Full wwPDB EM Validation Report ⓘ

Jun 29, 2023 – 06:18 PM EDT

PDB ID	:	8EYK
EMDB ID	:	EMD-28691
Title	:	Atomic model of the core modifying region of human fatty acid synthase in complex with TVB-2640
Authors	:	Hasan, S.M.N.; Keszei, A.; Mazhab-Jafari, M.T.
Deposited on	:	2022-10-27
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

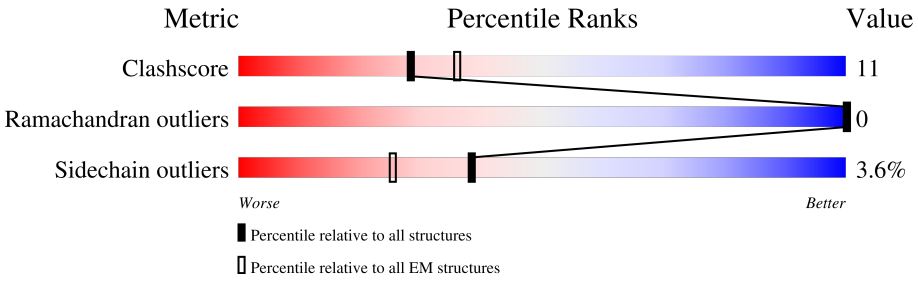
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	E	1670	44% 14% 42%
1	F	1670	48% 15% 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15386 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.

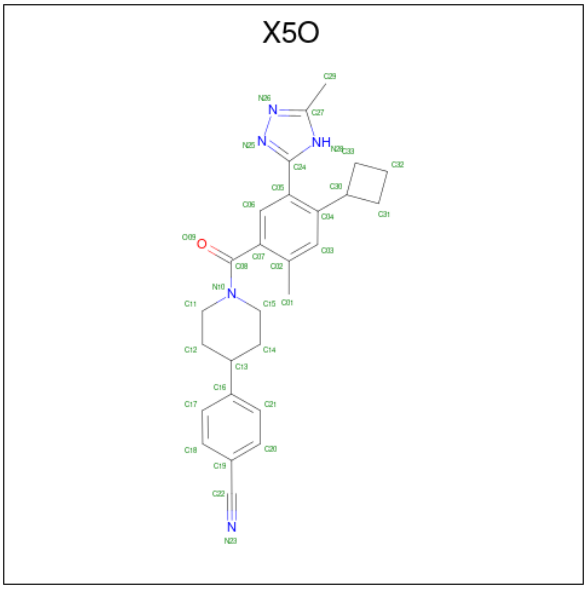
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	966	Total	C	N	O	S	0	0
			7179	4571	1268	1314	26		
1	F	1070	Total	C	N	O	S	0	0
			7949	5068	1398	1451	32		

There are 26 discrepancies between the modelled and reference sequences:

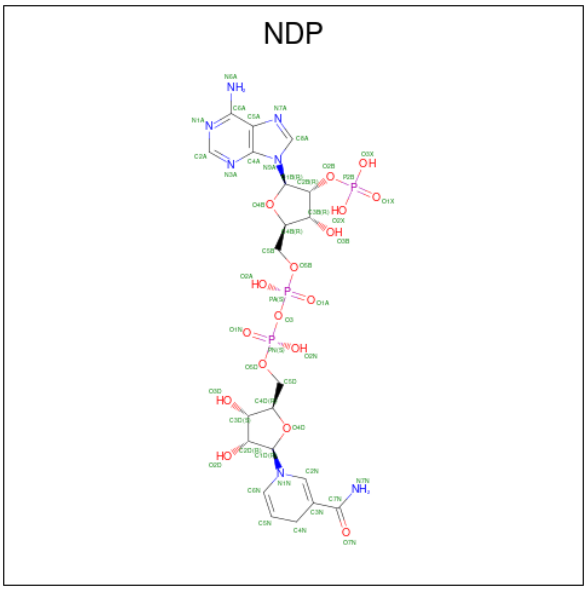
Chain	Residue	Modelled	Actual	Comment	Reference
E	854	GLY	-	cloning artifact	UNP P49327
E	2512	LEU	-	cloning artifact	UNP P49327
E	2513	GLU	-	cloning artifact	UNP P49327
E	2514	SER	-	cloning artifact	UNP P49327
E	2515	ARG	-	cloning artifact	UNP P49327
E	2516	GLY	-	cloning artifact	UNP P49327
E	2517	PRO	-	cloning artifact	UNP P49327
E	2518	HIS	-	expression tag	UNP P49327
E	2519	HIS	-	expression tag	UNP P49327
E	2520	HIS	-	expression tag	UNP P49327
E	2521	HIS	-	expression tag	UNP P49327
E	2522	HIS	-	expression tag	UNP P49327
E	2523	HIS	-	expression tag	UNP P49327
F	854	GLY	-	cloning artifact	UNP P49327
F	2512	LEU	-	cloning artifact	UNP P49327
F	2513	GLU	-	cloning artifact	UNP P49327
F	2514	SER	-	cloning artifact	UNP P49327
F	2515	ARG	-	cloning artifact	UNP P49327
F	2516	GLY	-	cloning artifact	UNP P49327
F	2517	PRO	-	cloning artifact	UNP P49327
F	2518	HIS	-	expression tag	UNP P49327
F	2519	HIS	-	expression tag	UNP P49327
F	2520	HIS	-	expression tag	UNP P49327
F	2521	HIS	-	expression tag	UNP P49327
F	2522	HIS	-	expression tag	UNP P49327
F	2523	HIS	-	expression tag	UNP P49327

- Molecule 2 is denifanstat (three-letter code: X5O) (formula: $C_{27}H_{29}N_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			33	27	5	1	
2	F	1	Total	C	N	O	0
			33	27	5	1	

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



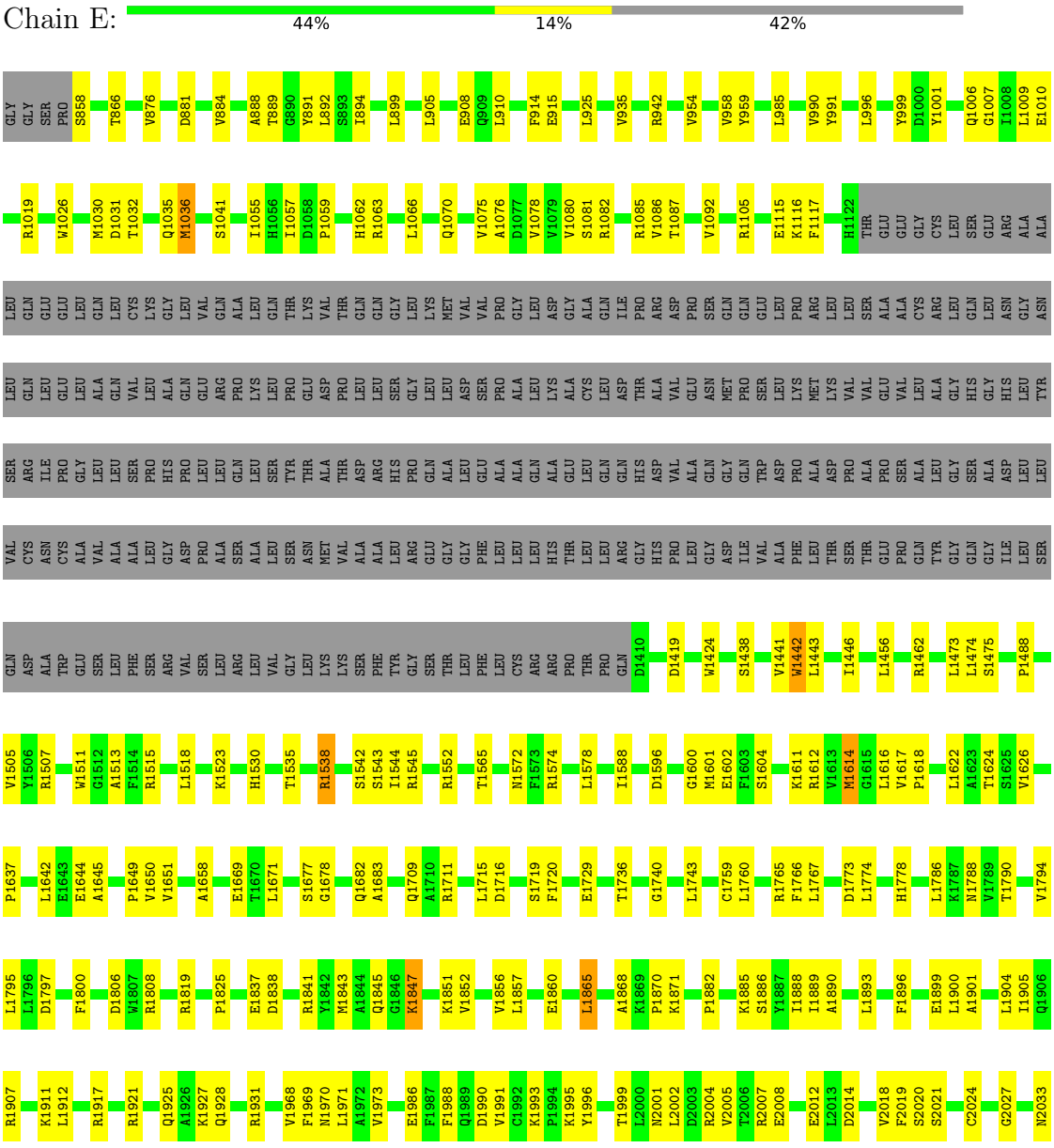
Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	F	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	F	1	Total	C	N	O	P	0
			48	21	7	17	3	

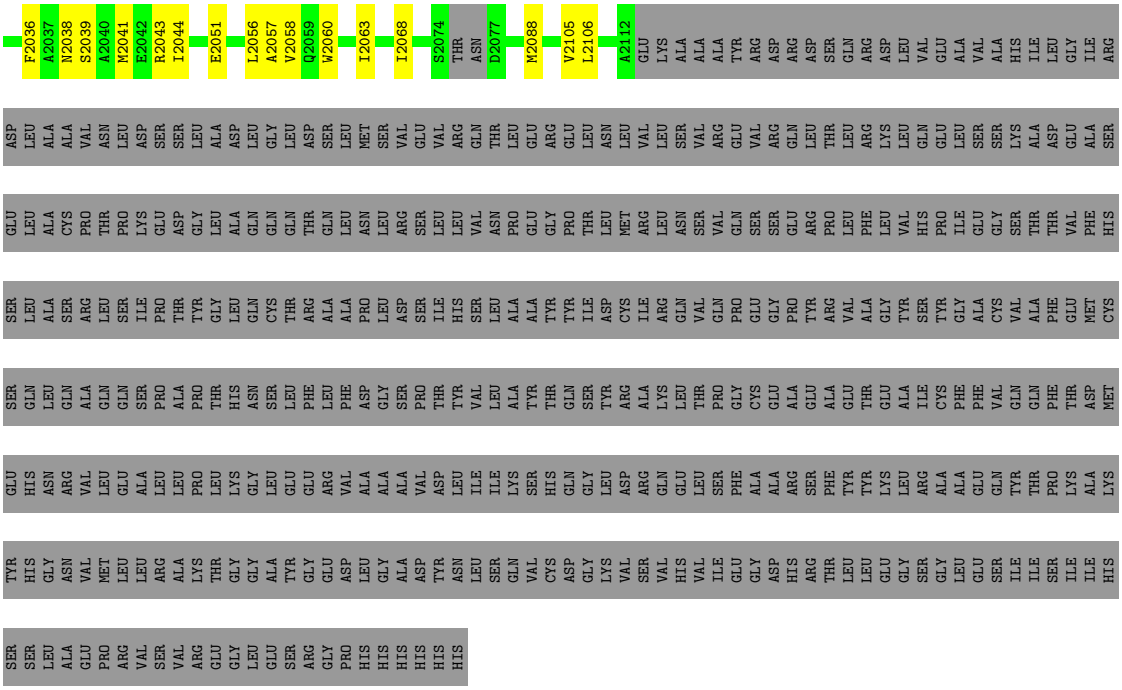
3 Residue-property plots (i)

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: Fatty acid synthase

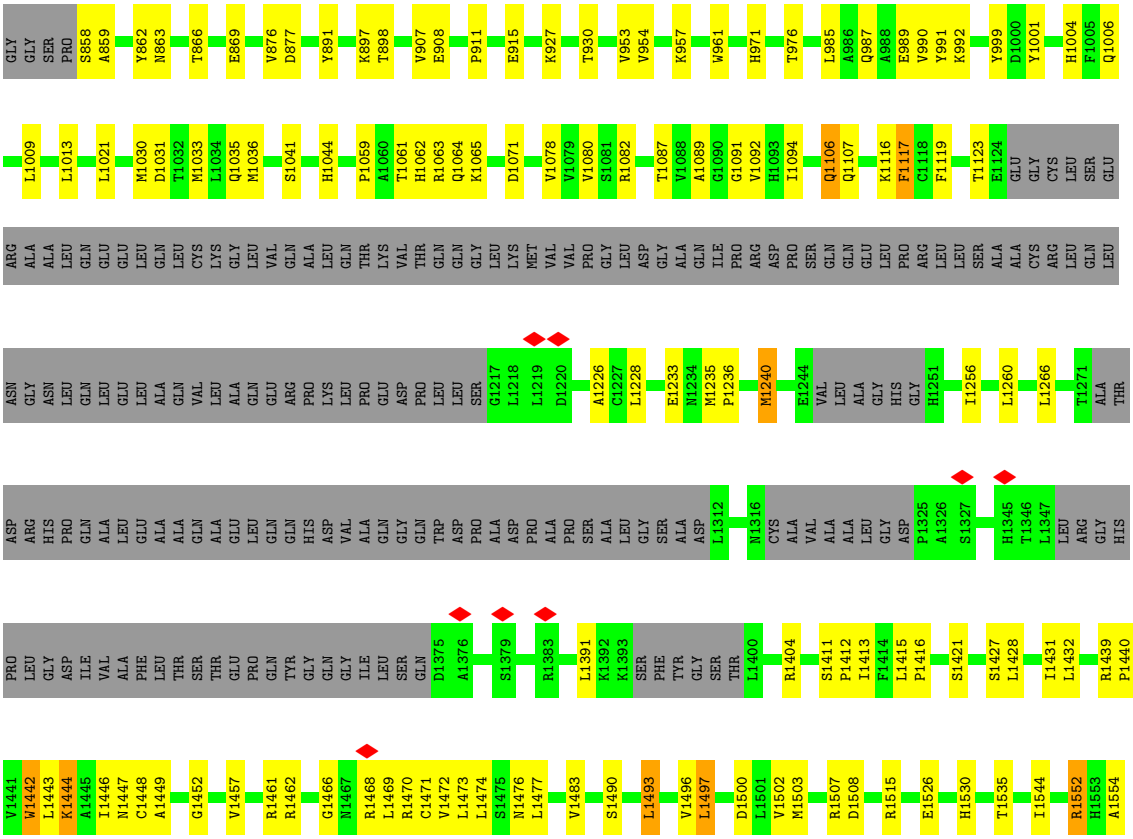
Chain E:

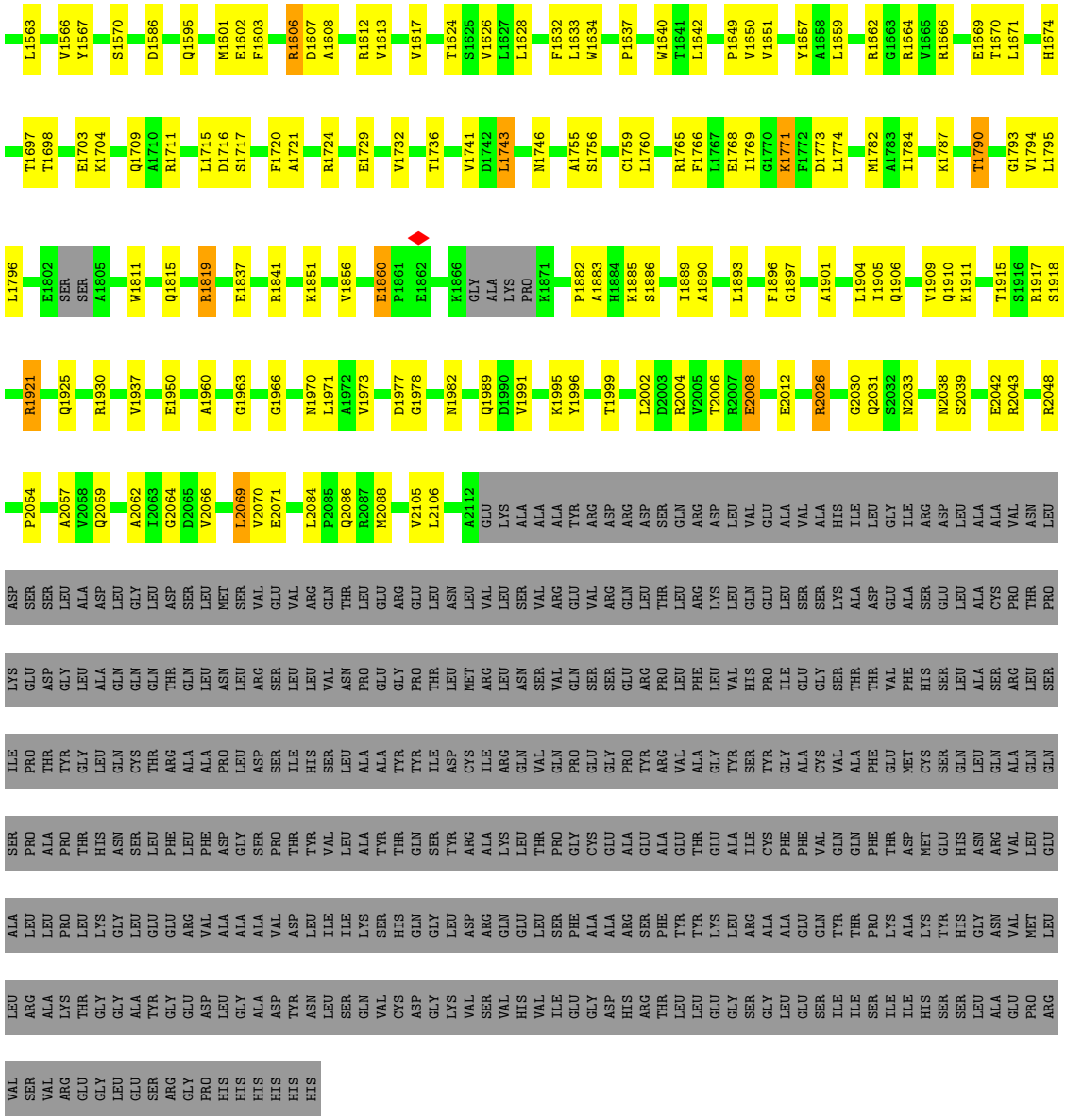




• Molecule 1: Fatty acid synthase

Chain F:




L1563 V1566 Y1567 S1570 D1586 Q1595 M1601 E1602 F1603 R1606 D1607 A1608 R1612 V1613 V1617 T1624 S1625 V1626 L1627 L1628 F1632 L1633 W1634 P1637 W1640 T1641 L1642 P1649 V1650 V1651 Y1657 A1658 L1659 R1662 G1663 R1664 V1665 R1666 E1669 T1670 L1671 H1674
T1697 T1698 E1703 K1704 Q1709 A1710 R1711 L1715 D1716 S1717 F1720 A1721 R1724 E1729 V1732 T1736 V1741 D1742 L1743 N1746 A1755 S1756 C1759 L1760 R1765 F1766 L1767 E1768 I1769 G1770 K1771 F1772 D1773 L1774 M1782 A1783 I1784 K1787 T1790 G1793 V1794 L1795
L1796 E1802 SER SER A1805 W1811 Q1815 R1819 E1837 R1841 K1851 V1856 E1860 P1861 E1862 K1866 GLY ALA LYS PRO K1871 P1882 A1883 H1884 K1885 S1886 I1889 A1890 L1893 F1896 G1897 A1901 L1904 I1905 Q1906 V1909 Q1910 K1911 T1915 S1916 R1917 S1918
R1921 Q1925 R1930 V1937 E1950 A1960 G1963 G1966 N1970 L1971 A1972 V1973 D1977 G1978 N1982 Q1989 D1990 V1991 K1995 Y1996 T1999 L2002 D2003 R2004 V2005 T2006 R2007 E2008 E2012 R2026 G2030 Q2031 S2032 N2033 N2038 S2039 E2042 R2043 R2048
P2054 A2057 V2058 Q2059 A2062 I2063 G2064 D2065 V2066 L2069 V2070 E2071 L2084 P2085 Q2086 R2087 M2088 V2105 L2106 A2112 GLU LYS ALA ALA ALA TYR ARG ASP ARG GLN ASP SER GLN ARG ASP LEU VAL GLU ALA VAL ALA HIS ILE LEU GLY SER PHE ILE ARG ASP LEU ALA ALA CYS PRO THR PRO
ASP SER SER LEU ALA ASP LEU GLY LEU ASP SER LEU MET SER VAL GLU VAL ARG GLN LEU THR LEU GLU ARG GLN LEU GLN GLU GLU LEU GLU SER SER LYS ALA ASP GLU ALA SER GLU LEU ALA CYS PRO THR PRO
LYS GLU ASP GLY LEU ALA GLN GLN GLN THR GLN LEU ASN LEU VAL ASN PRO GLU GLY PRO THR LEU MET ARG LEU ASN SER VAL GLN SER SER GLU ARG PRO LEU PHE LEU VAL HIS PRO ILE GLU GLY SER THR THR VAL PHE HIS SER LEU ALA SER ARG LEU SER
ILE PRO THR TYR GLY LEU GLN CYS THR ARG ALA ALA PRO LEU ASP SER ILE HIS SER LEU ALA ALA TYR THR TYR ILE ASP CYS ILE ARG GLN VAL GLN PRO GLU GLY PRO TYR ARG VAL ALA ALA GLY TYR SER TYR GLY ALA CYS VAL ALA PHE GLU MET CYS SER GLN LEU ALA GLN GLN GLN
SER PRO ALA PRO THR HIS ASN SER LEU PHE LEU PHE ASP GLY SER PRO THR TYR VAL LEU ALA TYR THR GLN SER TYR ARG ALA LYS LEU THR PRO GLY CYS GLU ALA ALA GLU GLU THR GLU ALA ILE CYS PHE PHE VAL GLN GLN PHE THR ASP MET GLU HIS ASN ARG VAL LEU GLU
ALA LEU LEU PRO LEU LYS GLY LEU GLU ARG VAL ALA ASP LEU ILE ILE LYS SER HIS GLN GLY LEU ASP ARG GLN GLU LEU SER PHE ALA ALA ARG SER PHE TYR TYR LYS LEU ARG ALA ALA GLU GLN TYR THR PRO LYS ALA LYS TYR HIS GLY ASN VAL MET LEU
LEU ARG ALA LYS THR GLY GLY ALA TYR ASN LEU SER GLN VAL CYS ASP GLY LYS VAL SER VAL HIS VAL ILE GLU GLY ASP HIS ARG THR LEU LEU GLU GLY SER GLY LEU GLU SER ILE ILE SER ILE ILE HIS SER GLY LEU ALA GLU PRO ARG
VAL SER VAL ARG GLU GLY LEU GLU SER ARG GLY PRO HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	311983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.76	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.168	Depositor
Minimum map value	-3.725	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.341	Depositor
Map size (Å)	257.5, 257.5, 257.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, X5O

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	E	0.29	0/7344	0.50	0/10015
1	F	0.29	0/8119	0.51	2/11061 (0.0%)
All	All	0.29	0/15463	0.50	2/21076 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1071	ASP	CB-CG-OD1	6.05	123.74	118.30
1	F	1497	LEU	CA-CB-CG	5.23	127.34	115.30

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	E	7179	0	6896	149	0
1	F	7949	0	7691	173	0
2	E	33	0	0	0	0
2	F	33	0	0	1	0
3	E	96	0	47	7	0
3	F	96	0	50	10	0
All	All	15386	0	14684	317	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 11.

All (317) 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:F:1915:THR:HG22	3:F:2603:NDP:H2A	1.49	0.93
1:E:1991:VAL:HG11	1:E:2033:ASN:HB2	1.55	0.89
1:F:1991:VAL:HG11	1:F:2033:ASN:HB2	1.65	0.78
1:F:1716:ASP:OD1	1:F:1717:SER:N	2.18	0.77
1:F:1233:GLU:O	1:F:1461:ARG:NH1	2.18	0.77
1:F:1950:GLU:OE2	1:F:1950:GLU:N	2.17	0.75
1:F:1628:LEU:HD11	1:F:1632:PHE:HB2	1.71	0.73
1:F:1760:LEU:HD11	1:F:1766:PHE:HB2	1.70	0.72
1:F:1973:VAL:HG12	3:F:2603:NDP:H51A	1.73	0.70
1:F:1617:VAL:HG11	1:F:1626:VAL:HG11	1.73	0.70
1:F:1432:LEU:HD23	1:F:1469:LEU:HD23	1.74	0.69
1:F:1703:GLU:N	1:F:1703:GLU:OE2	2.24	0.69
1:F:1674:HIS:NE2	1:F:1756:SER:OG	2.25	0.69
1:E:1602:GLU:HB2	1:E:1650:VAL:HG23	1.76	0.67
1:E:1790:THR:OG1	1:F:1662:ARG:NH2	2.28	0.67
1:E:1986:GLU:N	1:E:1986:GLU:OE2	2.28	0.67
1:E:2012:GLU:OE2	1:E:2012:GLU:N	2.28	0.66
1:F:1624:THR:HA	1:F:1856:VAL:HG11	1.77	0.65
1:E:858:SER:HB2	1:F:858:SER:HA	1.77	0.65
1:E:1843:MET:HB2	1:E:1852:VAL:HG21	1.79	0.65
1:E:1709:GLN:NE2	1:E:1715:LEU:O	2.29	0.65
1:E:1760:LEU:HD11	1:E:1766:PHE:HB2	1.80	0.64
1:F:1771:LYS:HE3	1:F:1795:LEU:HD22	1.80	0.64
1:E:1973:VAL:HG12	3:E:2603:NDP:H51A	1.79	0.64
1:E:2007:ARG:NH1	1:E:2051:GLU:OE1	2.31	0.63
1:F:1724:ARG:NH1	3:F:2602:NDP:O3X	2.31	0.63
1:F:1662:ARG:HD3	1:F:1794:VAL:HG22	1.80	0.63
1:F:908:GLU:O	1:F:1063:ARG:NH2	2.32	0.63
1:F:1978:GLY:N	1:F:2030:GLY:O	2.31	0.63
1:F:1602:GLU:HG3	1:F:1649:PRO:HB2	1.81	0.62
1:E:1456:LEU:HD13	1:E:2036:PHE:HB2	1.80	0.62
1:F:1901:ALA:O	1:F:1905:ILE:HG12	2.00	0.61
1:F:1890:ALA:HA	1:F:1915:THR:HB	1.81	0.61
1:F:1446:ILE:HA	1:F:1476:ASN:HD22	1.65	0.61
1:E:1885:LYS:NZ	1:E:2014:ASP:OD2	2.29	0.61
1:F:1602:GLU:OE1	1:F:1851:LYS:NZ	2.34	0.61
1:E:1882:PRO:HG2	1:E:1885:LYS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1033:MET:HE2	1:F:1094:ILE:HD12	1.83	0.60
1:F:1634:TRP:HD1	1:F:1815:GLN:HG2	1.66	0.60
1:F:1404:ARG:NH1	1:F:1500:ASP:O	2.34	0.60
1:F:1030:MET:HG2	1:F:1092:VAL:HG11	1.84	0.60
1:E:1066:LEU:HD23	1:E:1076:ALA:HB2	1.84	0.60
1:E:1614:MET:HG2	1:E:1645:ALA:HB1	1.83	0.59
1:F:1468:ARG:HH12	1:F:1470:ARG:HH11	1.47	0.59
1:E:942:ARG:HG2	1:E:959:TYR:HB3	1.84	0.59
1:E:1617:VAL:HG11	1:E:1626:VAL:HG11	1.84	0.59
1:E:1612:ARG:NH2	1:E:1637:PRO:O	2.36	0.59
1:F:1977:ASP:N	1:F:1977:ASP:OD1	2.35	0.58
1:F:1885:LYS:NZ	1:F:2012:GLU:O	2.36	0.58
1:F:1709:GLN:NE2	1:F:1715:LEU:O	2.36	0.58
1:E:1080:VAL:HG22	1:E:1087:THR:HG23	1.86	0.58
1:E:1865:LEU:HD23	1:E:1868:ALA:H	1.70	0.57
1:E:991:TYR:CZ	1:E:1006:GLN:HA	2.39	0.57
1:F:1448:CYS:SG	1:F:1996:TYR:OH	2.63	0.57
1:F:1883:ALA:O	1:F:1911:LYS:NZ	2.37	0.57
1:F:991:TYR:CZ	1:F:1006:GLN:HA	2.40	0.57
1:F:1995:LYS:NZ	1:F:2038:ASN:OD1	2.31	0.57
1:E:2024:CYS:SG	1:E:2039:SER:OG	2.59	0.56
1:F:1602:GLU:HB2	1:F:1650:VAL:HG23	1.87	0.56
1:F:2064:GLY:N	1:F:2086:GLN:O	2.34	0.56
1:E:1446:ILE:HG13	1:E:1488:PRO:HG3	1.88	0.56
1:E:894:ILE:HG22	1:E:935:VAL:HG21	1.86	0.56
1:E:1443:LEU:HD23	1:E:1443:LEU:H	1.70	0.56
1:F:1236:PRO:HB3	1:F:1468:ARG:HD3	1.86	0.56
1:F:1662:ARG:NH1	1:F:1793:GLY:O	2.38	0.56
1:E:1572:ASN:OD1	1:E:1851:LYS:NZ	2.38	0.56
1:E:1928:GLN:OE1	1:E:1931:ARG:NH2	2.39	0.56
1:F:1415:LEU:HD12	1:F:1416:PRO:HD2	1.88	0.56
1:E:1774:LEU:HA	1:F:1782:MET:O	2.06	0.56
1:E:1999:THR:HB	1:E:2044:ILE:HD12	1.88	0.56
1:F:1228:LEU:HB3	1:F:1260:LEU:HD21	1.88	0.55
1:F:1893:LEU:O	1:F:1925:GLN:NE2	2.39	0.55
1:F:1554:ALA:HB2	1:F:1882:PRO:HA	1.87	0.55
1:E:1845:GLN:HB2	1:E:1847:LYS:NZ	2.22	0.55
1:F:1765:ARG:HG3	1:F:1790:THR:HG23	1.89	0.54
1:E:1970:ASN:HB3	1:E:2018:VAL:HG12	1.90	0.54
1:F:869:GLU:N	1:F:869:GLU:OE2	2.38	0.54
1:E:1041:SER:HB2	1:E:1082:ARG:HH22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1490:SER:H	1:F:1493:LEU:HD21	1.72	0.54
1:E:1888:ILE:HB	1:E:1968:VAL:HG12	1.90	0.53
1:E:1900:LEU:HD23	1:E:1971:LEU:HD11	1.89	0.53
1:E:1917:ARG:N	3:E:2603:NDP:O2X	2.42	0.53
1:F:1457:VAL:O	1:F:1461:ARG:HG2	2.09	0.53
1:F:1483:VAL:HG11	1:F:1508:ASP:HA	1.90	0.53
1:F:1570:SER:OG	1:F:1602:GLU:OE1	2.26	0.53
1:F:1535:THR:HG22	1:F:1544:ILE:HG12	1.91	0.53
1:F:1493:LEU:O	1:F:1497:LEU:HD22	2.09	0.53
1:F:1470:ARG:NH2	1:F:1500:ASP:O	2.43	0.52
1:E:1530:HIS:HB2	1:E:1552:ARG:HB2	1.91	0.52
1:F:1413:ILE:O	1:F:1442:TRP:N	2.41	0.52
1:E:914:PHE:HB2	1:E:1055:ILE:HB	1.91	0.52
1:F:1235:MET:O	1:F:1461:ARG:NH2	2.43	0.52
1:E:1578:LEU:HD11	1:E:1588:ILE:HD11	1.92	0.52
1:F:915:GLU:HB2	1:F:957:LYS:HB2	1.92	0.52
1:E:2021:SER:OG	1:E:2038:ASN:ND2	2.43	0.52
1:F:2012:GLU:OE2	1:F:2012:GLU:N	2.30	0.52
1:E:1893:LEU:O	1:E:1925:GLN:NE2	2.38	0.52
1:E:1677:SER:O	1:E:1682:GLN:NE2	2.39	0.51
1:F:1670:THR:HG22	1:F:1741:VAL:HG12	1.91	0.51
1:F:862:TYR:HH	1:F:898:THR:HG1	1.54	0.51
1:F:1421:SER:O	1:F:1989:GLN:NE2	2.35	0.51
1:F:1784:ILE:HD12	1:F:1787:LYS:HD2	1.91	0.51
1:E:888:ALA:HA	1:E:891:TYR:HD2	1.76	0.51
1:E:2018:VAL:HB	1:E:2041:MET:SD	2.50	0.51
1:E:889:THR:HB	1:E:1030:MET:HB2	1.92	0.51
1:E:915:GLU:OE2	1:E:959:TYR:OH	2.24	0.51
1:E:1671:LEU:HG	1:E:1743:LEU:HB2	1.92	0.51
1:F:1795:LEU:HA	3:F:2602:NDP:H72N	1.77	0.51
1:E:1644:GLU:HG2	1:E:1825:PRO:HG2	1.93	0.50
1:E:1624:THR:HA	1:E:1856:VAL:HG11	1.93	0.50
1:E:1743:LEU:HD23	1:E:1767:LEU:HD11	1.92	0.50
1:F:1732:VAL:O	1:F:1736:THR:OG1	2.21	0.50
1:E:1890:ALA:HB3	1:E:1970:ASN:HA	1.92	0.50
1:F:985:LEU:HB3	1:F:990:VAL:HG23	1.93	0.50
1:E:1837:GLU:O	1:E:1841:ARG:HG2	2.11	0.50
1:E:2039:SER:O	1:E:2043:ARG:HG2	2.12	0.50
1:F:1030:MET:HA	1:F:1033:MET:HG3	1.94	0.50
1:F:1444:LYS:HA	1:F:1474:LEU:HG	1.92	0.50
1:F:1973:VAL:CG1	3:F:2603:NDP:H51A	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1443:LEU:N	1:F:1472:VAL:O	2.35	0.50
1:E:2004:ARG:O	1:E:2008:GLU:HG2	2.12	0.49
1:E:1669:GLU:OE1	1:E:1765:ARG:NH2	2.33	0.49
1:F:1036:MET:HG3	1:F:1078:VAL:HG11	1.93	0.49
1:F:1606:ARG:NH1	1:F:1860:GLU:OE2	2.44	0.49
1:F:1440:PRO:HA	1:F:1470:ARG:HB2	1.94	0.49
1:E:1117:PHE:HB3	1:E:2105:VAL:HB	1.95	0.49
1:F:1595:GLN:NE2	1:F:1906:GLN:OE1	2.45	0.49
1:F:1815:GLN:O	1:F:1819:ARG:HG2	2.13	0.49
1:E:889:THR:HA	1:E:892:LEU:HD12	1.95	0.49
1:E:1442:TRP:CD1	1:E:1474:LEU:HD21	2.48	0.48
1:F:1973:VAL:O	3:F:2603:NDP:H8A	2.13	0.48
1:F:866:THR:HB	1:F:876:VAL:HG12	1.94	0.48
1:F:1905:ILE:HD12	1:F:1937:VAL:HG21	1.94	0.48
1:E:1857:LEU:HD21	1:E:1871:LYS:H	1.78	0.48
1:F:987:GLN:HB2	1:F:1009:LEU:HA	1.94	0.48
1:F:1811:TRP:CH2	1:F:1815:GLN:HG3	2.48	0.48
1:F:2048:ARG:HH21	1:F:2054:PRO:HD2	1.77	0.48
1:E:1535:THR:HG22	1:E:1544:ILE:HG12	1.96	0.48
1:F:877:ASP:OD2	1:F:1004:HIS:ND1	2.42	0.48
1:F:891:TYR:CG	1:F:954:VAL:HG21	2.49	0.48
1:F:1427:SER:O	1:F:1431:ILE:HD13	2.14	0.48
1:F:1009:LEU:HD21	1:F:1021:LEU:HB2	1.95	0.47
1:E:1709:GLN:HG2	1:E:1720:PHE:CE2	2.48	0.47
1:F:1116:LYS:HA	1:F:2106:LEU:HA	1.96	0.47
1:F:2002:LEU:O	1:F:2006:THR:OG1	2.23	0.47
1:F:1566:VAL:HG22	1:F:1603:PHE:CD2	2.50	0.47
1:F:1659:LEU:O	1:F:1664:ARG:N	2.47	0.47
1:E:1031:ASP:OD2	1:E:1035:GLN:NE2	2.47	0.47
1:F:1228:LEU:HD11	1:F:1256:ILE:HG12	1.96	0.47
1:F:1526:GLU:OE2	1:F:1552:ARG:NH1	2.48	0.47
1:E:1010:GLU:HB3	1:E:1019:ARG:HG2	1.96	0.47
1:E:1838:ASP:N	1:E:1838:ASP:OD1	2.47	0.47
1:F:1769:ILE:HG22	3:F:2602:NDP:C2N	2.45	0.47
1:F:1729:GLU:HA	1:F:1759:CYS:SG	2.55	0.47
1:F:1889:ILE:HD11	1:F:1904:LEU:HD12	1.97	0.47
1:F:1123:THR:HG23	1:F:1391:LEU:HD23	1.97	0.47
1:E:999:TYR:HB3	1:E:1001:TYR:CE2	2.50	0.47
1:E:1115:GLU:HG2	1:E:1518:LEU:HD23	1.97	0.46
1:E:2057:ALA:HB3	1:E:2105:VAL:HG22	1.97	0.46
1:F:1729:GLU:HB2	1:F:1755:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1971:LEU:HD22	1:E:2019:PHE:CD2	2.50	0.46
1:F:911:PRO:HB2	1:F:961:TRP:HB3	1.97	0.46
1:E:1616:LEU:HD13	1:E:1650:VAL:HG22	1.97	0.46
1:F:1566:VAL:HG21	1:F:1626:VAL:HG23	1.97	0.46
1:E:1081:SER:HB3	1:E:1086:VAL:HG12	1.98	0.46
1:E:1736:THR:HG21	1:E:1740:GLY:H	1.80	0.46
1:F:1768:GLU:HG2	1:F:1774:LEU:HD21	1.97	0.46
1:E:1988:PHE:CE1	1:E:2033:ASN:HB3	2.51	0.46
1:F:1769:ILE:O	3:F:2602:NDP:H2N	2.15	0.46
1:E:1538:ARG:H	1:E:1538:ARG:HG2	1.60	0.46
1:F:1033:MET:SD	1:F:1089:ALA:HB3	2.56	0.46
1:F:1704:LYS:NZ	3:F:2602:NDP:O3X	2.45	0.45
1:E:881:ASP:O	1:E:1105:ARG:NH1	2.49	0.45
1:E:2063:ILE:HG12	3:E:2603:NDP:H42N	1.98	0.45
1:F:1059:PRO:HA	1:F:1062:HIS:HB3	1.97	0.45
1:F:1657:TYR:CZ	1:F:1662:ARG:HD2	2.50	0.45
1:E:1026:TRP:O	1:E:1030:MET:HG3	2.16	0.45
1:E:1716:ASP:OD1	1:E:1719:SER:OG	2.28	0.45
1:F:1473:LEU:HD11	1:F:1503:MET:HA	1.99	0.45
1:F:1671:LEU:HG	1:F:1743:LEU:HB2	1.97	0.45
1:E:1565:THR:OG1	1:E:1868:ALA:O	2.26	0.45
1:F:1613:VAL:HG21	1:F:1633:LEU:HD21	1.99	0.45
1:F:1468:ARG:HD2	1:F:1468:ARG:HA	1.77	0.45
1:F:1411:SER:OG	1:F:1439:ARG:NH1	2.50	0.45
1:F:1607:ASP:OD1	1:F:1608:ALA:N	2.47	0.45
1:E:1462:ARG:NH1	1:E:2027:GLY:O	2.50	0.45
1:E:2033:ASN:OD1	1:E:2033:ASN:N	2.50	0.45
1:E:2060:TRP:HB3	1:E:2063:ILE:HD11	1.99	0.45
1:E:891:TYR:CG	1:E:954:VAL:HG21	2.52	0.44
1:E:1604:SER:HA	1:E:1614:MET:HA	1.97	0.44
1:E:1007:GLY:HA3	1:E:1032:THR:HG21	1.99	0.44
1:E:1475:SER:HB3	1:E:1505:VAL:HG23	1.98	0.44
1:E:1736:THR:CG2	1:E:1740:GLY:H	2.30	0.44
1:F:1013:LEU:HD12	1:F:1930:ARG:HH12	1.82	0.44
1:F:1446:ILE:HD12	1:F:1447:ASN:N	2.31	0.44
1:F:1709:GLN:HG2	1:F:1720:PHE:CE2	2.52	0.44
1:E:1651:VAL:HG12	1:E:1683:ALA:HB2	1.99	0.44
1:F:2057:ALA:HB3	1:F:2105:VAL:HG22	1.98	0.44
1:E:1456:LEU:HD22	1:E:2036:PHE:CD1	2.52	0.44
1:E:1515:ARG:HA	1:E:1515:ARG:HD2	1.88	0.44
1:F:1697:THR:O	1:F:1721:ALA:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1970:ASN:ND2	1:F:1999:THR:OG1	2.51	0.44
1:E:908:GLU:O	1:E:1063:ARG:NH2	2.51	0.44
1:E:1543:SER:O	1:E:1543:SER:OG	2.30	0.44
1:E:1565:THR:HG23	1:E:1870:PRO:HG3	2.00	0.44
1:E:1711:ARG:NH2	1:E:1825:PRO:O	2.45	0.44
1:F:1910:GLN:HA	1:F:1937:VAL:HG13	1.99	0.44
1:F:1918:SER:HB3	1:F:1921:ARG:NH1	2.32	0.44
1:F:2026:ARG:HD3	2:F:2601:X5O:N23	2.33	0.44
1:F:897:LYS:HG2	1:F:907:VAL:HG21	1.98	0.44
1:F:1472:VAL:HG22	1:F:1502:VAL:HA	1.99	0.44
1:E:1010:GLU:OE1	1:E:1019:ARG:NH1	2.51	0.44
1:E:1889:ILE:HD11	1:E:1904:LEU:HD12	1.99	0.44
1:F:1698:THR:HG22	1:F:1721:ALA:HB3	1.98	0.44
1:F:2039:SER:O	1:F:2043:ARG:HG2	2.17	0.43
1:E:899:LEU:HD22	1:E:958:VAL:HG22	2.00	0.43
1:E:1574:ARG:NH2	1:E:1618:PRO:O	2.40	0.43
1:F:989:GLU:HA	1:F:992:LYS:HE2	2.00	0.43
1:F:1466:GLY:HA2	1:F:1469:LEU:HB3	1.99	0.43
1:F:1674:HIS:HD2	1:F:1746:ASN:HA	1.82	0.43
1:E:1642:LEU:HD23	1:E:1642:LEU:HA	1.90	0.43
1:E:2020:SER:N	1:E:2058:VAL:O	2.52	0.43
1:F:1061:THR:HA	1:F:1064:GLN:HG2	2.00	0.43
1:E:1059:PRO:HA	1:E:1062:HIS:HB3	2.01	0.43
1:E:1085:ARG:HD2	1:E:1085:ARG:HA	1.67	0.43
1:F:1885:LYS:HD3	1:F:1966:GLY:HA3	2.00	0.43
1:F:1062:HIS:HB2	1:F:1091:GLY:HA3	1.99	0.43
1:F:2062:ALA:O	1:F:2086:GLN:N	2.41	0.43
1:E:1658:ALA:HB2	1:E:1794:VAL:HG11	2.00	0.43
1:E:1116:LYS:HB2	1:E:1116:LYS:HE2	1.79	0.43
1:E:1808:ARG:HD2	1:E:1808:ARG:HA	1.71	0.43
1:F:1449:ALA:HB1	1:F:1477:LEU:HA	2.00	0.43
1:F:1633:LEU:O	1:F:1811:TRP:NE1	2.48	0.43
1:E:1729:GLU:HA	1:E:1759:CYS:SG	2.58	0.43
1:E:1778:HIS:O	1:F:1782:MET:HB2	2.18	0.43
1:F:1567:TYR:CE1	1:F:1606:ARG:HB2	2.54	0.43
1:E:866:THR:HB	1:E:876:VAL:HG22	2.01	0.42
1:E:905:LEU:HD12	1:E:910:LEU:HD13	2.01	0.42
1:E:1973:VAL:CG1	3:E:2603:NDP:H51A	2.48	0.42
1:F:1240:MET:HA	1:F:1240:MET:CE	2.49	0.42
1:E:1009:LEU:HB2	1:E:1019:ARG:HG3	2.01	0.42
1:E:996:LEU:HD23	1:E:996:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1473:LEU:O	1:E:1474:LEU:HD13	2.19	0.42
1:E:1907:ARG:HD3	1:E:1907:ARG:HA	1.85	0.42
1:F:999:TYR:HB3	1:F:1001:TYR:CE2	2.54	0.42
1:E:1602:GLU:HG3	1:E:1649:PRO:HB2	2.00	0.42
1:F:1080:VAL:HG22	1:F:1087:THR:HG23	2.01	0.42
1:F:1428:LEU:HD13	1:F:1432:LEU:HD12	2.00	0.42
1:F:1031:ASP:O	1:F:1035:GLN:HG3	2.19	0.42
1:E:1860:GLU:HG3	1:E:1865:LEU:HD13	2.02	0.42
1:F:1897:GLY:HA2	1:F:1971:LEU:HD22	2.02	0.42
1:F:2042:GLU:OE1	1:F:2059:GLN:NE2	2.24	0.42
1:E:1614:MET:SD	1:E:1649:PRO:HG3	2.60	0.42
1:F:1472:VAL:HG13	1:F:1502:VAL:O	2.20	0.42
1:F:1612:ARG:HD2	1:F:1642:LEU:HG	2.01	0.42
1:E:1031:ASP:O	1:E:1035:GLN:HG3	2.19	0.42
1:E:1057:ILE:HG23	1:E:1092:VAL:HG22	2.02	0.42
1:E:1611:LYS:HB3	1:E:1611:LYS:HE2	1.82	0.42
1:F:1041:SER:OG	1:F:1082:ARG:NH1	2.53	0.42
1:F:1530:HIS:HB2	1:F:1552:ARG:HG2	2.02	0.42
1:E:1806:ASP:N	1:E:1806:ASP:OD1	2.53	0.41
1:F:953:VAL:HG12	1:F:954:VAL:HG23	2.02	0.41
1:E:1600:GLY:HA3	1:E:1622:LEU:N	2.34	0.41
1:E:985:LEU:HD11	1:E:1927:LYS:HD2	2.01	0.41
1:F:1637:PRO:HG2	1:F:1640:TRP:CG	2.55	0.41
1:F:1905:ILE:CD1	1:F:1937:VAL:HG11	2.51	0.41
1:F:2084:LEU:HA	1:F:2084:LEU:HD12	1.85	0.41
1:E:1438:SER:O	1:E:1441:VAL:HG23	2.19	0.41
1:F:1960:ALA:HA	1:F:1963:GLY:O	2.19	0.41
1:E:1995:LYS:NZ	3:E:2603:NDP:O2D	2.48	0.41
1:E:2068:ILE:HD13	1:E:2068:ILE:HA	1.82	0.41
1:F:1769:ILE:HD13	1:F:1794:VAL:HB	2.02	0.41
1:E:1070:GLN:OE1	1:E:1070:GLN:N	2.54	0.41
1:E:1419:ASP:HB3	1:E:1424:TRP:HD1	1.86	0.41
1:E:1523:LYS:HE2	1:E:1523:LYS:HB3	1.79	0.41
1:E:1786:LEU:HG	1:F:1774:LEU:HB3	2.02	0.41
1:E:1890:ALA:N	1:E:1969:PHE:O	2.50	0.41
1:E:1899:GLU:HG3	1:E:2088:MET:HG2	2.02	0.41
1:F:1119:PHE:CZ	1:F:1507:ARG:HB3	2.56	0.41
1:F:1461:ARG:HD2	1:F:1471:CYS:SG	2.61	0.41
1:E:1036:MET:HG3	1:E:1078:VAL:HG11	2.02	0.41
1:E:1505:VAL:HG12	1:E:1513:ALA:HA	2.03	0.41
1:E:1518:LEU:HD23	1:E:1518:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:863:ASN:HB3	1:F:930:THR:HG21	2.03	0.41
1:F:1882:PRO:HG2	1:F:1885:LYS:HB2	2.02	0.41
1:E:1794:VAL:O	1:E:1795:LEU:HD23	2.21	0.41
1:E:1995:LYS:O	1:E:1999:THR:OG1	2.28	0.41
1:E:2056:LEU:HD12	1:E:2057:ALA:N	2.36	0.41
1:F:1106:GLN:OE1	1:F:1107:GLN:N	2.53	0.41
1:F:1226:ALA:HA	1:F:1515:ARG:HD2	2.02	0.41
1:F:1442:TRP:HE1	1:F:1496:VAL:HG12	1.85	0.41
1:F:2004:ARG:O	1:F:2008:GLU:HG3	2.21	0.41
1:F:2066:VAL:HG22	1:F:2088:MET:HE3	2.03	0.41
1:E:1678:GLY:HA3	3:E:2602:NDP:H52A	2.03	0.40
1:E:1901:ALA:O	1:E:1905:ILE:HG12	2.20	0.40
1:F:1260:LEU:HB3	1:F:1266:LEU:HD23	2.02	0.40
1:F:1452:GLY:HA2	1:F:2039:SER:HB3	2.04	0.40
1:F:1669:GLU:CD	1:F:1765:ARG:HH22	2.25	0.40
1:F:1917:ARG:NE	3:F:2603:NDP:O3X	2.49	0.40
1:F:1411:SER:HA	1:F:1412:PRO:HD3	1.95	0.40
1:F:1651:VAL:HG23	1:F:1851:LYS:HE3	2.03	0.40
1:E:985:LEU:HB3	1:E:990:VAL:HG23	2.04	0.40
1:E:1797:ASP:HA	1:E:1800:PHE:CE2	2.56	0.40
1:E:1990:ASP:HA	1:E:1993:LYS:HE2	2.03	0.40
1:F:1117:PHE:HB3	1:F:2105:VAL:HB	2.03	0.40
1:F:1416:PRO:HA	1:F:1444:LYS:HG3	2.03	0.40
1:E:1019:ARG:HD3	1:E:1075:VAL:HG21	2.03	0.40
1:E:1886:SER:HA	1:E:1911:LYS:HB2	2.03	0.40
1:E:1912:LEU:HD23	1:E:1912:LEU:HA	1.94	0.40
1:E:1973:VAL:O	3:E:2603:NDP:H8A	2.20	0.40
1:E:2002:LEU:HD23	1:E:2002:LEU:HA	1.93	0.40
1:F:858:SER:HB2	1:F:859:ALA:H	1.77	0.40
1:F:1837:GLU:O	1:F:1841:ARG:HG2	2.22	0.40
1:E:884:VAL:HG12	1:E:925:LEU:HD12	2.03	0.40
1:E:2001:ASN:O	1:E:2005:VAL:HG23	2.22	0.40
1:F:1904:LEU:HB3	1:F:1909:VAL:HG21	2.04	0.40
1:F:2069:LEU:HD12	1:F:2070:VAL:N	2.36	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	E	960/1670 (58%)	942 (98%)	18 (2%)	0	100	100
1	F	1052/1670 (63%)	1027 (98%)	25 (2%)	0	100	100
All	All	2012/3340 (60%)	1969 (98%)	43 (2%)	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	E	719/1392 (52%)	700 (97%)	19 (3%)	46	75
1	F	801/1392 (58%)	766 (96%)	35 (4%)	28	56
All	All	1520/2784 (55%)	1466 (96%)	54 (4%)	38	64

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1036	MET
1	E	1442	TRP
1	E	1507	ARG
1	E	1511	TRP
1	E	1538	ARG
1	E	1542	SER
1	E	1545	ARG
1	E	1596	ASP

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Mol	Chain	Res	Type
1	E	1601	MET
1	E	1614	MET
1	E	1773	ASP
1	E	1788	ASN
1	E	1819	ARG
1	E	1847	LYS
1	E	1865	LEU
1	E	1896	PHE
1	E	1921	ARG
1	E	1996	TYR
1	E	2106	LEU
1	F	927	LYS
1	F	971	HIS
1	F	976	THR
1	F	1044	HIS
1	F	1065	LYS
1	F	1106	GLN
1	F	1117	PHE
1	F	1240	MET
1	F	1442	TRP
1	F	1444	LYS
1	F	1462	ARG
1	F	1493	LEU
1	F	1552	ARG
1	F	1563	LEU
1	F	1586	ASP
1	F	1601	MET
1	F	1606	ARG
1	F	1666	ARG
1	F	1711	ARG
1	F	1743	LEU
1	F	1771	LYS
1	F	1773	ASP
1	F	1790	THR
1	F	1796	LEU
1	F	1819	ARG
1	F	1860	GLU
1	F	1886	SER
1	F	1896	PHE
1	F	1921	ARG
1	F	1982	ASN
1	F	2008	GLU

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Mol	Chain	Res	Type
1	F	2026	ARG
1	F	2031	GLN
1	F	2069	LEU
1	F	2071	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1530	HIS
1	E	1555	GLN
1	F	1476	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 monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NDP	E	2603	-	45,52,52	3.80	21 (46%)	53,80,80	1.76	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NDP	F	2603	-	45,52,52	3.90	21 (46%)	53,80,80	1.81	11 (20%)
3	NDP	F	2602	-	45,52,52	3.79	17 (37%)	53,80,80	1.81	11 (20%)
3	NDP	E	2602	-	45,52,52	3.81	18 (40%)	53,80,80	1.57	9 (16%)
2	X5O	F	2601	-	36,37,37	1.94	8 (22%)	48,53,53	2.91	9 (18%)
2	X5O	E	2601	-	36,37,37	1.97	9 (25%)	48,53,53	2.94	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	E	2603	-	-	8/30/77/77	0/5/5/5
3	NDP	F	2603	-	-	11/30/77/77	0/5/5/5
3	NDP	F	2602	-	-	12/30/77/77	0/5/5/5
3	NDP	E	2602	-	-	12/30/77/77	0/5/5/5
2	X5O	F	2601	-	-	3/22/38/38	1/5/5/5
2	X5O	E	2601	-	-	4/22/38/38	1/5/5/5

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2602	NDP	O4B-C1B	13.46	1.59	1.41
3	F	2603	NDP	O4B-C1B	13.17	1.59	1.41
3	F	2602	NDP	O4B-C1B	12.76	1.58	1.41
3	E	2603	NDP	O4B-C1B	11.86	1.57	1.41
3	F	2602	NDP	C2D-C3D	-10.80	1.23	1.53
3	F	2603	NDP	C2D-C3D	-10.67	1.24	1.53
3	E	2603	NDP	C2D-C3D	-10.48	1.24	1.53
3	E	2602	NDP	C2D-C3D	-10.28	1.25	1.53
3	E	2603	NDP	O4B-C4B	-9.99	1.22	1.45
3	F	2603	NDP	O4B-C4B	-9.65	1.23	1.45
3	F	2602	NDP	O4B-C4B	-9.19	1.24	1.45
3	E	2602	NDP	O4B-C4B	-9.16	1.24	1.45
3	F	2603	NDP	C4N-C3N	-7.21	1.35	1.49
3	F	2602	NDP	O4D-C1D	-6.98	1.25	1.42
2	E	2601	X5O	C08-N10	6.95	1.50	1.34
2	F	2601	X5O	C08-N10	6.80	1.49	1.34
3	E	2602	NDP	C4N-C3N	-6.77	1.36	1.49
3	E	2603	NDP	C4N-C3N	-6.72	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2603	NDP	O4D-C1D	-6.65	1.26	1.42
3	E	2602	NDP	O4D-C1D	-6.62	1.26	1.42
3	F	2602	NDP	C4N-C3N	-6.41	1.37	1.49
3	F	2603	NDP	O4D-C1D	-6.38	1.26	1.42
3	F	2602	NDP	C5D-C4D	-5.38	1.34	1.51
3	E	2602	NDP	C5D-C4D	-5.28	1.35	1.51
3	E	2603	NDP	C5D-C4D	-5.23	1.35	1.51
3	F	2603	NDP	C5D-C4D	-5.08	1.35	1.51
2	E	2601	X5O	C07-C08	4.88	1.58	1.50
3	F	2602	NDP	C4N-C5N	-4.83	1.36	1.48
2	F	2601	X5O	C07-C08	4.71	1.57	1.50
3	E	2603	NDP	C4N-C5N	-4.57	1.36	1.48
3	E	2602	NDP	C4N-C5N	-4.54	1.37	1.48
3	F	2603	NDP	C4N-C5N	-4.52	1.37	1.48
3	E	2603	NDP	O3B-C3B	-4.19	1.33	1.43
3	F	2603	NDP	O3B-C3B	-4.10	1.33	1.43
2	E	2601	X5O	C19-C22	4.10	1.53	1.44
2	F	2601	X5O	C19-C22	4.08	1.53	1.44
3	F	2603	NDP	O7N-C7N	-4.01	1.15	1.24
3	E	2602	NDP	O7N-C7N	-3.96	1.15	1.24
3	F	2602	NDP	C7N-N7N	3.95	1.43	1.33
3	F	2602	NDP	O3B-C3B	-3.95	1.33	1.43
3	E	2603	NDP	C7N-N7N	3.74	1.43	1.33
3	E	2602	NDP	O3B-C3B	-3.74	1.34	1.43
3	E	2602	NDP	C7N-N7N	3.70	1.43	1.33
3	E	2602	NDP	C2D-C1D	3.61	1.65	1.53
3	F	2602	NDP	O7N-C7N	-3.58	1.16	1.24
3	E	2602	NDP	O4D-C4D	3.40	1.52	1.45
3	E	2603	NDP	O7N-C7N	-3.36	1.16	1.24
3	F	2603	NDP	C4A-N3A	-3.32	1.31	1.35
3	F	2603	NDP	C7N-N7N	3.31	1.42	1.33
3	E	2603	NDP	O4D-C4D	3.27	1.52	1.45
3	E	2603	NDP	C4A-N3A	-3.26	1.31	1.35
3	F	2603	NDP	C6N-N1N	-3.24	1.29	1.37
3	F	2603	NDP	O4D-C4D	3.22	1.52	1.45
3	F	2602	NDP	C6A-N6A	3.17	1.45	1.34
3	F	2602	NDP	C2D-C1D	3.15	1.63	1.53
3	E	2602	NDP	C6A-N6A	3.14	1.45	1.34
3	F	2602	NDP	C6N-N1N	-3.14	1.29	1.37
3	E	2603	NDP	C6N-N1N	-3.13	1.29	1.37
3	E	2603	NDP	C2D-C1D	2.99	1.63	1.53
3	F	2603	NDP	C2D-C1D	2.97	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2602	NDP	O4D-C4D	2.96	1.51	1.45
3	F	2602	NDP	C1D-N1N	-2.80	1.38	1.46
3	E	2602	NDP	C6N-N1N	-2.71	1.30	1.37
2	F	2601	X5O	C11-N10	2.68	1.51	1.47
2	E	2601	X5O	C11-N10	2.66	1.51	1.47
3	E	2603	NDP	C6A-N6A	2.62	1.43	1.34
3	E	2602	NDP	C4A-N3A	-2.60	1.32	1.35
3	E	2603	NDP	C5A-C4A	-2.56	1.34	1.40
3	F	2603	NDP	C1D-N1N	-2.51	1.39	1.46
3	E	2603	NDP	C1D-N1N	-2.51	1.39	1.46
3	F	2603	NDP	C6A-N6A	2.48	1.43	1.34
3	F	2603	NDP	C5A-C4A	-2.48	1.34	1.40
2	F	2601	X5O	C05-C24	2.46	1.54	1.48
2	E	2601	X5O	C15-N10	2.44	1.51	1.47
3	E	2602	NDP	C1D-N1N	-2.44	1.39	1.46
2	F	2601	X5O	C15-N10	2.43	1.51	1.47
2	E	2601	X5O	C05-C24	2.42	1.54	1.48
3	E	2603	NDP	O3D-C3D	2.34	1.48	1.43
2	E	2601	X5O	C16-C13	2.28	1.56	1.52
2	F	2601	X5O	C16-C13	2.28	1.56	1.52
3	F	2602	NDP	C4A-N3A	-2.26	1.32	1.35
3	F	2603	NDP	PN-O2N	-2.25	1.44	1.55
3	E	2603	NDP	C8A-N7A	-2.23	1.30	1.34
3	F	2603	NDP	C8A-N7A	-2.18	1.30	1.34
3	F	2603	NDP	O3D-C3D	2.15	1.48	1.43
3	F	2603	NDP	C5A-N7A	-2.12	1.32	1.39
3	E	2603	NDP	O5B-C5B	-2.11	1.36	1.44
3	E	2602	NDP	C6N-C5N	2.08	1.37	1.33
3	F	2602	NDP	O3D-C3D	2.05	1.47	1.43
2	F	2601	X5O	C04-C30	2.04	1.55	1.52
3	E	2603	NDP	C5A-N7A	-2.04	1.32	1.39
2	E	2601	X5O	C04-C30	2.04	1.55	1.52
3	E	2602	NDP	O3D-C3D	2.03	1.47	1.43
2	E	2601	X5O	C01-C02	2.00	1.55	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2601	X5O	C12-C13-C16	-13.49	81.17	112.79
2	F	2601	X5O	C12-C13-C16	-12.73	82.95	112.79
2	F	2601	X5O	C14-C13-C16	9.47	135.00	112.79
2	E	2601	X5O	C14-C13-C16	8.94	133.76	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2601	X5O	C27-N26-N25	7.16	108.80	105.31
2	E	2601	X5O	C27-N26-N25	7.08	108.77	105.31
3	F	2603	NDP	PN-O3-PA	-6.77	109.58	132.83
2	F	2601	X5O	C24-N28-C27	6.31	107.74	103.79
2	E	2601	X5O	C24-N28-C27	6.25	107.70	103.79
3	F	2602	NDP	O4B-C4B-C3B	-6.23	92.78	105.11
3	E	2603	NDP	O4B-C4B-C3B	-5.09	95.05	105.11
3	E	2603	NDP	N3A-C2A-N1A	-4.94	120.96	128.68
3	F	2603	NDP	O4B-C4B-C3B	-4.57	96.07	105.11
3	F	2603	NDP	N3A-C2A-N1A	-4.42	121.77	128.68
3	F	2602	NDP	N3A-C2A-N1A	-4.33	121.92	128.68
3	E	2603	NDP	O4B-C1B-C2B	-4.27	99.18	106.59
3	E	2602	NDP	N3A-C2A-N1A	-4.20	122.11	128.68
3	E	2602	NDP	O4B-C4B-C3B	-4.18	96.85	105.11
3	E	2602	NDP	O2B-C2B-C1B	-4.11	95.30	110.10
3	F	2602	NDP	O4D-C1D-C2D	-3.89	98.17	106.64
3	E	2602	NDP	C1D-N1N-C2N	-3.74	114.89	121.11
3	F	2602	NDP	O2B-C2B-C1B	-3.68	96.87	110.10
2	F	2601	X5O	C24-N25-N26	3.53	107.67	104.70
3	F	2603	NDP	O4B-C1B-C2B	-3.53	100.47	106.59
2	E	2601	X5O	C24-N25-N26	3.45	107.60	104.70
3	E	2603	NDP	O3B-C3B-C4B	-3.42	101.15	111.05
3	E	2603	NDP	PN-O3-PA	-3.24	121.72	132.83
3	F	2602	NDP	O3D-C3D-C4D	-3.14	101.96	111.05
3	F	2602	NDP	C3N-C2N-N1N	-2.83	119.06	123.10
3	F	2603	NDP	O3B-C3B-C4B	-2.83	102.87	111.05
3	E	2603	NDP	C4A-C5A-N7A	-2.68	106.61	109.40
3	F	2602	NDP	O4D-C1D-N1N	-2.62	102.93	108.06
3	F	2602	NDP	C4D-O4D-C1D	-2.52	103.92	109.47
2	E	2601	X5O	C03-C02-C07	2.50	119.93	118.03
3	F	2603	NDP	C4A-C5A-N7A	-2.50	106.80	109.40
3	E	2602	NDP	C3N-C7N-N7N	2.49	122.09	117.67
2	F	2601	X5O	C15-C14-C13	-2.44	108.15	111.04
3	E	2603	NDP	O2D-C2D-C1D	-2.44	101.85	110.02
3	F	2603	NDP	C1D-N1N-C2N	-2.44	117.05	121.11
3	E	2603	NDP	C3D-C2D-C1D	2.40	105.99	101.43
2	F	2601	X5O	C31-C30-C04	-2.38	115.76	119.43
3	E	2602	NDP	C4D-O4D-C1D	-2.35	104.30	109.47
3	E	2602	NDP	O3D-C3D-C4D	-2.32	104.35	111.05
3	E	2602	NDP	PN-O3-PA	-2.25	125.09	132.83
2	F	2601	X5O	C29-C27-N28	2.23	126.08	120.49
2	F	2601	X5O	C03-C02-C07	2.22	119.72	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2603	NDP	C4D-O4D-C1D	-2.22	104.58	109.47
2	E	2601	X5O	C29-C27-N28	2.21	126.01	120.49
3	E	2603	NDP	C4D-O4D-C1D	-2.19	104.63	109.47
3	E	2603	NDP	C5D-C4D-C3D	-2.19	106.99	115.18
3	F	2602	NDP	C3N-C7N-N7N	2.15	121.49	117.67
3	F	2603	NDP	O2D-C2D-C1D	-2.15	102.82	110.02
3	F	2602	NDP	C2B-C3B-C4B	-2.15	97.32	101.99
3	E	2602	NDP	C4A-C5A-N7A	-2.13	107.17	109.40
3	F	2603	NDP	O4D-C1D-C2D	-2.11	102.03	106.64
3	F	2602	NDP	O2B-C2B-C3B	-2.09	104.11	111.68
2	E	2601	X5O	C31-C30-C04	-2.08	116.22	119.43
3	F	2603	NDP	O2B-C2B-C1B	-2.03	102.80	110.10

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2601	X5O	C06-C05-C24-N25
2	E	2601	X5O	C06-C05-C24-N28
2	F	2601	X5O	C06-C05-C24-N28
3	E	2602	NDP	C5B-O5B-PA-O2A
3	E	2602	NDP	C5B-O5B-PA-O3
3	E	2602	NDP	C5D-O5D-PN-O3
3	E	2602	NDP	C5D-O5D-PN-O1N
3	E	2603	NDP	C5B-O5B-PA-O1A
3	E	2603	NDP	C2B-O2B-P2B-O1X
3	E	2603	NDP	O4D-C1D-N1N-C6N
3	F	2602	NDP	C5B-O5B-PA-O1A
3	F	2602	NDP	C5B-O5B-PA-O2A
3	F	2602	NDP	C5B-O5B-PA-O3
3	F	2602	NDP	C5D-O5D-PN-O3
3	F	2603	NDP	C5B-O5B-PA-O3
3	F	2603	NDP	O4B-C4B-C5B-O5B
3	E	2603	NDP	O4B-C4B-C5B-O5B
3	E	2603	NDP	O4D-C4D-C5D-O5D
3	F	2603	NDP	O4D-C4D-C5D-O5D
3	F	2603	NDP	O4D-C1D-N1N-C6N
3	F	2602	NDP	O4D-C4D-C5D-O5D
2	F	2601	X5O	C06-C05-C24-N25
3	F	2603	NDP	C3D-C4D-C5D-O5D
3	E	2602	NDP	C2D-C1D-N1N-C2N
3	E	2602	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	E	2603	NDP	C5B-O5B-PA-O3
3	E	2603	NDP	PN-O3-PA-O1A
3	F	2602	NDP	PN-O3-PA-O2A
3	F	2602	NDP	O4D-C1D-N1N-C2N
3	E	2602	NDP	C5B-O5B-PA-O1A
3	F	2602	NDP	C5D-O5D-PN-O1N
3	F	2603	NDP	C5B-O5B-PA-O1A
3	F	2603	NDP	C5B-O5B-PA-O2A
3	E	2603	NDP	C3D-C4D-C5D-O5D
3	F	2602	NDP	C3B-C4B-C5B-O5B
2	E	2601	X5O	C04-C05-C24-N25
2	F	2601	X5O	C04-C05-C24-N25
3	E	2602	NDP	C2D-C1D-N1N-C6N
3	E	2602	NDP	O4D-C1D-N1N-C2N
3	E	2602	NDP	PN-O3-PA-O2A
3	F	2602	NDP	C2D-C1D-N1N-C2N
3	F	2602	NDP	C3D-C4D-C5D-O5D
3	F	2602	NDP	C2B-O2B-P2B-O1X
3	F	2603	NDP	C2B-O2B-P2B-O1X
3	E	2602	NDP	O4D-C1D-N1N-C6N
2	E	2601	X5O	C14-C13-C16-C21
3	E	2602	NDP	C2B-O2B-P2B-O3X
3	F	2603	NDP	C2B-O2B-P2B-O2X
3	F	2603	NDP	C2B-O2B-P2B-O3X
3	F	2603	NDP	C5D-O5D-PN-O1N

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2601	X5O	C11-C12-C13-C14-C15-N10
2	F	2601	X5O	C11-C12-C13-C14-C15-N10

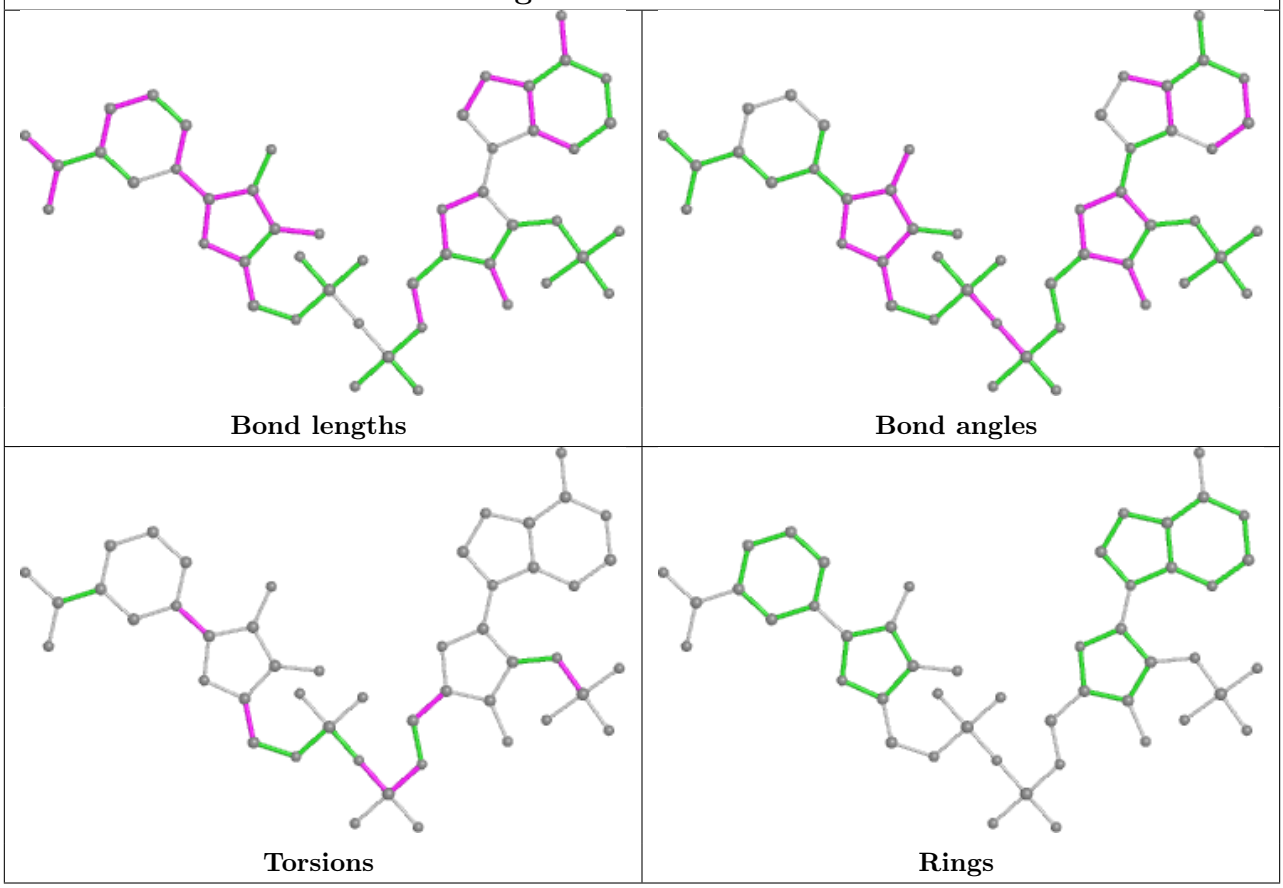
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2603	NDP	6	0
3	F	2603	NDP	5	0
3	F	2602	NDP	5	0
3	E	2602	NDP	1	0
2	F	2601	X5O	1	0

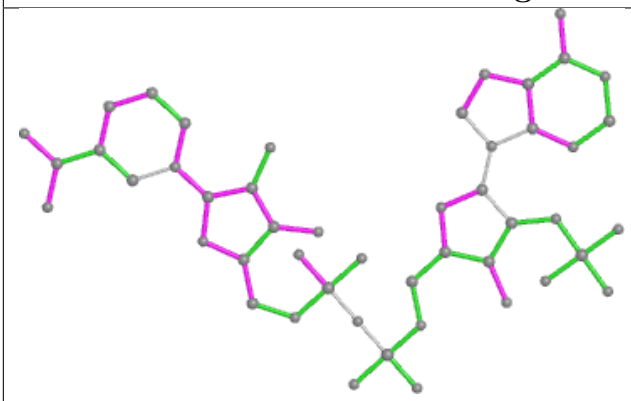
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

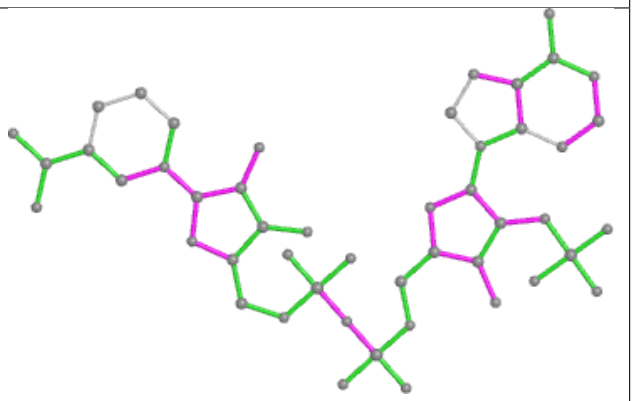
Ligand NDP E 2603



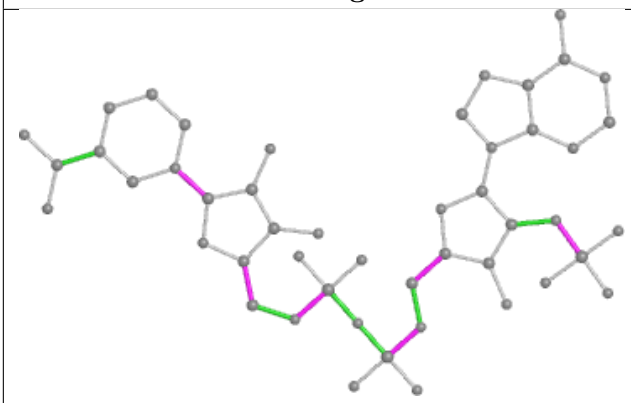
Ligand NDP F 2603



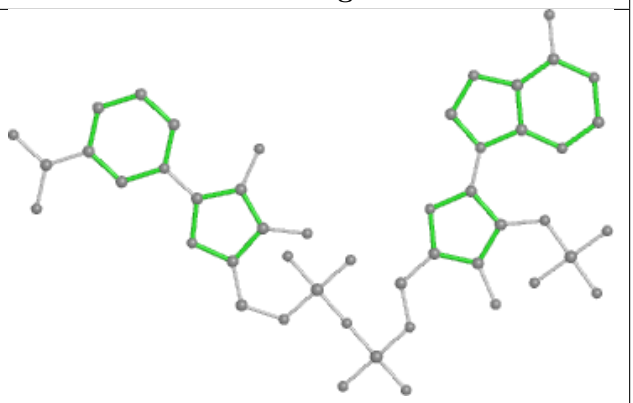
Bond lengths



Bond angles

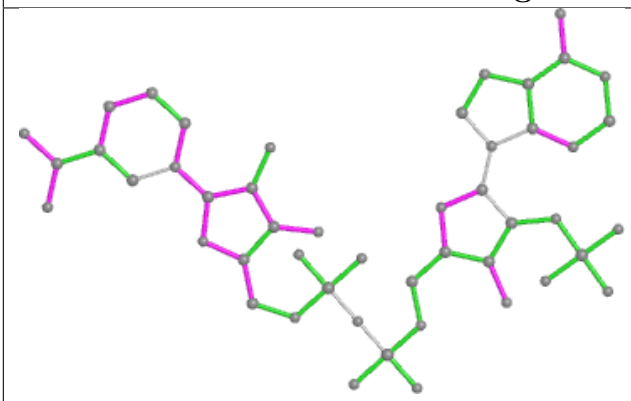


Torsions

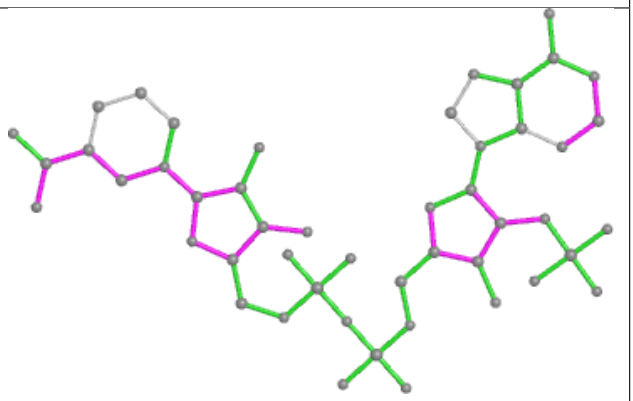


Rings

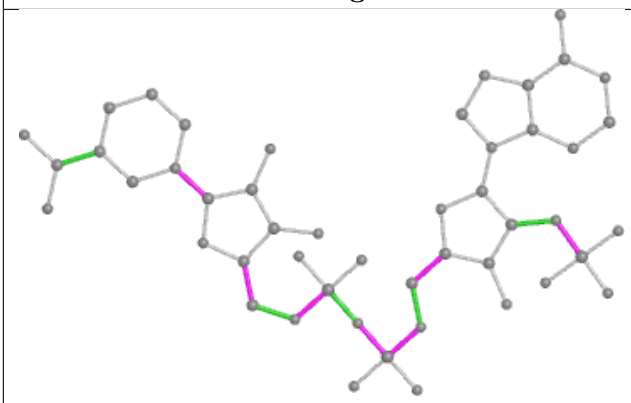
Ligand NDP F 2602



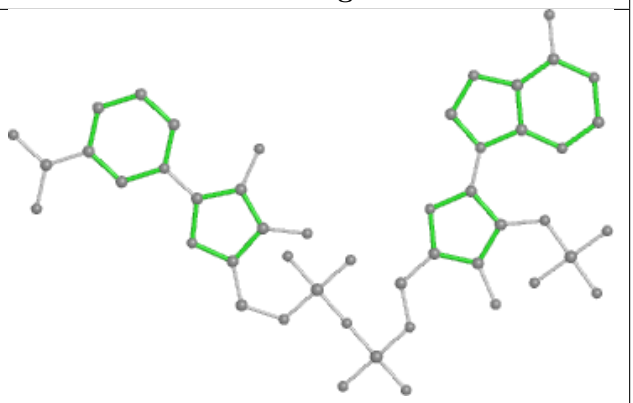
Bond lengths



Bond angles

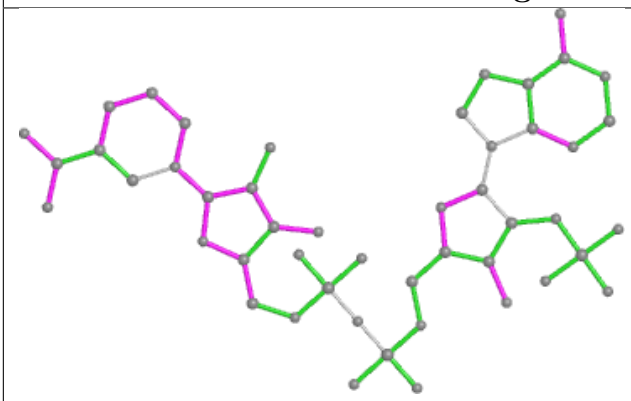


Torsions

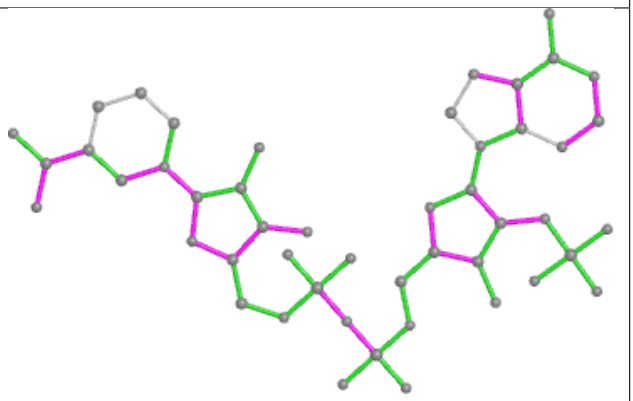


Rings

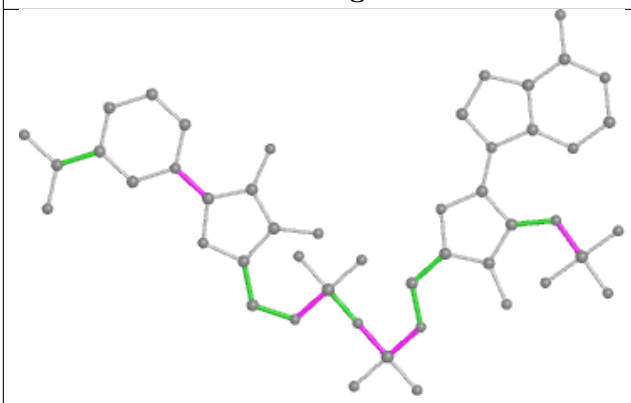
Ligand NDP E 2602



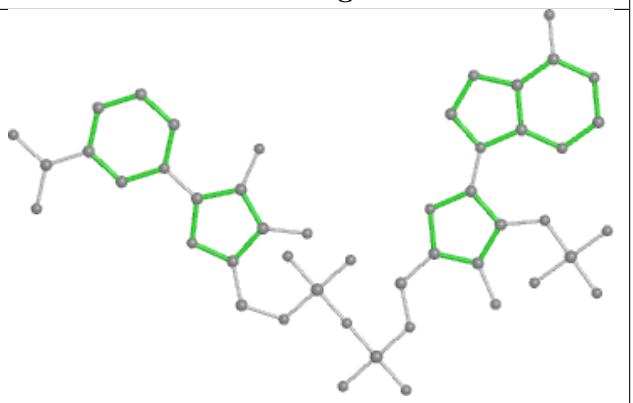
Bond lengths



Bond angles

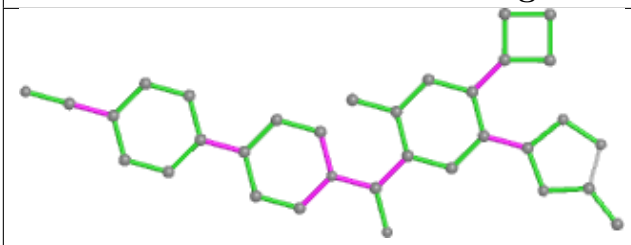


Torsions

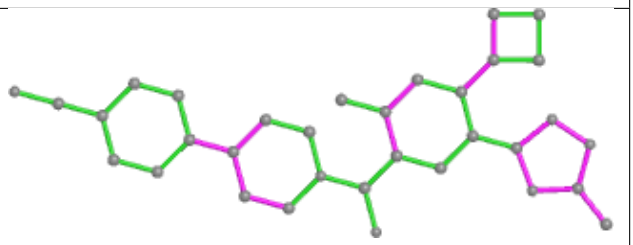


Rings

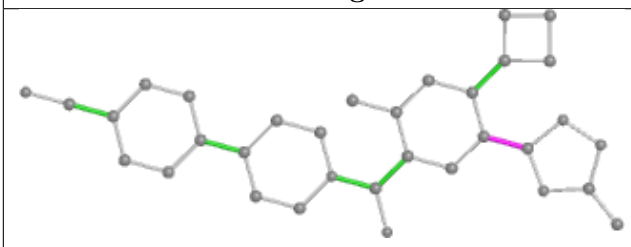
Ligand X5O F 2601



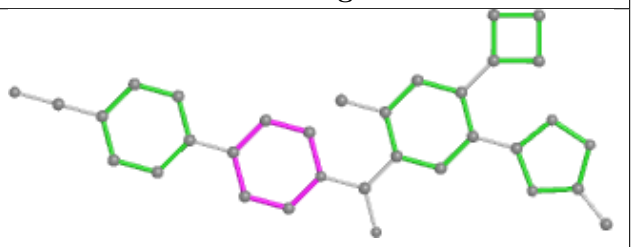
Bond lengths



Bond angles

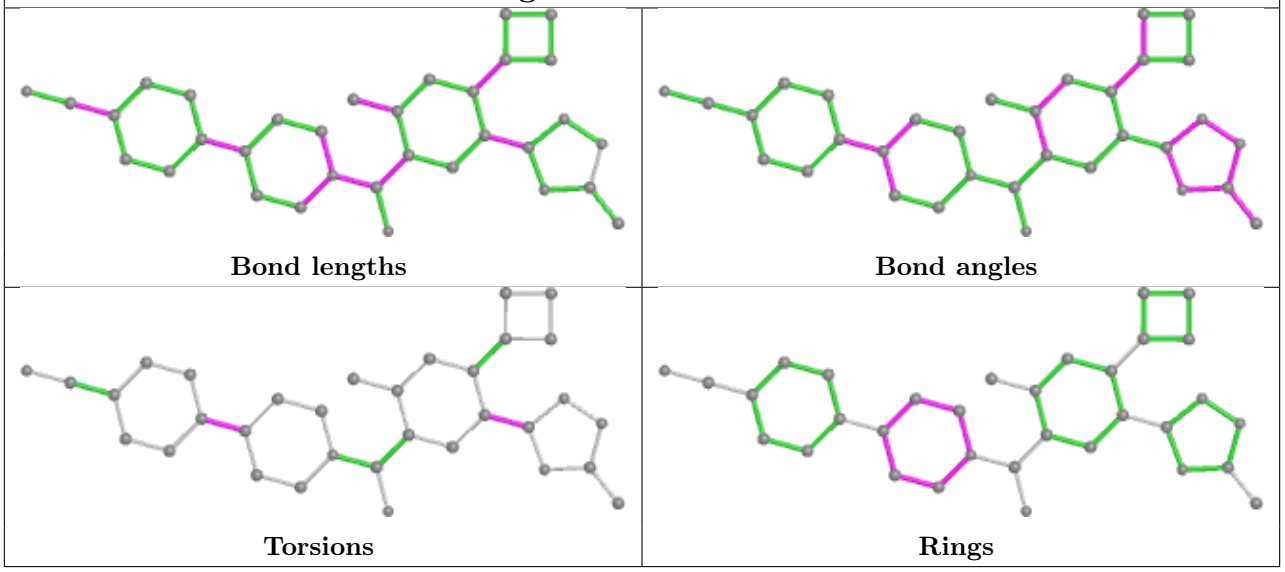


Torsions



Rings

Ligand X5O E 2601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

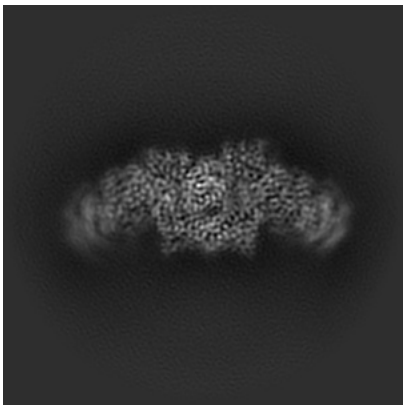
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28691. These allow visual inspection of the internal detail of the map and identification of artifacts.

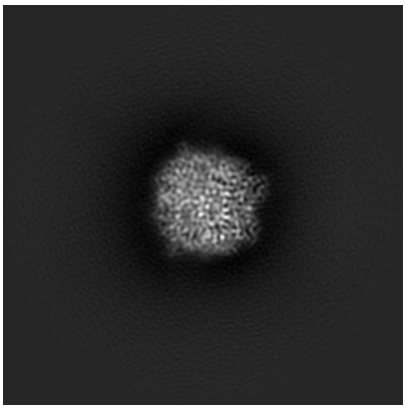
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

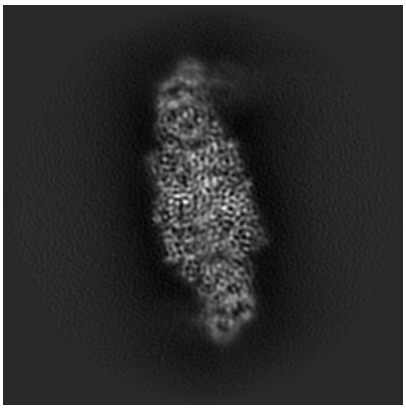
6.1.1 Primary map



X

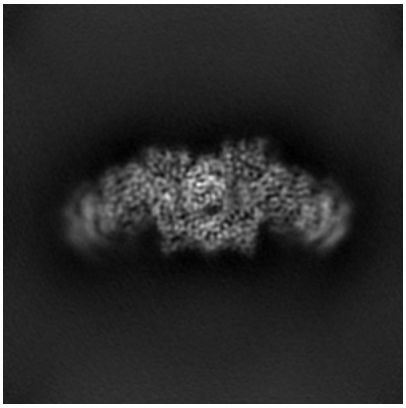


Y

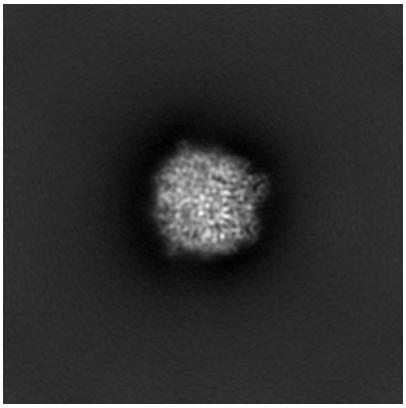


Z

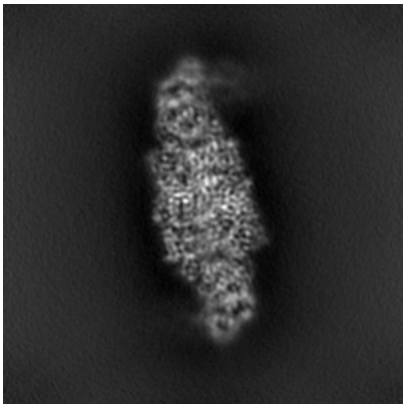
6.1.2 Raw map



X



Y

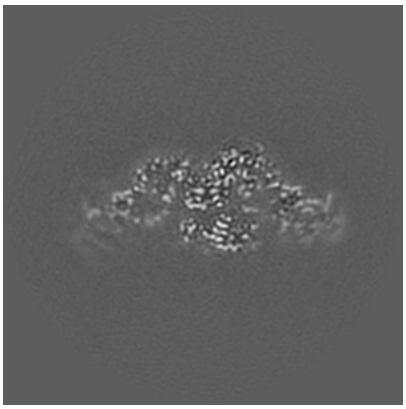


Z

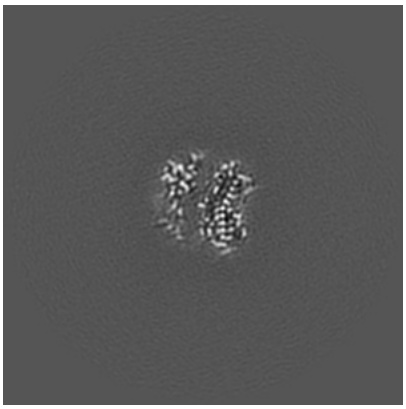
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

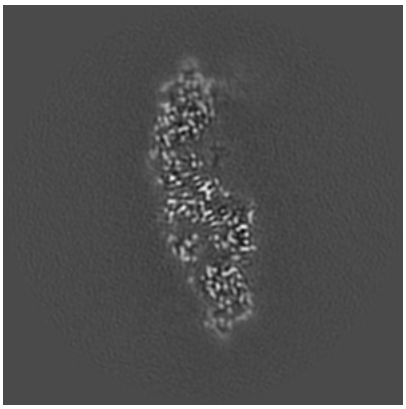
6.2.1 Primary map



X Index: 125

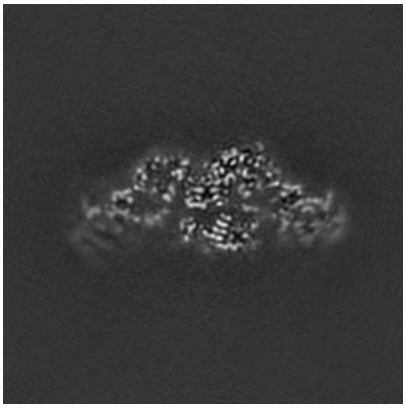


Y Index: 125

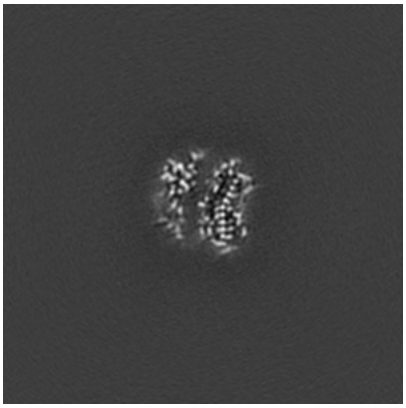


Z Index: 125

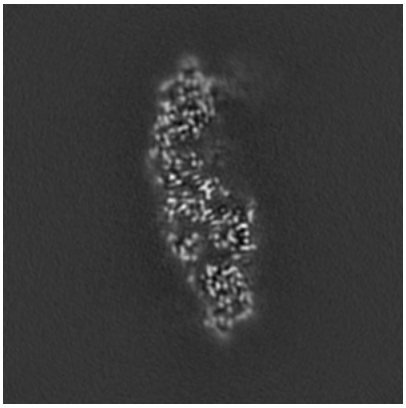
6.2.2 Raw map



X Index: 125



Y Index: 125

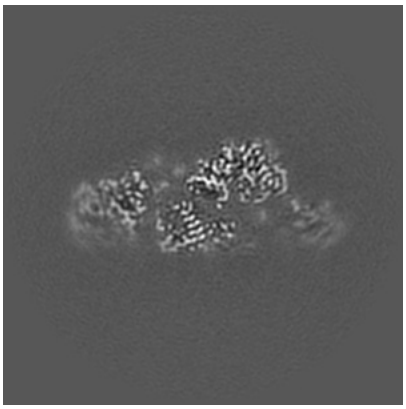


Z Index: 125

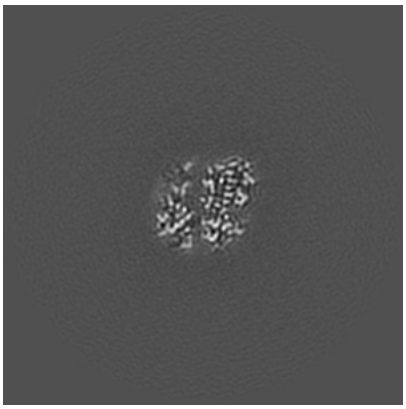
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

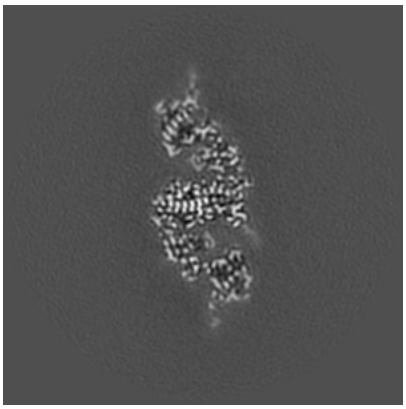
6.3.1 Primary map



X Index: 131

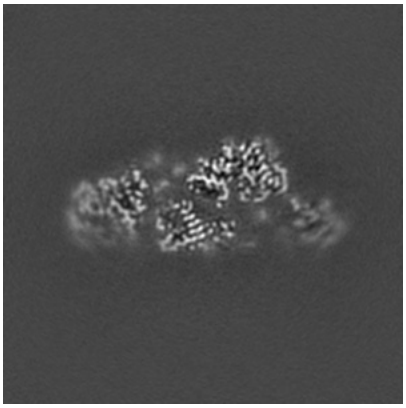


Y Index: 131

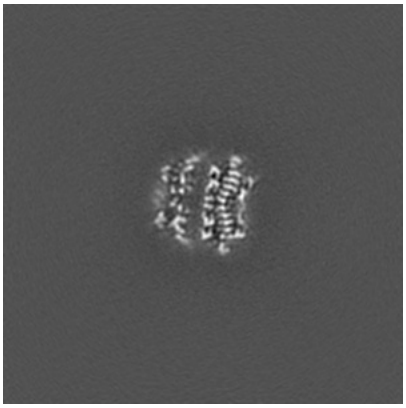


Z Index: 137

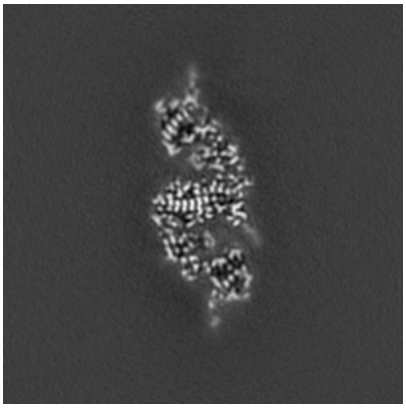
6.3.2 Raw map



X Index: 131



Y Index: 127

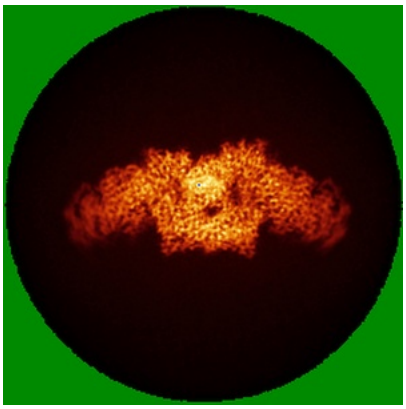


Z Index: 137

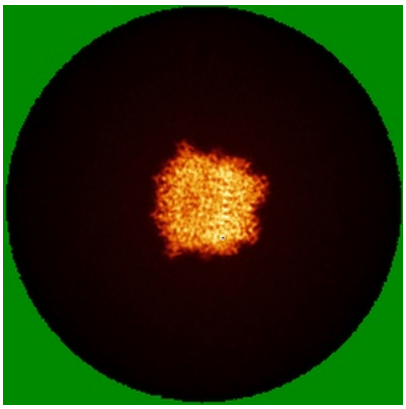
The images above show the largest variance slices of the map in three orthogonal directions.

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

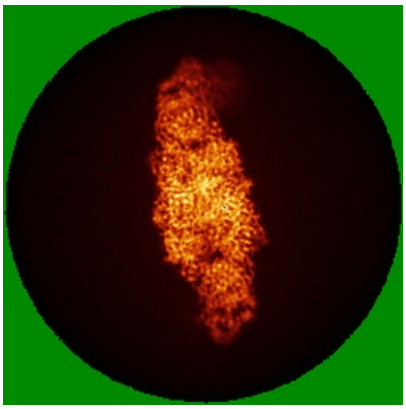
6.4.1 Primary map



X

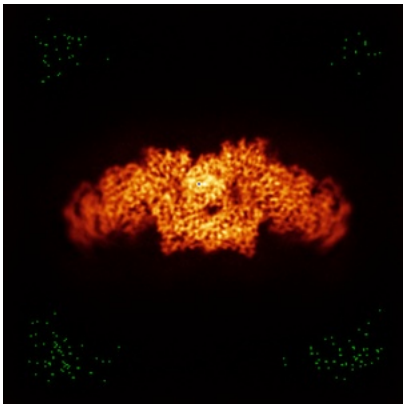


Y

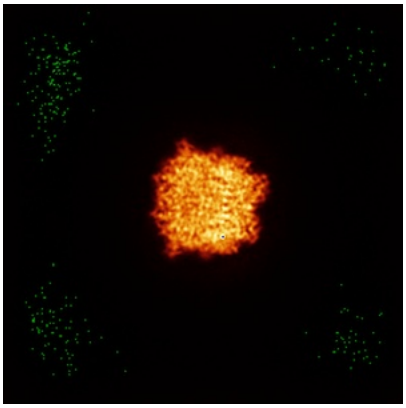


Z

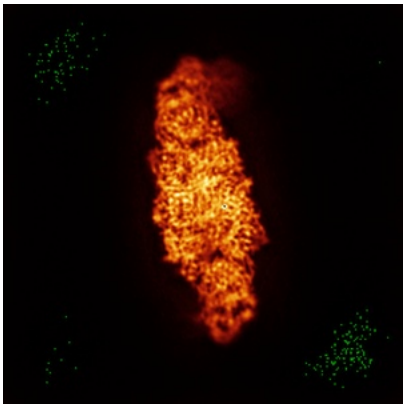
6.4.2 Raw map



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.

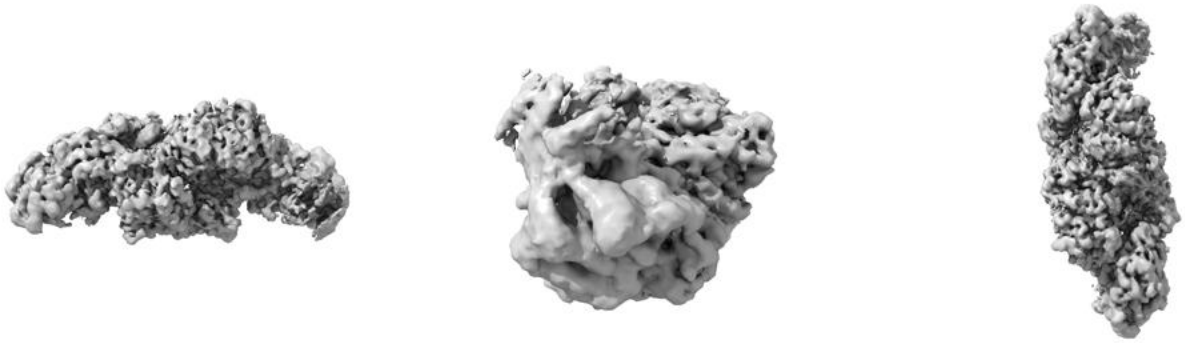
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.341. 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



X Y Z

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.

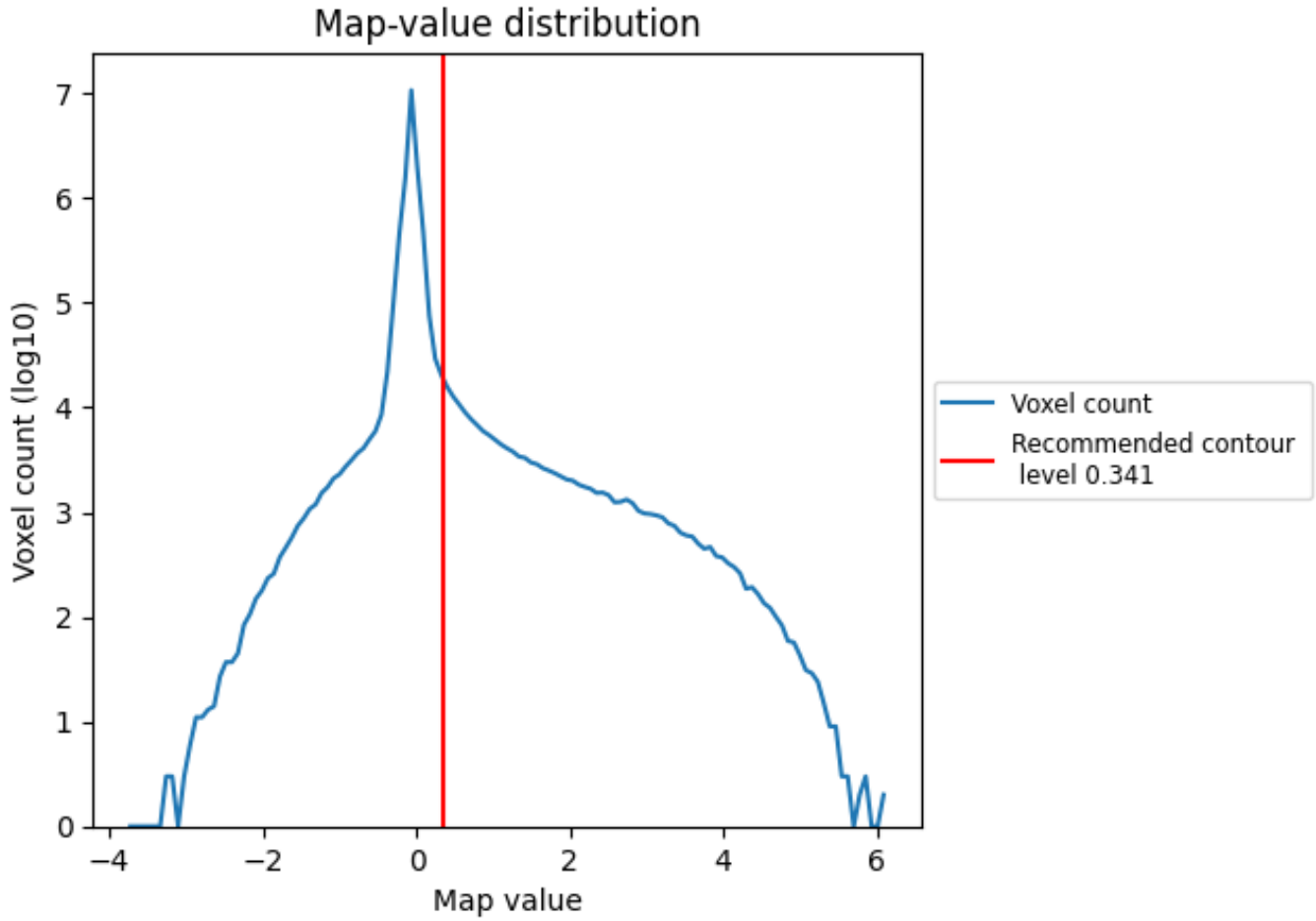
6.6 Mask visualisation (i)

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

7 Map analysis

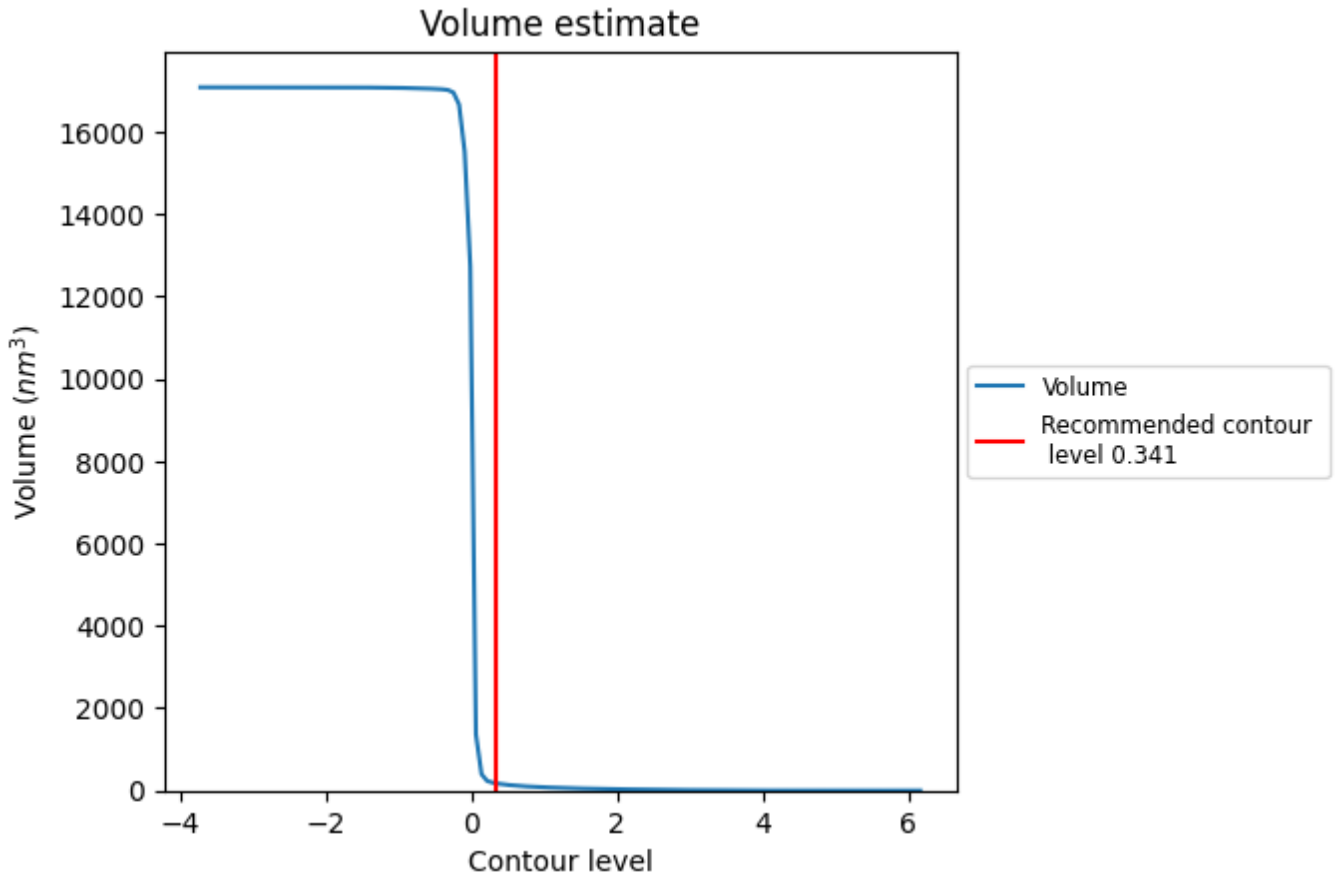
This section contains the results of statistical analysis of the map.

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.

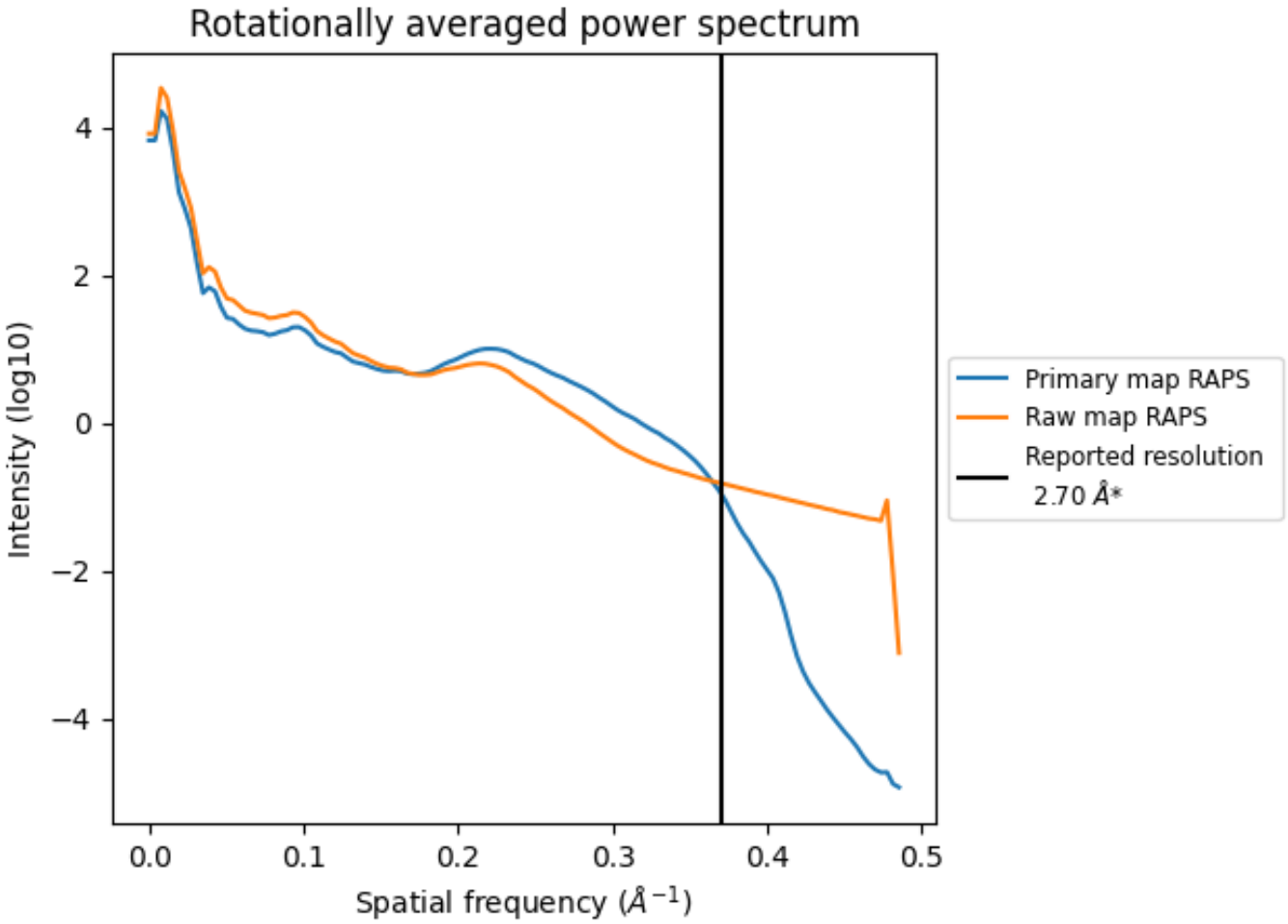
7.2 Volume estimate



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 160 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)

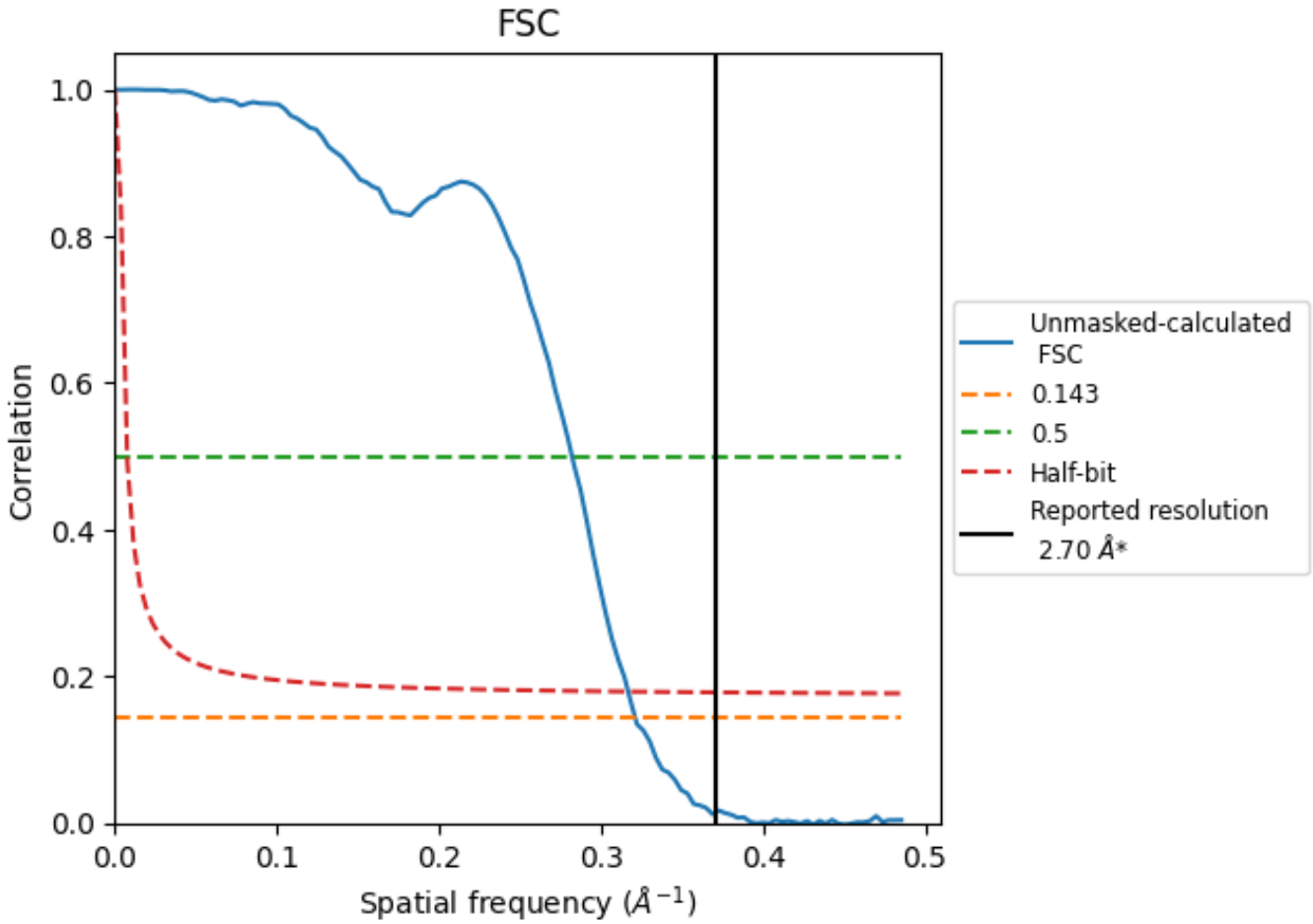


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

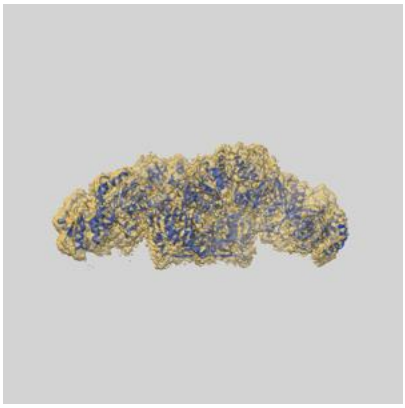
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.54	3.16

*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 3.11 differs from the reported value 2.7 by more than 10 %

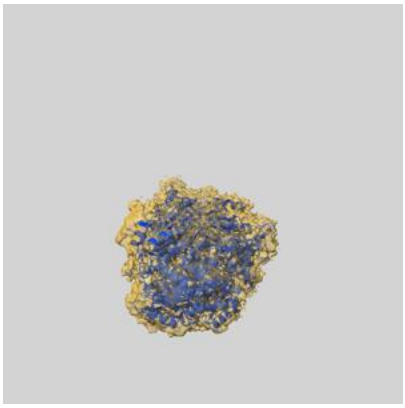
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28691 and PDB model 8EYK. Per-residue inclusion information can be found in section 3 on page 6.

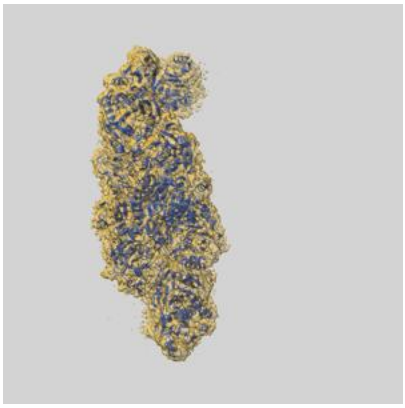
9.1 Map-model overlay



X



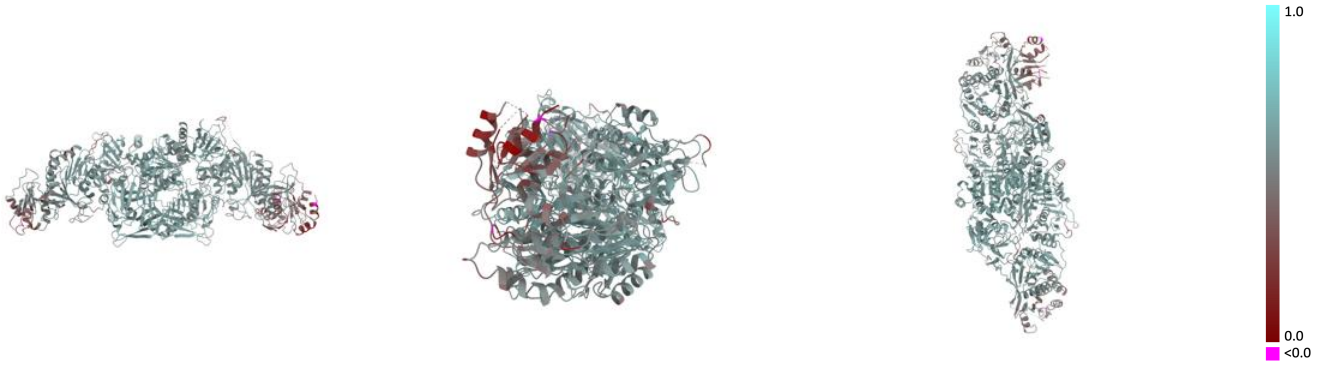
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

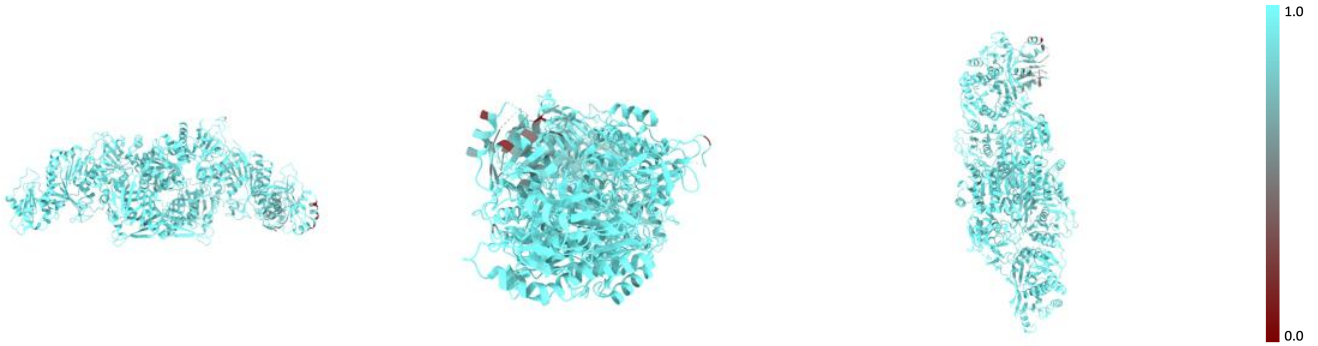
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

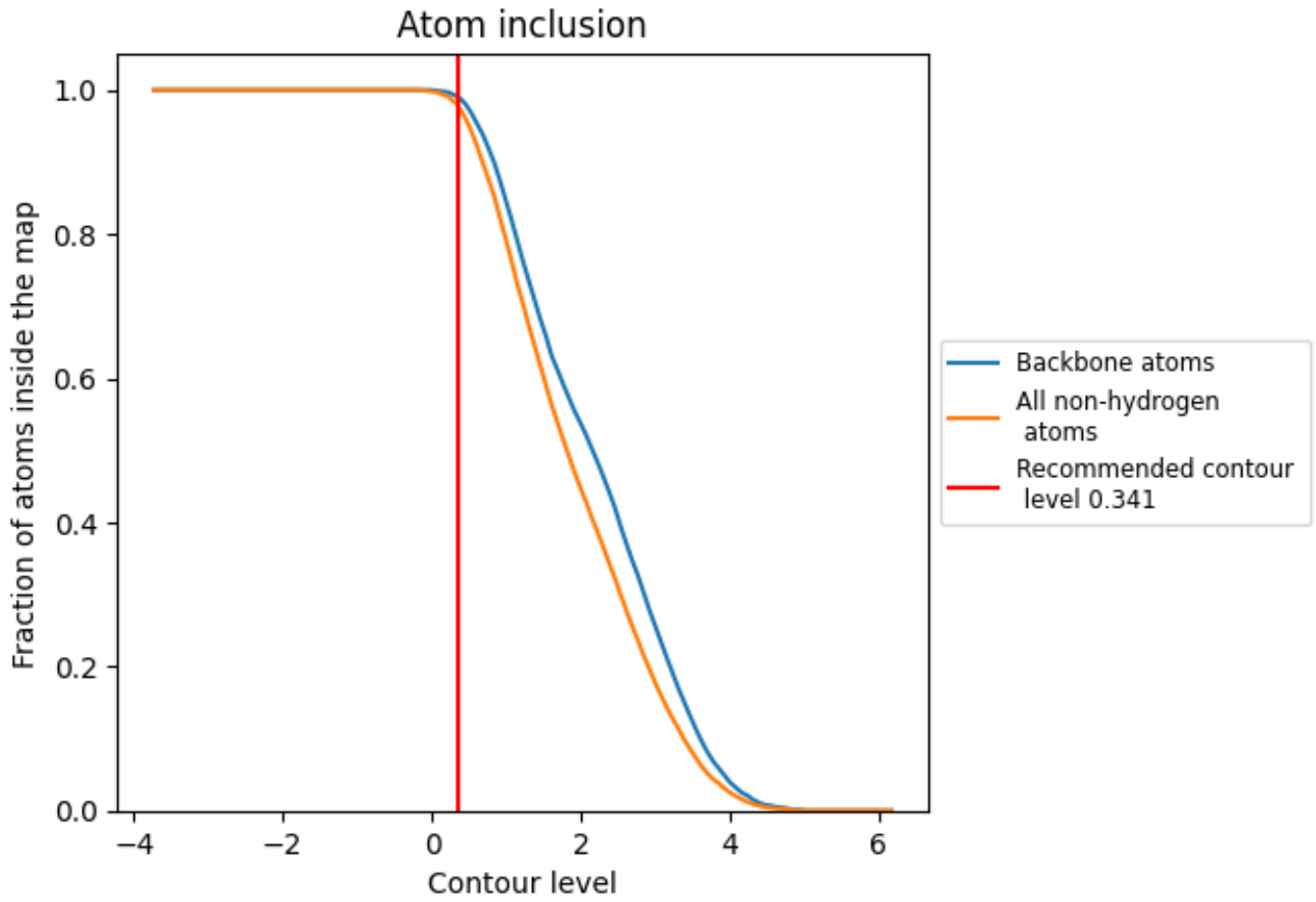
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.341).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9800	0.5550
E	0.9910	0.5690
F	0.9690	0.5420