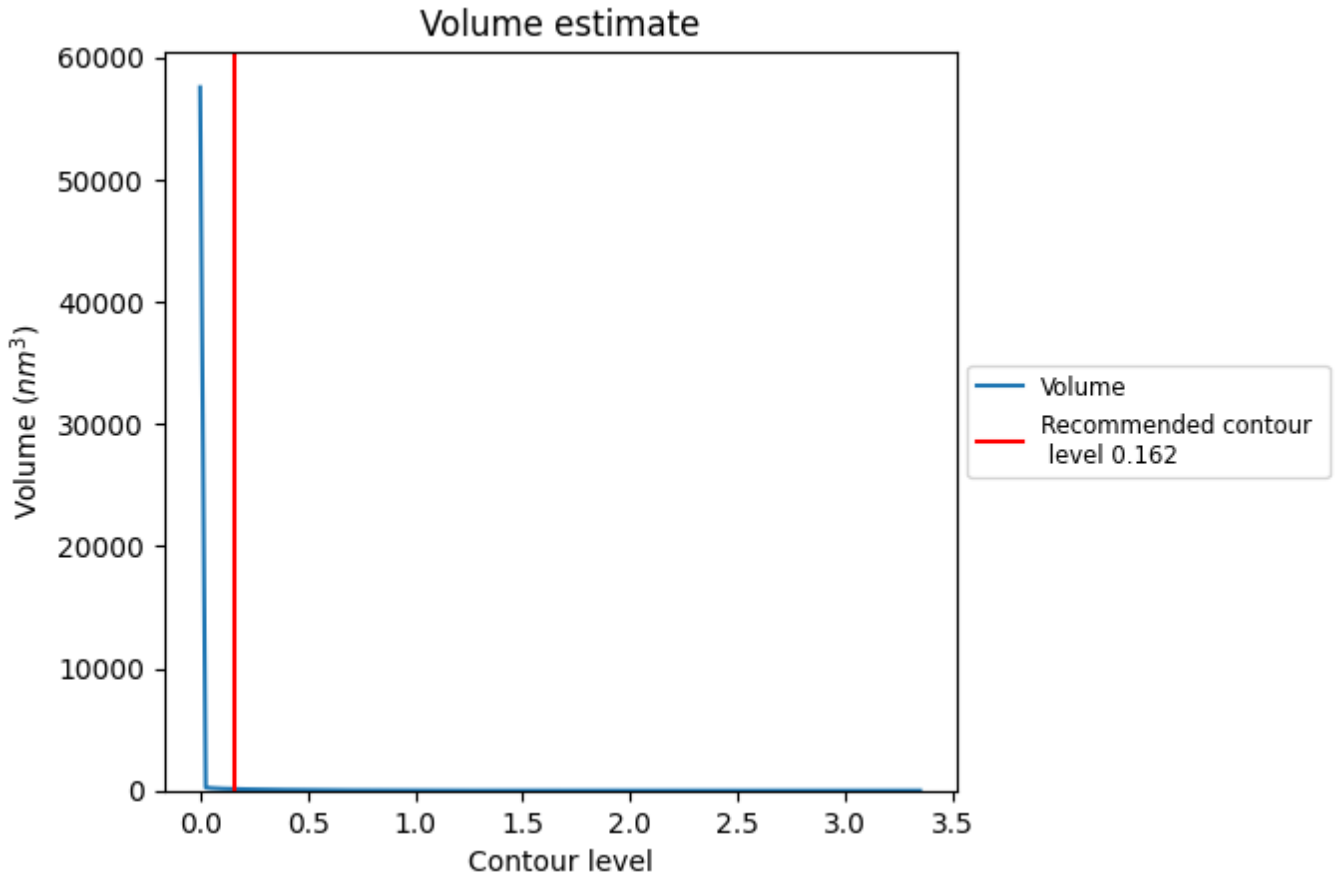
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

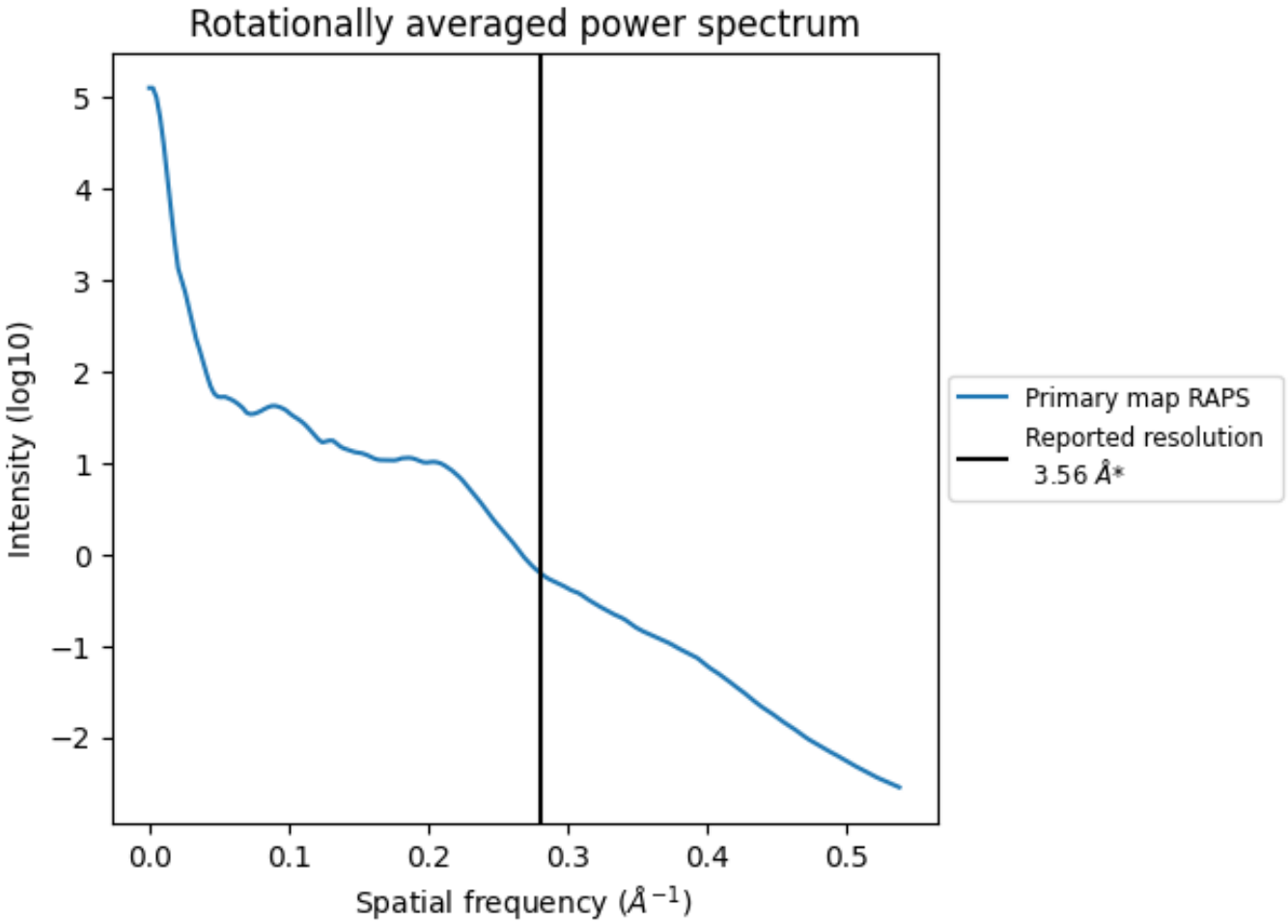
7.2 Volume estimate



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.281 Å^{-1}

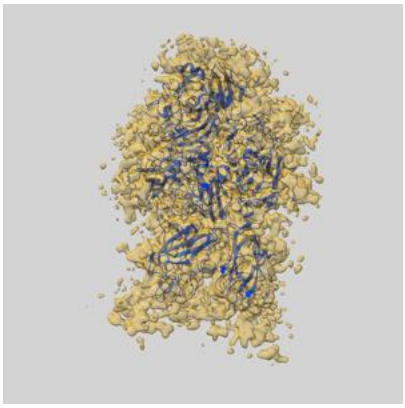
8 Fourier-Shell correlation (i)

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

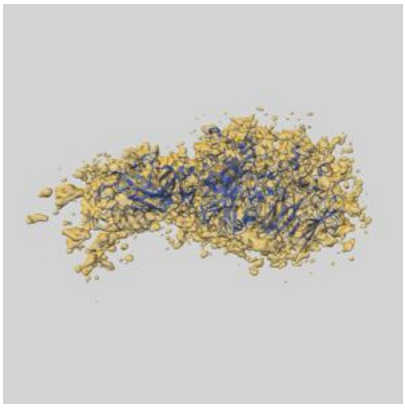
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76497 and PDB model 12JV. Per-residue inclusion information can be found in section 3 on page 5.

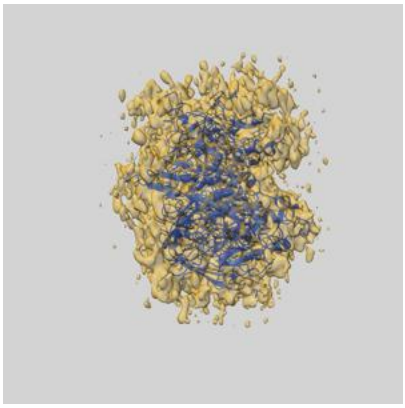
9.1 Map-model overlay



X



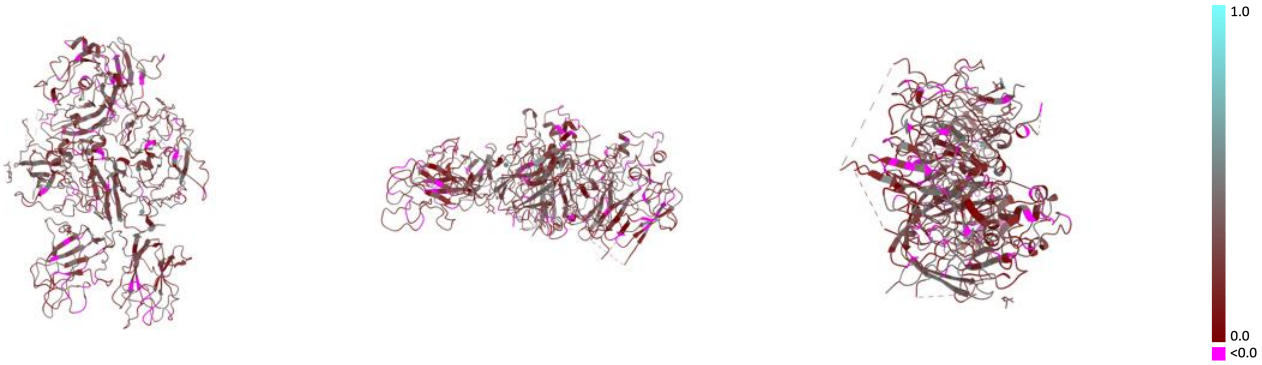
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.162 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

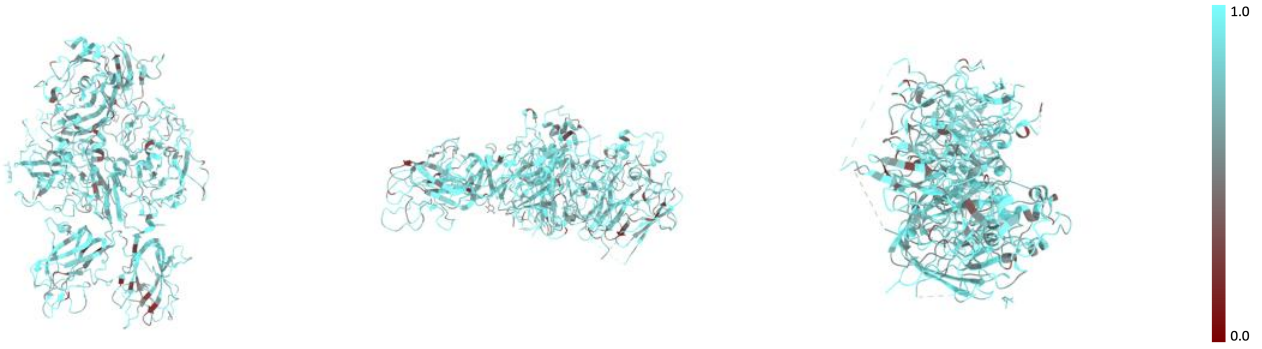
9.2 Q-score mapped to coordinate model



X Y Z

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

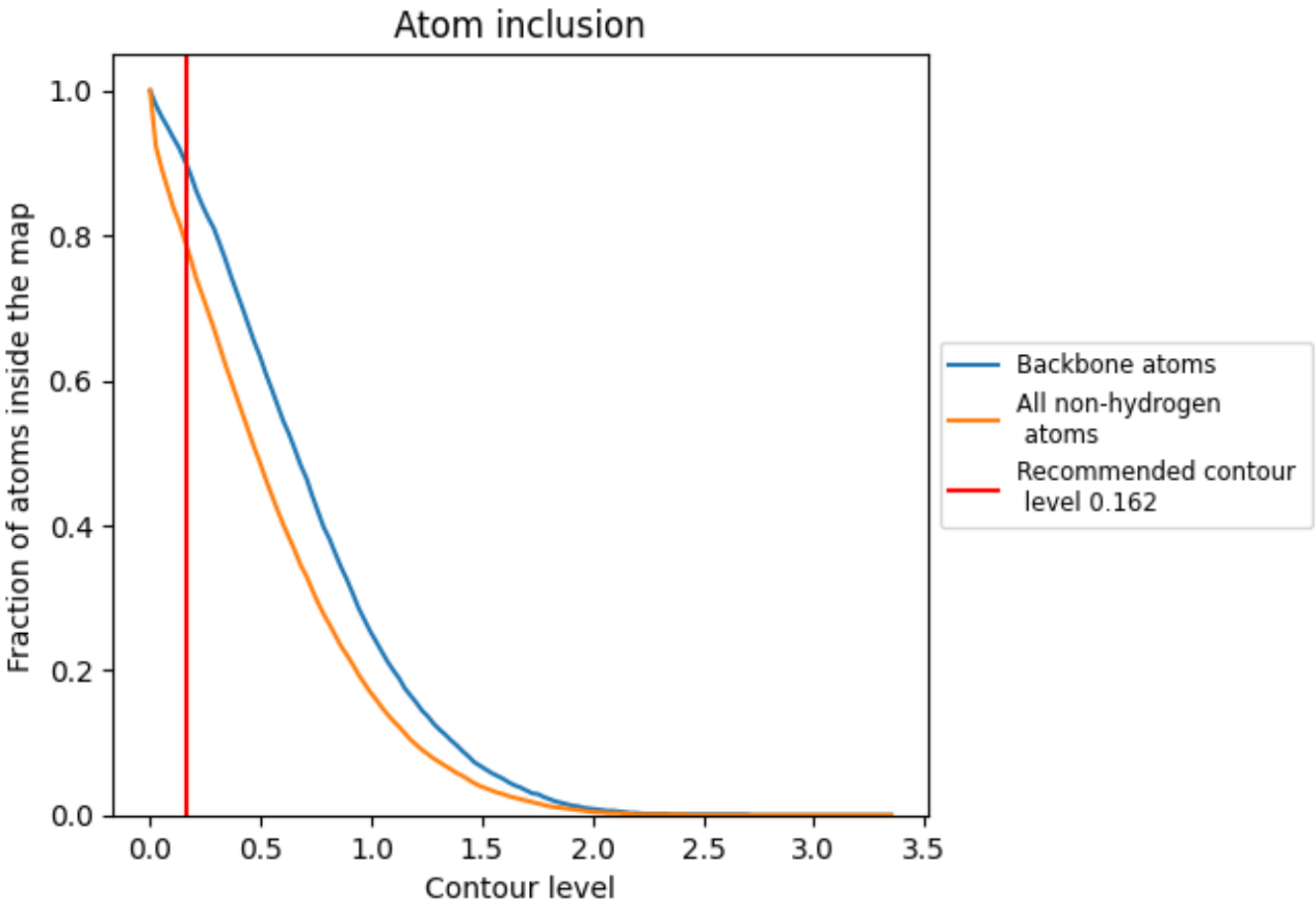
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.162).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.162) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7870	0.2550
A	0.7870	0.2550