



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:38 AM UTC

PDB ID : 8RDE / pdb_00008rde
EMDB ID : EMD-19070
Title : STRUCTURE OF THE MOUSE FCGBP DIMER PROTEIN IN ITS COMPACT CONFORMATION
Authors : Gallego, P.; Hansson, G.C.; Johansson, M.E.V.
Deposited on : 2023-12-08
Resolution : 3.70 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

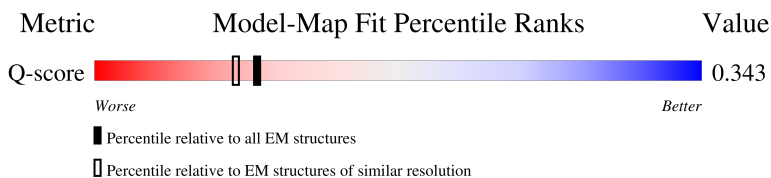
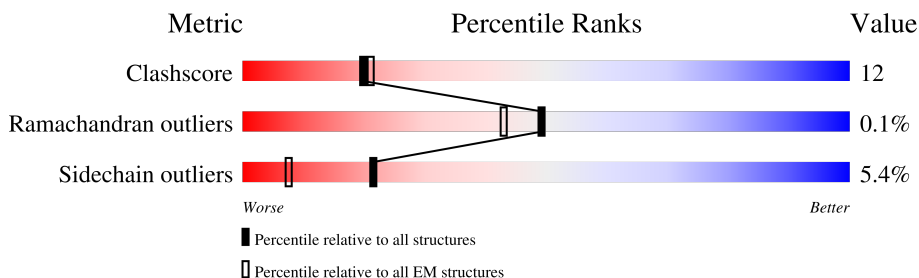
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	2587	
1	D	2587	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20050 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 Fc fragment of IgG binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1342	Total	C	N	O	S	1	0
			9937	6174	1721	1921	121		
1	D	1342	Total	C	N	O	S	1	0
			9937	6174	1721	1921	121		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2584	THR	-	expression tag	UNP E9Q0B5
A	2585	ARG	-	expression tag	UNP E9Q0B5
A	2586	THR	-	expression tag	UNP E9Q0B5
A	2587	ARG	-	expression tag	UNP E9Q0B5
D	2584	THR	-	expression tag	UNP E9Q0B5
D	2585	ARG	-	expression tag	UNP E9Q0B5
D	2586	THR	-	expression tag	UNP E9Q0B5
D	2587	ARG	-	expression tag	UNP E9Q0B5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

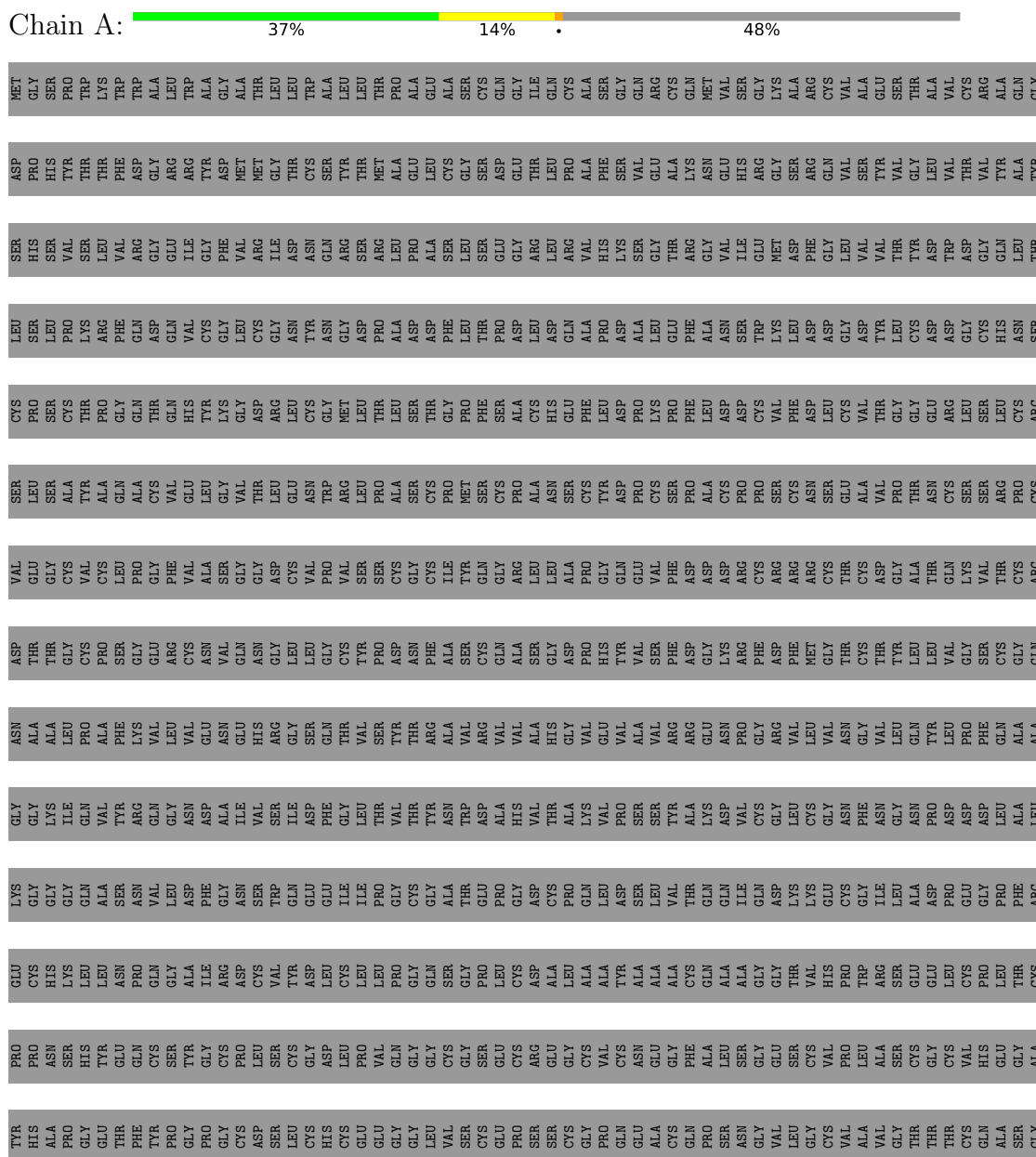
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	4	Total 4	Ca 4	0
3	D	4	Total 4	Ca 4	0

3 Residue-property plots

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

- Molecule 1: Fc fragment of IgG binding protein



S2293	L2180	L2060	L1937	E1826	T1689	G1540	D1374	L1283	ASP	GLY	LEU	ASP	THR	ASN	ASP
R2310	C2161	V2063	V1941	P1827	E1690	P1548	R1378	L1285	HIS	CYS	CYS	ASP	PRO	THR	THR
A2316	L2163	K2067	E1944	P1828	C1828	C1828	V1379	P1285	CYS	GLU	ILE	ASP	GLY	LEU	ILE
A2317	G2165	P2068	T1945	P1829	V1694	A1551	D1380	A1289	LYS	GLY	ILE	THR	ASN	ARG	VAL
A2318	N2166	G2069	I1946	C1832	R1701	T1587	V1381	T1293	PRO	CYS	ALA	CYS	THR	LEU	THR
S2319	F2167	D2070	C1947	T1833	R1710	V1558	L1382	T1293	GLN	GLY	ALA	SER	GLN	GLU	PHE
S2320	N2168	D2070	R1948	P1834	R1710	C1563	L1383	P1294	VAL	CYS	THR	PRO	GLN	SER	ASP
N2170	L1959	F2073	L1949	E1835	L1714	C1563	Y1387	F1295	GLY	GLY	VAL	GLY	GLN	GLN	GLY
D2173	S1960	L2077	S1960	F1840	L1714	V1564	Y1387	F1296	PRO	PHE	CYS	GLY	GLY	LYS	PHE
E2078	G1961	E2078	G1961	F1840	Y1717	E1565	V1391	V1297	LYS	LEU	GLN	ASP	GLY	VAL	ASP
K2079	D1962	K2079	D1962	P1843	G1718	G1566	C1392	T1298	ARG	GLY	ALA	GLY	TRP	ARG	ARG
T1963	T1963	G2080	C1964	P1834	L1719	C1569	G1393	T1299	GLY	ASN	ALA	TYR	GLY	VAL	PHE
C1964	C1964	S2081	C1964	G1847	L1719	D1570	L1394	K1300	VAL	GLY	ALA	GLY	ASP	ASN	GLY
V1965	V1965	V1965	V1965	E1848	Q1726	D1570	C1395	S1306	THR	LYS	GLY	GLY	THR	THR	THR
G1968	G1968	G2082	G1968	I1849	Q1726	S1576	C1395	S1306	THR	ALA	GLN	GLY	GLY	VAL	CYS
P1966	P1966	K2084	P1966	T1850	R1729	V1581	V1407	V1309	CYS	VAL	GLU	ASP	GLY	ASP	VAL
C1970	C1970	P2085	C1970	A1851	K1730	V1581	M1413	Q1314	VAL	PRO	GLU	PHE	ASP	THR	THR
G1971	G1971	Q2086	G1971	P1852	F1736	G1588	I1417	V1315	LYS	ILE	TRP	CYS	PRO	VAL	VAL
V1980	V1980	R2087	V1980	E1853	F1737	C1589	P1418	T1316	ASP	GLU	LEU	GLY	ARG	PRO	ALA
F1985	F1985	V2090	F1985	A1857	L1740	V1596	W1424	T1318	PRO	GLN	THR	THR	ASP	VAL	VAL
Y1986	Y1986	T2091	Y1986	C1858	P1741	Y1596	W1424	T1319	CYS	CYS	GLU	THR	GLN	LEU	THR
P1987	P1987	V2096	P1987	C1859	F1742	Y1596	W1434	I1324	GLY	CYS	PHE	PRO	GLY	ASP	GLY
G1998	G1998	V2097	G1998	T1866	H1743	E1601	W1434	I1324	THR	THR	CYS	THR	PRO	GLY	ASN
P1998	P1998	G2098	P1998	Q1867	L1744	E1601	C1441	H1327	CYS	ASN	MET	PRO	GLY	LYS	ARG
D2000	D2000	L2099	D2000	Y1868	K1747	R1610	C1441	H1327	ILE	GLY	GLU	LEU	SER	ILE	GLY
G2001	G2001	A2100	G2001	F1869	L1748	R1611	D1447	K1329	ARG	GLY	CYS	ALA	ARG	LEU	LEU
Q2002	Q2002	R2101	Q2002	A1876	S1749	C1612	R1446	E1350	PRO	VAL	PRO	ALA	GLN	HIS	HIS
Q2104	Q2104	Q2104	Q2104	Q1880	V1750	L1621	C1458	I1331	THR	GLU	PRO	ALA	THR	GLN	GLN
V2105	V2105	Q2105	A2009	Q1880	V1751	L1621	C1458	I1331	THR	GLU	PRO	ALA	THR	GLN	GLN
T2106	T2106	T2107	D2010	G1885	I1752	C1623	L1461	V1334	LYS	CYS	LYS	LEU	THR	GLY	VAL
D2108	D2108	V2107	C2011	G1885	D1756	C1623	L1461	V1334	VAL	VAL	THR	LEU	ASP	SER	LEU
E2110	E2110	E2110	E2012	P1888	V1759	A1626	F1469	L1340	GLN	SER	GLU	ASP	PHE	ASP	GLN
V2111	V2111	V2112	P2013	A1889	V1759	L1636	G1493	L1343	GLY	VAL	VAL	PRO	GLY	VAL	GLU
V2112	V2112	V2112	Y2014	T1892	F1774	L1636	G1493	P1344	ILE	LEU	CYS	GLN	ASN	VAL	ASN
E2126	E2126	E2126	Y2014	Y1893	V1775	I1642	L1499	V1346	GLY	GLU	ASP	PRO	GLU	ALA	ALA
G2127	G2127	G2127	G2022	L1904	G1792	A1654	A1502	L1347	VAL	CYS	CYS	GLN	THR	THR	THR
R2128	R2128	R2128	V2023	G1905	N1793	W1655	A1502	L1347	CYS	GLN	CYS	ASP	GLY	ASP	GLY
L2132	L2132	L2132	Q2024	E1906	Y1794	G1656	C1510	G1349	ALA	GLN	SER	ALA	VAL	PHE	ASN
V2140	V2140	V2140	C2031	K1909	K1796	D1657	C1510	G1349	VAL	HIS	GLY	VAL	PRO	GLY	GLY
D2145	D2145	D2145	L2045	P1910	N1799	H1659	E1518	V1354	CYS	VAL	TRP	ASP	ARG	VAL	VAL
P2153	P2153	P2153	L2045	P1914	N1799	H1659	E1518	V1354	ALA	CYS	ALA	ASP	VAL	SER	SER
S2154	S2154	S2154	D2046	C1917	K1808	D1664	D1532	L1363	THR	GLN	LEU	LEU	PRO	ALA	THR
F2156	F2156	F2156	G2047	P1918	E1810	Q1671	N1533	D1366	LYS	PRO	GLY	LEU	ASP	LYS	VAL
R2157	R2157	R2157	L2052	P1918	E1810	C1674	N1533	D1366	VAL	VAL	VAL	VAL	LEU	VAL	VAL
Q2280	Q2280	Q2280	H2052	S1929	C1820	C1674	H1535	L1369	THR	GLY	GLN	GLY	PRO	THR	THR
V2289	V2289	V2289	G2054	C1929	D1821	L1678	Y1536	Q1370	VAL	ASN	GLN	ASN	PRO	TYR	VAL
R2290	R2290	R2290	G2054	C1929	D1821	L1678	E1536	Q1370	GLY	GLN	GLN	GLY	PRO	TYR	VAL
Q2291	Q2291	Q2291	P1935	P1935	Q1822	L1538	E1538	T1372	THR	GLN	CYS	VAL	VAL	VAL	VAL
D2292	D2292	D2292	S2057	S1936	C1823	P1685	C1539	Y1373	ILE	GLN	PRO	SER	THR	ARG	VAL





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0495	Depositor
Map size (Å)	302.72, 302.72, 302.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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, 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	0.36	2/10201 (0.0%)	0.63	20/13926 (0.1%)
1	D	0.36	2/10201 (0.0%)	0.63	20/13926 (0.1%)
All	All	0.36	4/20402 (0.0%)	0.63	40/27852 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1582	PRO	N-CD	9.17	1.60	1.47
1	D	1582	PRO	N-CD	9.14	1.60	1.47
1	A	2234	PRO	N-CD	-7.90	1.36	1.47
1	D	2234	PRO	N-CD	-7.89	1.36	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2292	ASP	CB-CA-C	-9.86	105.21	116.54
1	D	2292	ASP	CB-CA-C	-9.84	105.22	116.54
1	A	2107	VAL	N-CA-C	-8.01	99.24	109.58
1	D	2107	VAL	N-CA-C	-8.01	99.25	109.58
1	A	1743	HIS	N-CA-C	7.09	120.08	108.52
1	D	1743	HIS	N-CA-C	7.07	120.04	108.52
1	D	2361	MET	N-CA-CB	7.04	119.11	110.17
1	A	2361	MET	N-CA-CB	7.01	119.07	110.17
1	D	2359	GLN	N-CA-C	6.91	118.60	108.86
1	A	2359	GLN	N-CA-C	6.89	118.57	108.86
1	D	2001	GLY	N-CA-C	6.62	124.14	115.47
1	A	2001	GLY	N-CA-C	6.61	124.13	115.47
1	D	1590	TRP	CB-CA-C	-6.52	102.17	111.95
1	A	1590	TRP	CB-CA-C	-6.50	102.20	111.95
1	A	2047	GLY	N-CA-C	6.34	120.69	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2047	GLY	N-CA-C	6.33	120.67	111.24
1	A	2360	TYR	N-CA-C	5.86	117.75	108.67
1	D	2360	TYR	N-CA-C	5.86	117.75	108.67
1	D	2165	GLY	CA-C-O	-5.58	118.30	122.37
1	A	2165	GLY	CA-C-O	-5.57	118.30	122.37
1	D	1792	GLY	CA-C-O	-5.54	118.41	122.23
1	A	1792	GLY	CA-C-O	-5.52	118.42	122.23
1	A	1582	PRO	CA-N-CD	-5.38	104.47	112.00
1	D	1582	PRO	CA-N-CD	-5.38	104.47	112.00
1	D	1582	PRO	N-CA-CB	5.37	108.02	103.35
1	A	1582	PRO	N-CA-CB	5.33	107.98	103.35
1	D	1394	LEU	CA-C-N	-5.26	115.93	123.20
1	D	1394	LEU	C-N-CA	-5.26	115.93	123.20
1	A	1394	LEU	CA-C-N	-5.24	115.97	123.20
1	A	1394	LEU	C-N-CA	-5.24	115.97	123.20
1	A	2169	GLY	N-CA-C	5.13	118.88	112.73
1	D	2169	GLY	N-CA-C	5.13	118.88	112.73
1	A	2000	ASP	CB-CA-C	-5.12	102.52	111.23
1	D	2000	ASP	CB-CA-C	-5.12	102.52	111.23
1	D	2293	SER	N-CA-C	5.11	119.37	113.18
1	A	2293	SER	N-CA-C	5.11	119.36	113.18
1	A	2045	LEU	N-CA-C	-5.09	105.81	111.36
1	D	2045	LEU	N-CA-C	-5.06	105.84	111.36
1	A	1794	TYR	CB-CA-C	5.02	119.64	112.12
1	D	1794	TYR	CB-CA-C	5.01	119.63	112.12

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	A	9937	0	9279	236	0
1	D	9937	0	9279	244	0
2	A	84	0	78	8	0
2	D	84	0	78	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	D	4	0	0	0	0
All	All	20050	0	18714	480	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 12.

All (480) 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:2316:CYS:SG	1:A:2360:TYR:CE1	2.29	1.26
1:D:2316:CYS:SG	1:D:2360:TYR:CE1	2.28	1.26
1:A:1621:LEU:HD12	1:A:1621:LEU:O	1.50	1.11
1:D:1621:LEU:HD12	1:D:1621:LEU:O	1.50	1.10
1:D:2352:CYS:SG	1:D:2360:TYR:OH	2.27	0.92
1:A:2352:CYS:SG	1:A:2360:TYR:OH	2.27	0.92
1:A:1621:LEU:HD13	1:A:1623:CYS:HB2	1.56	0.88
1:A:2316:CYS:SG	1:A:2360:TYR:CZ	2.67	0.88
1:D:1621:LEU:HD13	1:D:1623:CYS:HB2	1.56	0.87
1:D:2316:CYS:SG	1:D:2360:TYR:CZ	2.67	0.87
1:D:2374:GLU:HG2	1:D:2375:ARG:HG2	1.66	0.78
1:A:1374:ASP:HB3	1:A:1378:ARG:HB2	1.66	0.77
1:A:2374:GLU:HG2	1:A:2375:ARG:HG2	1.66	0.76
1:D:1654:ALA:HB3	1:D:1775:VAL:HG12	1.68	0.75
1:D:1374:ASP:HB3	1:D:1378:ARG:HB2	1.66	0.75
1:A:1493:GLY:HA3	1:A:1968:GLY:HA3	1.70	0.74
1:D:1254:TRP:HB3	1:D:1262:ASN:HB3	1.68	0.74
1:A:2450:VAL:HG21	1:A:2542:LEU:HD11	1.70	0.73
1:D:2450:VAL:HG21	1:D:2542:LEU:HD11	1.70	0.73
1:D:2277:ALA:O	1:D:2280:GLN:HG2	1.90	0.72
1:A:2277:ALA:O	1:A:2280:GLN:HG2	1.90	0.71
1:A:1970:CYS:SG	1:A:1971:GLY:N	2.64	0.71
1:D:2491:VAL:HG21	1:D:2502:VAL:HG21	1.72	0.71
1:D:1970:CYS:SG	1:D:1971:GLY:N	2.64	0.70
1:D:1284:CYS:N	1:D:1392:CYS:SG	2.58	0.70
1:D:2446:LEU:HD13	1:D:2545:MET:HG3	1.73	0.70
1:A:2491:VAL:HG21	1:A:2502:VAL:HG21	1.71	0.70
1:D:1317:VAL:HG22	1:D:1324:ILE:HB	1.72	0.69
1:A:1284:CYS:N	1:A:1392:CYS:SG	2.58	0.69
1:A:1317:VAL:HG22	1:A:1324:ILE:HB	1.72	0.69
1:A:2446:LEU:HD13	1:A:2545:MET:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2352:CYS:SG	1:D:2360:TYR:CZ	2.86	0.69
1:A:1370:GLN:HB2	1:A:1382:THR:HB	1.75	0.69
1:D:1370:GLN:HB2	1:D:1382:THR:HB	1.75	0.69
1:A:1654:ALA:HB3	1:A:1775:VAL:HG12	1.74	0.69
1:A:2352:CYS:SG	1:A:2360:TYR:CZ	2.86	0.68
1:D:2157:ARG:HD3	1:D:2167:PHE:HB3	1.75	0.68
1:A:2108:ASP:HB2	1:A:2112:VAL:HG12	1.76	0.68
1:D:2108:ASP:HB2	1:D:2112:VAL:HG12	1.76	0.67
1:A:1740:LEU:HD22	1:A:1961:GLY:HA3	1.76	0.67
1:D:1740:LEU:HD22	1:D:1961:GLY:HA3	1.76	0.67
1:A:2352:CYS:SG	1:A:2360:TYR:CE1	2.88	0.67
1:D:1756:ASP:OD1	1:D:1948:ARG:NH2	2.29	0.66
1:D:2352:CYS:SG	1:D:2360:TYR:CE1	2.88	0.66
1:A:2101:ARG:CZ	1:A:2106:THR:HG21	2.25	0.66
1:D:2087:ARG:HG2	1:D:2100:ALA:HB1	1.75	0.66
1:D:2101:ARG:CZ	1:D:2106:THR:HG21	2.25	0.66
1:A:1253:CYS:SG	1:A:1395:CYS:HB2	2.34	0.66
1:A:2087:ARG:NH1	1:A:2087:ARG:O	2.28	0.66
1:A:2087:ARG:HG2	1:A:2100:ALA:HB1	1.75	0.66
1:A:2157:ARG:HD3	1:A:2167:PHE:HB3	1.75	0.66
1:D:1612:CYS:H	1:D:1623:CYS:HA	1.61	0.66
1:A:2212:PRO:HA	1:A:2215:LEU:HD13	1.77	0.65
1:A:1756:ASP:OD1	1:A:1948:ARG:NH2	2.29	0.65
1:A:2579:SER:O	1:D:2471:LYS:NZ	2.28	0.65
1:A:1362:VAL:HG11	1:A:1558:VAL:HG11	1.78	0.65
1:D:1255:LEU:HB3	1:D:1379:VAL:HB	1.78	0.65
1:D:2087:ARG:O	1:D:2087:ARG:NH1	2.28	0.65
1:D:2155:SER:O	1:D:2159:ARG:NH2	2.29	0.65
1:D:2012[A]:GLU:HG2	1:D:2013:PRO:HD2	1.78	0.65
1:D:1362:VAL:HG11	1:D:1558:VAL:HG11	1.78	0.65
1:A:2155:SER:O	1:A:2159:ARG:NH2	2.29	0.64
1:A:1612:CYS:H	1:A:1623:CYS:HA	1.61	0.64
1:D:2212:PRO:HA	1:D:2215:LEU:HD13	1.77	0.64
1:D:2420:ASN:HB2	2:D:5608:NAG:H2	1.80	0.64
1:A:2012[A]:GLU:HG2	1:A:2013:PRO:HD2	1.78	0.64
1:D:1621:LEU:O	1:D:1621:LEU:CD1	2.38	0.64
1:A:2416:SER:HB3	1:A:2419:ALA:HA	1.80	0.64
1:D:2416:SER:HB3	1:D:2419:ALA:HA	1.80	0.64
1:A:2420:ASN:HB2	2:A:5608:NAG:H2	1.80	0.64
1:D:1283:LEU:HD12	1:D:1289:ALA:HB2	1.79	0.64
1:A:1283:LEU:HD12	1:A:1289:ALA:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2351:ASP:OD1	1:D:2352:CYS:N	2.28	0.63
1:D:1363:LEU:HB3	1:D:1371:VAL:HG13	1.80	0.63
1:A:1363:LEU:HB3	1:A:1371:VAL:HG13	1.80	0.62
1:A:1621:LEU:O	1:A:1621:LEU:CD1	2.38	0.62
1:D:1284:CYS:SG	1:D:1285:PRO:HD3	2.39	0.62
1:A:1284:CYS:SG	1:A:1285:PRO:HD3	2.39	0.62
1:D:2398:GLU:OE1	1:D:2407:GLN:NE2	2.33	0.62
1:A:1826:GLU:HG2	1:A:1829:PRO:HG3	1.82	0.61
1:A:2398:GLU:OE1	1:A:2407:GLN:NE2	2.33	0.61
1:A:1458:CYS:H	1:A:1499:LEU:HD11	1.66	0.61
1:A:2351:ASP:OD1	1:A:2352:CYS:N	2.28	0.61
1:D:1293:THR:N	1:D:1387:TYR:OH	2.34	0.61
1:A:1293:THR:N	1:A:1387:TYR:OH	2.34	0.60
1:D:1253:CYS:SG	1:D:1395:CYS:HB2	2.40	0.60
1:A:2363:VAL:HG21	2:A:5607:NAG:H82	1.83	0.60
1:A:1657:ASP:OD1	1:A:1671:GLN:NE2	2.33	0.60
1:D:1826:GLU:HG2	1:D:1829:PRO:HG3	1.82	0.60
1:D:1959:LEU:HD21	1:D:1980:VAL:HG13	1.83	0.60
1:D:2363:VAL:HG21	2:D:5607:NAG:H82	1.83	0.60
1:D:1458:CYS:H	1:D:1499:LEU:HD11	1.66	0.60
1:A:1959:LEU:HD21	1:A:1980:VAL:HG13	1.83	0.59
1:A:1843:PRO:HA	1:A:1847:GLY:HA3	1.84	0.59
1:D:1654:ALA:HB3	1:D:1775:VAL:CG1	2.33	0.59
1:A:1610:LYS:HB3	1:A:1623:CYS:SG	2.43	0.58
1:A:2437:TYR:OH	1:A:2574:ARG:NH2	2.37	0.58
1:A:1254:TRP:HH2	1:A:1378:ARG:HH21	1.49	0.58
1:D:1959:LEU:HD13	1:D:1965:VAL:HG11	1.85	0.58
1:D:1493:GLY:HA3	1:D:1968:GLY:HA3	1.83	0.58
1:A:1959:LEU:HD13	1:A:1965:VAL:HG11	1.85	0.58
1:A:2423:THR:HB	1:A:2550:CYS:O	2.03	0.58
1:D:2077:LEU:HB3	1:D:2086:GLN:HG2	1.85	0.58
1:A:1345:VAL:HG13	1:A:1354:VAL:HB	1.86	0.58
1:A:2458:ASP:OD1	1:A:2460:GLN:NE2	2.35	0.58
1:A:1832:CYS:SG	1:A:1833:THR:N	2.77	0.58
1:A:1740:LEU:HD13	1:A:1961:GLY:HA3	1.85	0.58
1:A:2077:LEU:HB3	1:A:2086:GLN:HG2	1.85	0.58
1:D:1314:GLN:OE1	1:D:1327:HIS:NE2	2.37	0.58
1:D:1345:VAL:HG13	1:D:1354:VAL:HB	1.86	0.58
1:D:1843:PRO:HA	1:D:1847:GLY:HA3	1.84	0.57
1:D:2191:THR:O	1:D:2194:ARG:NH1	2.32	0.57
1:D:2423:THR:HB	1:D:2550:CYS:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:PHE:HA	1:A:1319:THR:HG22	1.86	0.57
1:D:1295:PHE:HA	1:D:1319:THR:HG22	1.86	0.57
1:A:1372:THR:CG2	1:A:1380:ASP:HB3	2.35	0.57
1:D:1610:LYS:HB3	1:D:1623:CYS:SG	2.43	0.57
1:A:1314:GLN:OE1	1:A:1327:HIS:NE2	2.37	0.57
1:D:2458:ASP:OD1	1:D:2460:GLN:NE2	2.35	0.57
1:D:1249:TYR:CZ	1:D:1400:LYS:HG2	2.39	0.57
1:D:1372:THR:CG2	1:D:1380:ASP:HB3	2.35	0.57
1:D:1740:LEU:HD22	1:D:1961:GLY:CA	2.35	0.57
1:D:2437:TYR:OH	1:D:2574:ARG:NH2	2.37	0.56
1:A:2323:THR:HB	1:A:2326:THR:HA	1.86	0.56
1:A:1275:CYS:HA	1:A:1300:LYS:HE2	1.88	0.56
1:A:2320:SER:HB3	1:A:2322:LEU:HG	1.88	0.56
1:D:1740:LEU:HD13	1:D:1961:GLY:HA3	1.85	0.56
1:D:2108:ASP:HA	1:D:2112:VAL:HA	1.87	0.56
1:A:2081:SER:H	1:A:2084:ASP:HB2	1.69	0.56
1:D:1298:THR:HG1	1:D:1316:THR:HG1	1.51	0.56
1:D:1611:ARG:NH1	1:D:1626:ALA:O	2.37	0.56
1:D:1832:CYS:SG	1:D:1833:THR:N	2.77	0.56
1:D:1275:CYS:HA	1:D:1300:LYS:HE2	1.88	0.56
1:D:2081:SER:H	1:D:2084:ASP:HB2	1.69	0.56
1:D:2323:THR:HB	1:D:2326:THR:HA	1.86	0.56
1:A:1740:LEU:HD22	1:A:1961:GLY:CA	2.35	0.56
1:A:1868:TYR:HD2	1:A:1893:TYR:HD1	1.53	0.55
1:A:2052:LEU:HD23	1:A:2054:GLY:H	1.72	0.55
1:D:2316:CYS:HA	1:D:2340:LEU:HD22	1.88	0.55
1:A:2108:ASP:HA	1:A:2112:VAL:HA	1.87	0.55
1:A:2316:CYS:SG	1:A:2360:TYR:CD1	2.96	0.55
1:A:2316:CYS:HA	1:A:2340:LEU:HD22	1.88	0.55
1:D:2442:ARG:HD3	1:D:2450:VAL:HB	1.89	0.55
1:A:2108:ASP:OD1	1:A:2109:GLY:N	2.40	0.55
1:A:2442:ARG:HD3	1:A:2450:VAL:HB	1.89	0.55
1:D:2320:SER:HB3	1:D:2322:LEU:HG	1.88	0.55
1:A:2108:ASP:CA	1:A:2112:VAL:HA	2.37	0.55
1:A:2369:SER:HB3	1:A:2373:SER:HB2	1.89	0.55
1:D:1868:TYR:HD2	1:D:1893:TYR:HD1	1.53	0.55
1:D:1853:GLU:HA	1:D:1857:ALA:HB2	1.88	0.55
1:A:2158:GLY:H	1:A:2167:PHE:HB2	1.72	0.54
1:A:1298:THR:HG1	1:A:1316:THR:HG1	1.50	0.54
1:A:1621:LEU:CD1	1:A:1623:CYS:HB2	2.33	0.54
1:D:2158:GLY:H	1:D:2167:PHE:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:GLN:O	1:A:1880:GLN:HG3	2.08	0.54
1:A:2108:ASP:CB	1:A:2112:VAL:HA	2.38	0.54
1:D:2415:ILE:HG23	1:D:2416:SER:H	1.72	0.54
1:A:2415:ILE:HG23	1:A:2416:SER:H	1.72	0.54
1:D:1589:CYS:HB2	1:D:1596:TYR:HB2	1.89	0.54
1:D:2060:LEU:HD12	1:D:2163:LEU:HB2	1.89	0.54
1:A:1853:GLU:HA	1:A:1857:ALA:HB2	1.88	0.54
1:D:2108:ASP:CA	1:D:2112:VAL:HA	2.37	0.54
1:D:2369:SER:HB3	1:D:2373:SER:HB2	1.89	0.54
1:A:1255:LEU:HB3	1:A:1379:VAL:HB	1.89	0.54
1:A:1589:CYS:HB2	1:A:1596:TYR:HB2	1.89	0.54
1:A:1654:ALA:HB3	1:A:1775:VAL:CG1	2.37	0.54
1:D:1655:TRP:HZ3	1:D:1889:ALA:HA	1.73	0.54
1:A:2060:LEU:HD12	1:A:2163:LEU:HB2	1.89	0.54
1:A:2191:THR:O	1:A:2194:ARG:NH1	2.32	0.54
1:D:2108:ASP:OD1	1:D:2109:GLY:N	2.40	0.54
1:D:2316:CYS:SG	1:D:2360:TYR:CD1	2.96	0.53
1:A:1655:TRP:HZ3	1:A:1889:ALA:HA	1.72	0.53
1:D:2052:LEU:HD23	1:D:2054:GLY:H	1.72	0.53
1:D:2108:ASP:CB	1:D:2112:VAL:HA	2.38	0.53
1:D:2128:ARG:HH22	1:D:2145:ASP:HB2	1.74	0.53
1:D:1685:PRO:HB2	1:D:1689:THR:HB	1.90	0.53
1:A:2240:ALA:HA	1:A:2243:LYS:HE2	1.89	0.53
1:A:1710:ARG:HH12	1:A:1726:GLN:HB3	1.73	0.53
1:A:1536:TYR:OH	1:A:1565:GLU:OE2	2.26	0.53
1:A:1694:VAL:HG22	1:A:1714:LEU:HD13	1.91	0.53
1:D:2240:ALA:HA	1:D:2243:LYS:HE2	1.89	0.53
1:A:2490:TRP:NE1	1:A:2495:ARG:HG2	2.25	0.52
1:A:1611:ARG:NH1	1:A:1626:ALA:O	2.37	0.52
1:D:1536:TYR:OH	1:D:1565:GLU:OE2	2.26	0.52
1:D:1710:ARG:HH12	1:D:1726:GLN:HB3	1.73	0.52
1:A:1685:PRO:HB2	1:A:1689:THR:HB	1.90	0.52
1:D:1694:VAL:HG22	1:D:1714:LEU:HD13	1.91	0.52
1:D:1880:GLN:O	1:D:1880:GLN:HG3	2.08	0.52
1:A:1273:GLY:HA3	1:A:1277:TYR:HE2	1.75	0.52
1:A:2485:PRO:HD3	1:A:2528:LEU:HD21	1.90	0.52
1:D:1636:LEU:HA	1:D:1642:ILE:HG22	1.92	0.52
1:D:2490:TRP:NE1	1:D:2495:ARG:HG2	2.25	0.52
1:D:1372:THR:HG22	1:D:1380:ASP:HB3	1.92	0.52
1:A:2014:TYR:HE1	1:A:2157:ARG:HH21	1.58	0.51
1:D:2126:GLU:HG3	1:D:2330:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1589:CYS:H	1:D:1596:TYR:H	1.59	0.51
1:A:1417:ILE:N	1:A:1418:PRO:HD2	2.25	0.51
1:D:1621:LEU:CD1	1:D:1623:CYS:HB2	2.33	0.51
1:D:2485:PRO:HD3	1:D:2528:LEU:HD21	1.90	0.51
1:A:2126:GLU:HG3	1:A:2330:PHE:CE1	2.46	0.51
1:A:2455:VAL:HG12	1:A:2474:ILE:HG23	1.92	0.51
1:D:2108:ASP:HB2	1:D:2112:VAL:HA	1.92	0.51
1:D:2177:LEU:HD23	1:D:2182:VAL:HA	1.92	0.51
1:A:1274:THR:OG1	1:A:1434:TRP:O	2.27	0.51
1:A:1372:THR:HG22	1:A:1380:ASP:HB3	1.92	0.51
1:D:1306:SER:HB2	1:D:1309:VAL:HG22	1.92	0.51
1:D:1678:LEU:N	1:D:1694:VAL:O	2.44	0.51
1:A:2101:ARG:HD3	1:A:2106:THR:HG22	1.93	0.51
1:A:2177:LEU:HD23	1:A:2182:VAL:HA	1.92	0.51
1:A:1254:TRP:HB3	1:A:1262:ASN:HB3	1.91	0.51
1:A:1589:CYS:H	1:A:1596:TYR:H	1.59	0.51
1:A:1636:LEU:HA	1:A:1642:ILE:HG22	1.93	0.51
1:A:1678:LEU:N	1:A:1694:VAL:O	2.44	0.51
1:D:1273:GLY:HA3	1:D:1277:TYR:HE2	1.75	0.51
1:D:1417:ILE:N	1:D:1418:PRO:HD2	2.25	0.51
1:D:2101:ARG:HD3	1:D:2106:THR:HG22	1.93	0.50
1:D:2509:ARG:NH2	1:D:2511:MET:SD	2.77	0.50
1:A:1333:LYS:HA	1:A:1340:LEU:HA	1.94	0.50
1:D:2014:TYR:HE1	1:D:2157:ARG:HH21	1.58	0.50
1:A:1306:SER:HB2	1:A:1309:VAL:HG22	1.92	0.50
1:A:1730:LYS:HA	1:A:1740:LEU:HD11	1.94	0.50
1:A:2128:ARG:HH22	1:A:2145:ASP:HB2	1.74	0.50
1:A:2108:ASP:HB2	1:A:2112:VAL:HA	1.92	0.50
1:D:2031:CYS:HA	1:D:2153:PRO:HA	1.93	0.50
1:A:1324:ILE:HG23	1:A:1334:VAL:HB	1.94	0.50
1:A:1384:PRO:HB3	2:A:5601:NAG:H62	1.93	0.50
1:D:1730:LYS:HA	1:D:1740:LEU:HD11	1.94	0.50
1:D:1750:VAL:HG13	1:D:1759:VAL:HG12	1.93	0.50
1:D:2455:VAL:HG12	1:D:2474:ILE:HG23	1.92	0.50
1:A:1548:PRO:HB2	1:A:1551:ALA:HA	1.94	0.49
2:A:5608:NAG:O7	2:A:5608:NAG:O4	2.25	0.49
1:A:1737:PHE:HD1	1:A:2022:GLY:HA3	1.77	0.49
1:A:1750:VAL:HG13	1:A:1759:VAL:HG12	1.93	0.49
1:A:2031:CYS:HA	1:A:2153:PRO:HA	1.93	0.49
1:D:1548:PRO:HB2	1:D:1551:ALA:HA	1.94	0.49
1:D:1737:PHE:HD1	1:D:2022:GLY:HA3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2565:GLN:HG3	1:D:2572:LYS:HD3	1.95	0.49
1:A:1906:GLU:O	1:A:1909:LYS:NZ	2.45	0.49
1:A:2091:THR:HG22	1:A:2096:VAL:HG22	1.95	0.49
1:A:2397:CYS:SG	1:A:2406:CYS:HB3	2.52	0.49
1:D:1906:GLU:O	1:D:1909:LYS:NZ	2.45	0.49
1:A:1655:TRP:HB2	1:A:1659:HIS:O	2.11	0.49
1:A:1910:PRO:HA	1:A:1914:PRO:HB3	1.94	0.49
1:D:1324:ILE:HG23	1:D:1334:VAL:HB	1.94	0.49
1:A:1866:THR:HG23	1:A:1867:GLN:N	2.28	0.49
1:D:1333:LYS:HA	1:D:1340:LEU:HA	1.94	0.49
1:D:2335:CYS:HB3	1:D:2339:PHE:CD2	2.47	0.49
1:A:2509:ARG:NH2	1:A:2511:MET:SD	2.77	0.49
1:D:1880:GLN:HE21	1:D:2350:GLN:HG3	1.78	0.49
1:A:2335:CYS:HB3	1:A:2339:PHE:CD2	2.47	0.49
1:D:2352:CYS:HA	1:D:2360:TYR:CE1	2.48	0.49
1:A:1729:ARG:HH22	1:A:1962:ASP:HA	1.79	0.48
1:A:1880:GLN:HE21	1:A:2350:GLN:HG3	1.78	0.48
1:A:2019:ILE:HB	1:A:2024:GLN:HG2	1.95	0.48
1:A:2364:ASN:HD22	2:A:5607:NAG:H62	1.78	0.48
1:A:1823:CYS:SG	1:A:1828:CYS:N	2.86	0.48
1:A:2352:CYS:HA	1:A:2360:TYR:CE1	2.48	0.48
1:D:1655:TRP:HZ2	1:D:1868:TYR:CG	2.31	0.48
1:D:2091:THR:HG22	1:D:2096:VAL:HG22	1.95	0.48
1:A:2565:GLN:HG3	1:A:2572:LYS:HD3	1.95	0.48
1:D:1823:CYS:SG	1:D:1828:CYS:N	2.86	0.48
1:D:2577:ASP:OD1	1:D:2577:ASP:N	2.45	0.48
1:A:2362:PRO:O	1:A:2365:SER:OG	2.29	0.48
1:A:1998:GLY:HA3	1:A:2002:GLN:HG3	1.95	0.48
1:A:2577:ASP:OD1	1:A:2577:ASP:N	2.45	0.48
1:D:1998:GLY:HA3	1:D:2002:GLN:HG3	1.95	0.48
1:D:1910:PRO:HA	1:D:1914:PRO:HB3	1.94	0.48
1:D:2019:ILE:HB	1:D:2024:GLN:HG2	1.95	0.48
1:D:2397:CYS:SG	1:D:2406:CYS:HB3	2.52	0.48
1:A:2322:LEU:HB2	1:A:2325:CYS:H	1.78	0.48
1:D:1274:THR:OG1	1:D:1434:TRP:O	2.27	0.48
1:D:1249:TYR:OH	1:D:1400:LYS:HG2	2.14	0.47
1:A:2498:LEU:HD13	1:A:2510:ARG:HE	1.79	0.47
1:D:1273:GLY:HA3	1:D:1277:TYR:CE2	2.50	0.47
1:D:1729:ARG:HH22	1:D:1962:ASP:HA	1.79	0.47
1:D:2364:ASN:HD22	2:D:5607:NAG:H62	1.78	0.47
1:A:1324:ILE:HD12	1:A:1334:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1610:LYS:HD2	1:A:1623:CYS:SG	2.55	0.47
1:D:1324:ILE:HD12	1:D:1334:VAL:HB	1.96	0.47
1:D:1610:LYS:HD2	1:D:1623:CYS:SG	2.55	0.47
1:D:1866:THR:HG23	1:D:1867:GLN:N	2.28	0.47
1:D:2322:LEU:HB2	1:D:2325:CYS:H	1.78	0.47
1:D:2310:ARG:HG3	1:D:2325:CYS:SG	2.55	0.47
1:D:2398:GLU:HB3	1:D:2407:GLN:HE22	1.80	0.47
1:A:2415:ILE:HG23	1:A:2416:SER:N	2.30	0.47
1:A:2471:LYS:NZ	1:D:2577:ASP:O	2.43	0.47
1:A:1366:ASP:OD1	1:A:1366:ASP:N	2.48	0.47
1:A:2132:LEU:HB3	1:A:2140:VAL:HG13	1.97	0.47
1:D:1469:PHE:HB3	1:D:1517:ILE:HG23	1.97	0.47
1:A:2310:ARG:HG3	1:A:2325:CYS:SG	2.55	0.46
1:D:2415:ILE:HG21	1:D:2534:LEU:HB3	1.96	0.46
1:A:1740:LEU:O	1:A:1742:PHE:N	2.45	0.46
1:D:2086:GLN:N	1:D:2086:GLN:OE1	2.48	0.46
1:D:2111:VAL:HG13	1:D:2403:VAL:HA	1.97	0.46
1:D:2277:ALA:O	1:D:2280:GLN:CG	2.60	0.46
1:D:2415:ILE:HG23	1:D:2416:SER:N	2.30	0.46
1:D:2498:LEU:HD13	1:D:2510:ARG:HE	1.79	0.46
1:D:2132:LEU:HB3	1:D:2140:VAL:HG13	1.97	0.46
1:A:2277:ALA:O	1:A:2280:GLN:CG	2.60	0.46
1:A:2352:CYS:CB	1:A:2360:TYR:HE1	2.28	0.46
1:D:1366:ASP:OD1	1:D:1366:ASP:N	2.48	0.46
1:D:2352:CYS:CB	1:D:2360:TYR:HE1	2.28	0.46
1:A:1273:GLY:HA3	1:A:1277:TYR:CE2	2.50	0.46
1:A:1820:CYS:SG	1:A:1821:ASP:N	2.89	0.46
1:A:2415:ILE:HG21	1:A:2534:LEU:HB3	1.96	0.46
1:D:1327:HIS:HB2	1:D:1329:ASN:ND2	2.31	0.46
1:A:1327:HIS:HB2	1:A:1329:ASN:ND2	2.31	0.46
1:A:1750:VAL:HG22	1:A:1759:VAL:HG12	1.98	0.46
1:A:2053:HIS:O	1:A:2053:HIS:ND1	2.49	0.46
1:A:2111:VAL:HG13	1:A:2403:VAL:HA	1.97	0.46
1:A:2214:CYS:SG	1:A:2259:CYS:N	2.89	0.46
1:D:1740:LEU:O	1:D:1742:PHE:N	2.45	0.46
1:A:2086:GLN:OE1	1:A:2086:GLN:N	2.48	0.46
1:A:2491:VAL:HG21	1:A:2502:VAL:HG11	1.98	0.45
1:D:1373:TYR:HD1	1:D:1379:VAL:HG22	1.81	0.45
1:D:1775:VAL:HG13	1:D:1775:VAL:O	2.15	0.45
1:A:1880:GLN:HE22	1:A:2350:GLN:NE2	2.15	0.45
1:A:2073:PHE:HA	1:A:2091:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1540:GLY:N	1:D:1563:CYS:SG	2.90	0.45
1:D:1808:LYS:HG2	1:D:1810:GLU:H	1.82	0.45
1:A:1373:TYR:HD1	1:A:1379:VAL:HG22	1.81	0.45
1:A:1469:PHE:HB3	1:A:1517:ILE:HG23	1.97	0.45
1:A:1655:TRP:HB2	1:A:1659:HIS:HB2	1.97	0.45
1:A:2045:LEU:N	1:A:2164:CYS:O	2.47	0.45
1:D:2053:HIS:O	1:D:2053:HIS:ND1	2.49	0.45
1:D:2173:ASP:O	1:D:2176:VAL:HG22	2.17	0.45
1:D:2214:CYS:SG	1:D:2259:CYS:N	2.89	0.45
1:D:1880:GLN:HE22	1:D:2350:GLN:NE2	2.15	0.45
1:D:2491:VAL:HG21	1:D:2502:VAL:HG11	1.98	0.45
1:A:1540:GLY:N	1:A:1563:CYS:SG	2.90	0.45
1:A:1744:LEU:HD12	1:A:1744:LEU:HA	1.91	0.45
1:A:2398:GLU:HB3	1:A:2407:GLN:HE22	1.80	0.45
1:D:1750:VAL:HG22	1:D:1759:VAL:HG12	1.98	0.45
1:D:1835:GLU:H	1:D:1835:GLU:CD	2.25	0.45
1:A:2090:VAL:HB	1:A:2097:VAL:HG13	1.98	0.45
1:A:1796:LYS:HD3	1:A:1796:LYS:HA	1.53	0.45
1:A:1917:CYS:SG	1:A:1918:PRO:HD2	2.57	0.45
1:D:1347:LEU:HD23	1:D:1349:GLY:H	1.82	0.45
1:A:1775:VAL:O	1:A:1775:VAL:HG13	2.15	0.44
1:D:1820:CYS:SG	1:D:1821:ASP:N	2.89	0.44
1:D:2431:ILE:HG23	1:D:2570:ILE:HG21	1.99	0.44
1:A:2156:PHE:HB3	1:A:2160:LEU:HB2	2.00	0.44
1:A:2173:ASP:HB3	2:A:5609:NAG:H82	1.99	0.44
1:D:1917:CYS:SG	1:D:1918:PRO:HD2	2.57	0.44
1:A:1808:LYS:HG2	1:A:1810:GLU:H	1.82	0.44
1:D:1929:SER:HB2	1:D:1946:ILE:O	2.17	0.44
1:A:1347:LEU:HD23	1:A:1349:GLY:H	1.82	0.44
1:A:2431:ILE:HG23	1:A:2570:ILE:HG21	1.99	0.44
1:D:1796:LYS:HA	1:D:1796:LYS:HD3	1.53	0.44
1:D:1850:THR:OG1	1:D:1869:PHE:HB2	2.18	0.44
1:A:1929:SER:HB2	1:A:1946:ILE:O	2.17	0.44
1:D:1719:LEU:HD23	1:D:1748:LEU:HD13	2.00	0.44
1:D:1774:PHE:CE2	1:D:1892:THR:HG23	2.53	0.44
1:A:2173:ASP:O	1:A:2176:VAL:HG22	2.17	0.44
1:D:2073:PHE:HA	1:D:2091:THR:O	2.16	0.44
1:A:2418:GLY:HA3	2:A:5608:NAG:H83	1.99	0.44
1:D:2156:PHE:HB3	1:D:2160:LEU:HB2	1.99	0.44
1:D:2242:HIS:HA	1:D:2245:LEU:O	2.18	0.44
1:D:2418:GLY:HA3	2:D:5608:NAG:H83	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1570:ASP:OD1	1:A:1570:ASP:N	2.51	0.44
1:D:1962:ASP:N	1:D:1962:ASP:OD1	2.51	0.44
1:A:1719:LEU:HD23	1:A:1748:LEU:HD13	2.00	0.44
1:A:1848:ILE:O	1:A:1852:PRO:HG3	2.18	0.44
1:A:1850:THR:OG1	1:A:1869:PHE:HB2	2.18	0.44
1:D:1717:TYR:CD2	1:D:1747:LYS:HD3	2.53	0.44
1:D:2090:VAL:HB	1:D:2097:VAL:HG13	1.98	0.44
1:A:2242:HIS:HA	1:A:2245:LEU:O	2.18	0.43
1:D:1826:GLU:OE1	1:D:1826:GLU:N	2.41	0.43
1:D:1880:GLN:HE22	1:D:2350:GLN:HE21	1.66	0.43
1:D:2045:LEU:N	1:D:2164:CYS:O	2.47	0.43
1:D:1535:HIS:ND1	1:D:1537:GLU:HG3	2.33	0.43
1:D:1657:ASP:HB3	1:D:1708:TYR:HE1	1.83	0.43
1:D:2173:ASP:HB3	2:D:5609:NAG:H82	1.98	0.43
1:A:1331:ILE:HD13	1:A:1340:LEU:HB2	2.01	0.43
1:A:2439:LEU:HB2	1:A:2455:VAL:HG23	2.00	0.43
1:D:1662:THR:OG1	1:D:1666:HIS:N	2.48	0.43
1:A:1535:HIS:ND1	1:A:1537:GLU:HG3	2.33	0.43
1:A:1588:GLY:HA2	1:A:1596:TYR:C	2.44	0.43
1:A:1880:GLN:HE22	1:A:2350:GLN:HE21	1.66	0.43
1:D:1848:ILE:O	1:D:1852:PRO:HG3	2.18	0.43
1:D:2079:LYS:HD3	1:D:2083:GLY:HA2	2.01	0.43
1:D:2101:ARG:NH1	1:D:2106:THR:HG21	2.33	0.43
1:A:2101:ARG:NH1	1:A:2106:THR:HG21	2.33	0.43
1:D:1588:GLY:HA2	1:D:1596:TYR:C	2.44	0.43
1:D:1935:PRO:O	1:D:1937:LEU:N	2.51	0.43
1:A:1935:PRO:O	1:A:1937:LEU:N	2.51	0.43
2:D:5608:NAG:O7	2:D:5608:NAG:O4	2.25	0.43
1:A:1263:SER:HA	1:A:1395:CYS:HB3	2.01	0.43
1:A:1297:VAL:HG12	1:A:1317:VAL:HG12	2.00	0.43
1:A:1774:PHE:CE2	1:A:1892:THR:HG23	2.53	0.43
1:A:1962:ASP:N	1:A:1962:ASP:OD1	2.51	0.43
1:D:1263:SER:HA	1:D:1395:CYS:HB3	2.01	0.43
1:D:1297:VAL:HG12	1:D:1317:VAL:HG12	2.00	0.43
1:D:1621:LEU:HD13	1:D:1623:CYS:CB	2.39	0.43
1:D:2364:ASN:ND2	2:D:5607:NAG:H62	2.34	0.43
1:D:2439:LEU:HB2	1:D:2455:VAL:HG23	2.01	0.43
1:A:1407:VAL:HA	1:A:1413:MET:HA	2.01	0.42
1:A:1835:GLU:CD	1:A:1835:GLU:H	2.25	0.42
1:D:2337:ASP:OD1	1:D:2338:HIS:N	2.53	0.42
1:A:1532:ASP:HB3	1:A:1533:ASN:H	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1717:TYR:CD2	1:A:1747:LYS:HD3	2.53	0.42
1:A:2057:SER:HB2	1:A:2195:ALA:HB3	2.02	0.42
1:A:2222:TYR:O	1:A:2225:ASN:ND2	2.52	0.42
1:D:1331:ILE:HD13	1:D:1340:LEU:HB2	2.01	0.42
1:D:2222:TYR:O	1:D:2225:ASN:ND2	2.52	0.42
1:A:1518:GLU:OE1	1:A:1518:GLU:N	2.53	0.42
1:A:1533:ASN:HB2	1:A:1569:CYS:HA	2.01	0.42
1:D:1370:GLN:HE21	1:D:1370:GLN:HB3	1.65	0.42
1:D:1533:ASN:HB2	1:D:1569:CYS:HA	2.01	0.42
1:D:2057:SER:HB3	1:D:2078:GLU:HG3	2.01	0.42
1:A:2067:LYS:HD2	1:A:2068:PRO:HD2	2.02	0.42
1:A:2342:SER:O	1:A:2343:HIS:ND1	2.52	0.42
1:A:2337:ASP:OD1	1:A:2338:HIS:N	2.53	0.42
1:D:1840:PHE:CD2	1:D:1876:ALA:HB1	2.55	0.42
1:D:2570:ILE:HD12	1:D:2570:ILE:H	1.85	0.42
1:A:1392:CYS:HB3	1:A:1424:TRP:HZ3	1.85	0.42
1:A:1736:GLU:HA	1:A:2022:GLY:HA2	2.01	0.42
1:A:2376:CYS:HA	1:A:2386:CYS:HA	2.01	0.42
1:A:2570:ILE:HD12	1:A:2570:ILE:H	1.85	0.42
1:D:1407:VAL:HA	1:D:1413:MET:HA	2.01	0.42
1:D:1701:ARG:HH21	1:D:2318:ALA:HB2	1.85	0.42
1:A:1826:GLU:OE1	1:A:1826:GLU:N	2.41	0.42
1:A:2057:SER:HB3	1:A:2078:GLU:HG3	2.01	0.42
1:D:1570:ASP:N	1:D:1570:ASP:OD1	2.51	0.42
1:D:1985:PHE:CE2	1:D:1987:PRO:HG3	2.55	0.42
1:A:1372:THR:HG23	1:A:1380:ASP:HB3	2.01	0.41
1:A:1701:ARG:HH21	1:A:2318:ALA:HB2	1.85	0.41
1:A:1985:PHE:CE2	1:A:1987:PRO:HG3	2.55	0.41
1:D:1576:SER:HB2	1:D:1581:VAL:HG11	2.02	0.41
1:D:2342:SER:O	1:D:2343:HIS:ND1	2.52	0.41
1:A:2079:LYS:HD3	1:A:2083:GLY:HA2	2.01	0.41
1:D:1664:ASP:OD1	1:D:1664:ASP:N	2.52	0.41
1:D:1736:GLU:HA	1:D:2022:GLY:HA2	2.01	0.41
1:A:2276:THR:HG21	1:A:2289:TRP:CD1	2.55	0.41
1:D:1372:THR:HG23	1:D:1380:ASP:HB3	2.01	0.41
1:D:1392:CYS:HB3	1:D:1424:TRP:HZ3	1.85	0.41
1:A:1740:LEU:HD23	1:A:1752:ILE:HB	2.02	0.41
1:D:2057:SER:HB2	1:D:2195:ALA:HB3	2.02	0.41
1:D:1655:TRP:HE3	1:D:1656:GLY:H	1.68	0.41
1:D:2276:THR:HG21	1:D:2289:TRP:CD1	2.55	0.41
1:A:1447:ASP:OD1	1:A:1448:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1710:ARG:NH2	1:D:1726:GLN:OE1	2.49	0.41
1:A:2364:ASN:ND2	2:A:5607:NAG:H62	2.34	0.41
1:D:2472:VAL:HG23	1:D:2528:LEU:HD22	2.02	0.41
1:A:1576:SER:HB2	1:A:1581:VAL:HG11	2.02	0.41
1:A:1885:GLY:O	1:A:1888:PRO:HD2	2.20	0.41
1:A:2441:SER:HA	1:A:2453:TYR:O	2.21	0.41
1:D:1885:GLY:O	1:D:1888:PRO:HD2	2.20	0.41
1:D:2316:CYS:SG	1:D:2360:TYR:HE1	2.23	0.41
1:A:1840:PHE:CD2	1:A:1876:ALA:HB1	2.55	0.41
1:A:2078:GLU:OE1	1:A:2078:GLU:N	2.54	0.41
1:D:1343:LEU:HB3	1:D:1344:PRO:HD3	2.02	0.41
1:D:1518:GLU:OE1	1:D:1518:GLU:N	2.53	0.41
1:D:1519:ASP:HA	1:D:1538:LEU:HD21	2.03	0.41
1:D:1565:GLU:HG2	1:D:1566:GLY:N	2.36	0.41
1:D:1991:CYS:N	1:D:2017:CYS:SG	2.94	0.41
1:D:2067:LYS:HD2	1:D:2068:PRO:HD2	2.02	0.41
1:D:2376:CYS:HA	1:D:2386:CYS:HA	2.01	0.41
1:A:1519:ASP:HA	1:A:1538:LEU:HD21	2.03	0.41
1:D:2108:ASP:O	1:D:2109:GLY:C	2.64	0.41
1:A:1565:GLU:HG2	1:A:1566:GLY:N	2.36	0.40
1:D:2397:CYS:HA	1:D:2406:CYS:HA	2.04	0.40
1:D:2473:HIS:HB3	1:D:2480:LEU:HD11	2.03	0.40
1:A:1256:TRP:HZ2	1:A:1502:ALA:HB1	1.86	0.40
1:A:1343:LEU:HB3	1:A:1344:PRO:HD3	2.02	0.40
1:A:2070:ASP:OD2	1:A:2159:ARG:NH2	2.54	0.40
1:A:2473:HIS:HB3	1:A:2480:LEU:HD11	2.03	0.40
1:A:2273:ALA:HA	1:A:2276:THR:HG22	2.04	0.40
1:A:2531:ASP:OD1	1:A:2531:ASP:N	2.55	0.40
1:D:2078:GLU:N	1:D:2078:GLU:OE1	2.54	0.40
1:D:2188:ALA:O	1:D:2191:THR:OG1	2.27	0.40
1:D:2415:ILE:HG22	1:D:2534:LEU:O	2.22	0.40
1:A:2503:LEU:HB3	1:A:2504:THR:H	1.69	0.40
1:D:1744:LEU:HD12	1:D:1744:LEU:HA	1.91	0.40
1:D:1267:TRP:HB2	1:D:1402:HIS:HB2	2.04	0.40
1:D:1280:ALA:HA	1:D:1393:GLY:HA3	2.04	0.40
1:D:1285:PRO:HB2	1:D:1287:VAL:HG23	2.04	0.40
1:D:1368:GLY:HA3	1:D:1384:PRO:HG3	2.04	0.40
1:D:2070:ASP:OD2	1:D:2159:ARG:NH2	2.54	0.40
1:D:2441:SER:HA	1:D:2453:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1337/2587 (52%)	1253 (94%)	83 (6%)	1 (0%)	48	78
1	D	1337/2587 (52%)	1253 (94%)	83 (6%)	1 (0%)	48	78
All	All	2674/5174 (52%)	2506 (94%)	166 (6%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2109	GLY
1	D	2109	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1085/2113 (51%)	1025 (94%)	60 (6%)	19	46
1	D	1085/2113 (51%)	1025 (94%)	60 (6%)	19	46
All	All	2170/4226 (51%)	2050 (94%)	120 (6%)	21	46

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1317	VAL
1	A	1345	VAL
1	A	1369	LEU
1	A	1370	GLN

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Mol	Chain	Res	Type
1	A	1371	VAL
1	A	1391	VAL
1	A	1395	CYS
1	A	1441	CYS
1	A	1461	LEU
1	A	1510	CYS
1	A	1532	ASP
1	A	1557	THR
1	A	1601	GLU
1	A	1623	CYS
1	A	1664	ASP
1	A	1674	CYS
1	A	1690	GLU
1	A	1752	ILE
1	A	1796	LYS
1	A	1799	ASN
1	A	1823	CYS
1	A	1850	THR
1	A	1859	CYS
1	A	1904	LEU
1	A	1941	VAL
1	A	1944	GLU
1	A	1959	LEU
1	A	1963	THR
1	A	1965	VAL
1	A	2011	CYS
1	A	2012[A]	GLU
1	A	2012[B]	GLU
1	A	2063	VAL
1	A	2087	ARG
1	A	2099	LEU
1	A	2104	GLN
1	A	2105	VAL
1	A	2140	VAL
1	A	2161	CYS
1	A	2170	ASN
1	A	2173	ASP
1	A	2200	LEU
1	A	2202	CYS
1	A	2211	CYS
1	A	2241	CYS
1	A	2291	THR

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Mol	Chain	Res	Type
1	A	2345	VAL
1	A	2355	VAL
1	A	2376	CYS
1	A	2399	ILE
1	A	2462	CYS
1	A	2475	PHE
1	A	2501	THR
1	A	2502	VAL
1	A	2504	THR
1	A	2518	VAL
1	A	2534	LEU
1	A	2560	ASP
1	A	2567	LYS
1	A	2577	ASP
1	D	1317	VAL
1	D	1345	VAL
1	D	1369	LEU
1	D	1370	GLN
1	D	1371	VAL
1	D	1391	VAL
1	D	1395	CYS
1	D	1441	CYS
1	D	1461	LEU
1	D	1510	CYS
1	D	1532	ASP
1	D	1557	THR
1	D	1601	GLU
1	D	1623	CYS
1	D	1664	ASP
1	D	1674	CYS
1	D	1690	GLU
1	D	1752	ILE
1	D	1796	LYS
1	D	1799	ASN
1	D	1823	CYS
1	D	1850	THR
1	D	1859	CYS
1	D	1904	LEU
1	D	1941	VAL
1	D	1944	GLU
1	D	1959	LEU
1	D	1963	THR

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Mol	Chain	Res	Type
1	D	1965	VAL
1	D	2011	CYS
1	D	2012[A]	GLU
1	D	2012[B]	GLU
1	D	2063	VAL
1	D	2087	ARG
1	D	2099	LEU
1	D	2104	GLN
1	D	2105	VAL
1	D	2140	VAL
1	D	2161	CYS
1	D	2170	ASN
1	D	2173	ASP
1	D	2200	LEU
1	D	2202	CYS
1	D	2211	CYS
1	D	2241	CYS
1	D	2291	THR
1	D	2345	VAL
1	D	2355	VAL
1	D	2376	CYS
1	D	2399	ILE
1	D	2462	CYS
1	D	2475	PHE
1	D	2501	THR
1	D	2502	VAL
1	D	2504	THR
1	D	2518	VAL
1	D	2534	LEU
1	D	2560	ASP
1	D	2567	LYS
1	D	2577	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1880	GLN
1	A	2065	HIS
1	A	2120	HIS
1	A	2350	GLN
1	A	2465	ASN
1	D	1880	GLN

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Mol	Chain	Res	Type
1	D	1922	HIS
1	D	1924	GLN
1	D	2065	HIS
1	D	2350	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	5609	1	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	A	5610	1	14,14,15	0.32	0	17,19,21	0.44	0
2	NAG	D	5607	1	14,14,15	0.86	1 (7%)	17,19,21	1.27	1 (5%)
2	NAG	A	5601	1	14,14,15	0.80	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	A	5603	1	14,14,15	0.35	0	17,19,21	0.66	0
2	NAG	D	5608	1	14,14,15	0.67	1 (7%)	17,19,21	0.88	0
2	NAG	A	5607	1	14,14,15	0.85	1 (7%)	17,19,21	1.26	1 (5%)
2	NAG	D	5601	1	14,14,15	0.81	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	D	5610	1	14,14,15	0.32	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	5608	1	14,14,15	0.67	1 (7%)	17,19,21	0.88	0
2	NAG	D	5603	1	14,14,15	0.35	0	17,19,21	0.66	0
2	NAG	D	5609	1	14,14,15	0.28	0	17,19,21	0.44	0

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	5609	1	-	1/6/23/26	0/1/1/1
2	NAG	A	5610	1	-	1/6/23/26	0/1/1/1
2	NAG	D	5607	1	-	2/6/23/26	0/1/1/1
2	NAG	A	5601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	5603	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5608	1	-	3/6/23/26	0/1/1/1
2	NAG	A	5607	1	-	2/6/23/26	0/1/1/1
2	NAG	D	5601	1	-	2/6/23/26	0/1/1/1
2	NAG	D	5610	1	-	1/6/23/26	0/1/1/1
2	NAG	A	5608	1	-	3/6/23/26	0/1/1/1
2	NAG	D	5603	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5609	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5607	NAG	O5-C1	3.03	1.48	1.43
2	A	5607	NAG	O5-C1	3.00	1.48	1.43
2	D	5601	NAG	O5-C1	2.46	1.47	1.43
2	A	5601	NAG	O5-C1	2.46	1.47	1.43
2	D	5608	NAG	O5-C1	-2.26	1.39	1.43
2	A	5608	NAG	O5-C1	-2.25	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5607	NAG	C1-O5-C5	5.01	118.90	112.19
2	A	5607	NAG	C1-O5-C5	4.98	118.86	112.19
2	D	5601	NAG	C1-O5-C5	3.72	117.18	112.19
2	A	5601	NAG	C1-O5-C5	3.71	117.15	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5608	NAG	C1-C2-N2-C7
2	D	5608	NAG	C1-C2-N2-C7
2	A	5601	NAG	C4-C5-C6-O6
2	D	5601	NAG	C4-C5-C6-O6
2	A	5601	NAG	O5-C5-C6-O6
2	D	5601	NAG	O5-C5-C6-O6
2	A	5607	NAG	O5-C5-C6-O6
2	D	5607	NAG	O5-C5-C6-O6
2	D	5610	NAG	O5-C5-C6-O6
2	A	5610	NAG	O5-C5-C6-O6
2	A	5608	NAG	O5-C5-C6-O6
2	D	5608	NAG	O5-C5-C6-O6
2	D	5607	NAG	C4-C5-C6-O6
2	A	5607	NAG	C4-C5-C6-O6
2	A	5608	NAG	C3-C2-N2-C7
2	D	5608	NAG	C3-C2-N2-C7
2	D	5609	NAG	C4-C5-C6-O6
2	A	5609	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5609	NAG	1	0
2	D	5607	NAG	3	0
2	A	5601	NAG	1	0
2	D	5608	NAG	3	0
2	A	5607	NAG	3	0
2	A	5608	NAG	3	0
2	D	5609	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1657:ASP	C	1658:PRO	N	7.71
1	A	1657:ASP	C	1658:PRO	N	7.58
1	A	1258:ASP	C	1259:PRO	N	5.18
1	D	1258:ASP	C	1259:PRO	N	5.03

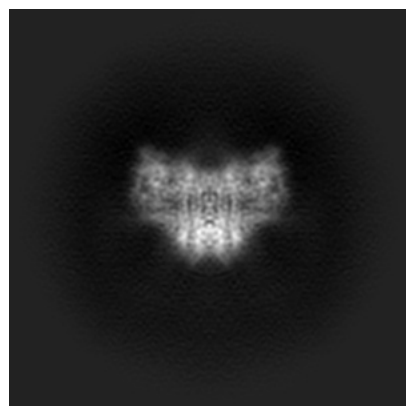
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19070. These allow visual inspection of the internal detail of the map and identification of artifacts.

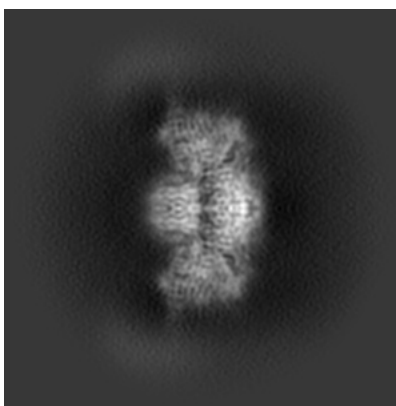
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

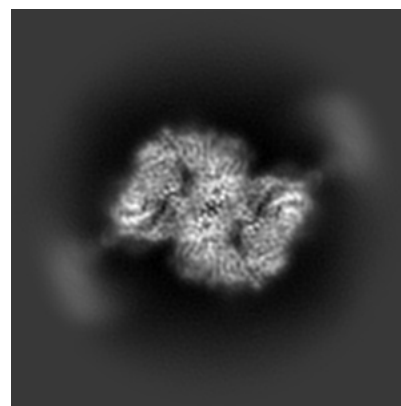
6.1.1 Primary map



X

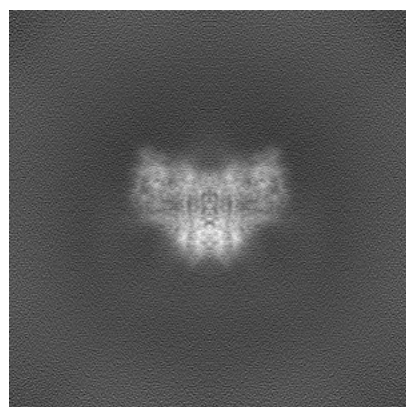


Y

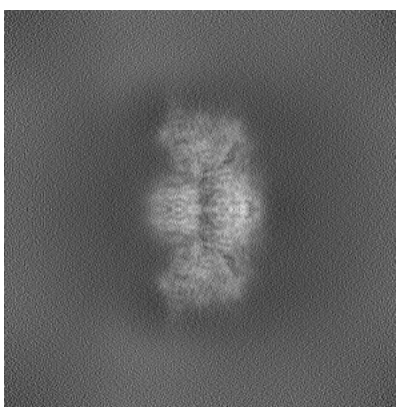


Z

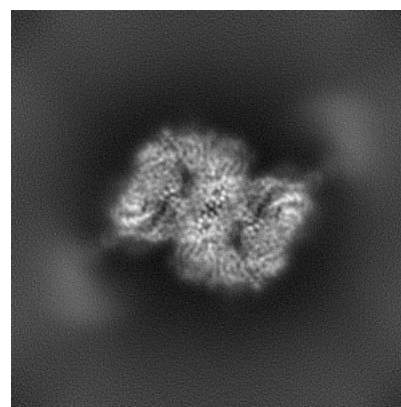
6.1.2 Raw map



X



Y



Z

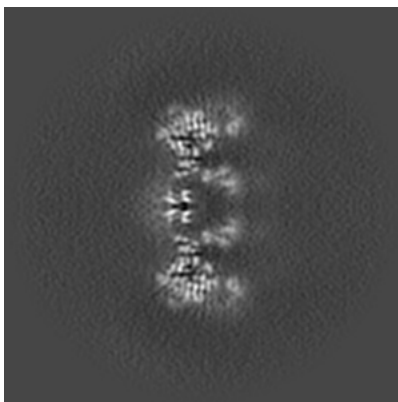
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

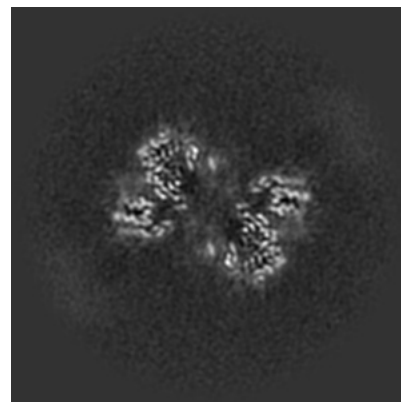
6.2.1 Primary map



X Index: 176

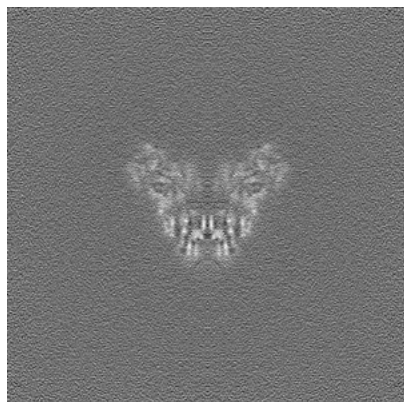


Y Index: 176

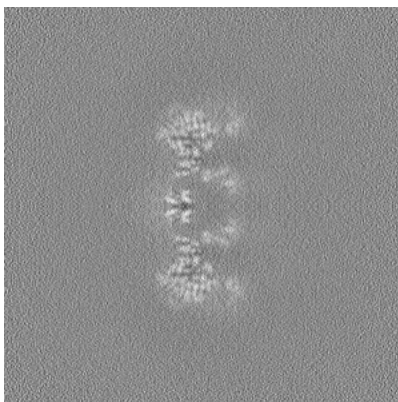


Z Index: 176

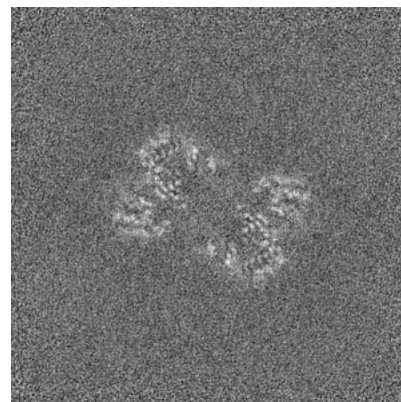
6.2.2 Raw map



X Index: 176



Y Index: 176



Z Index: 176

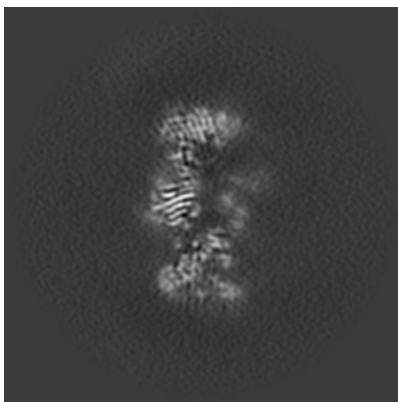
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

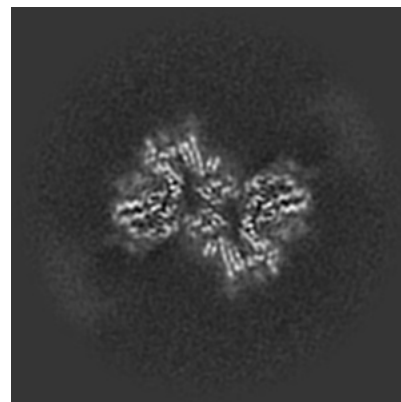
6.3.1 Primary map



X Index: 176

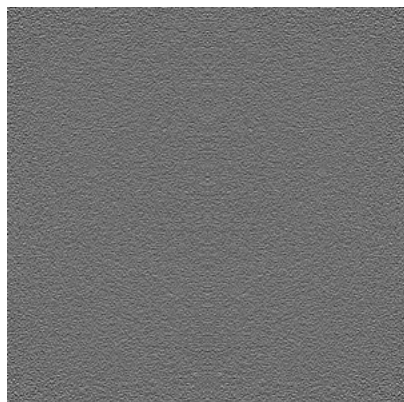


Y Index: 186

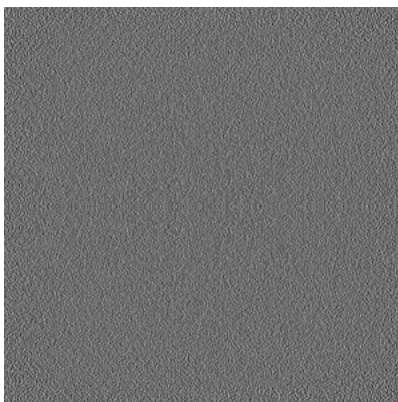


Z Index: 168

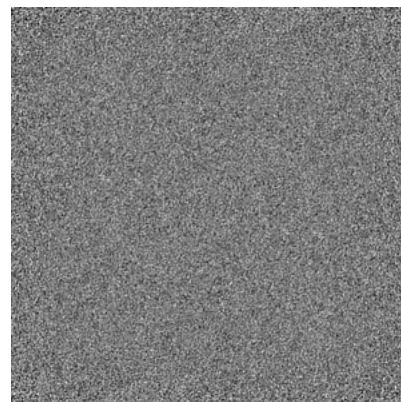
6.3.2 Raw map



X Index: 0



Y Index: 0

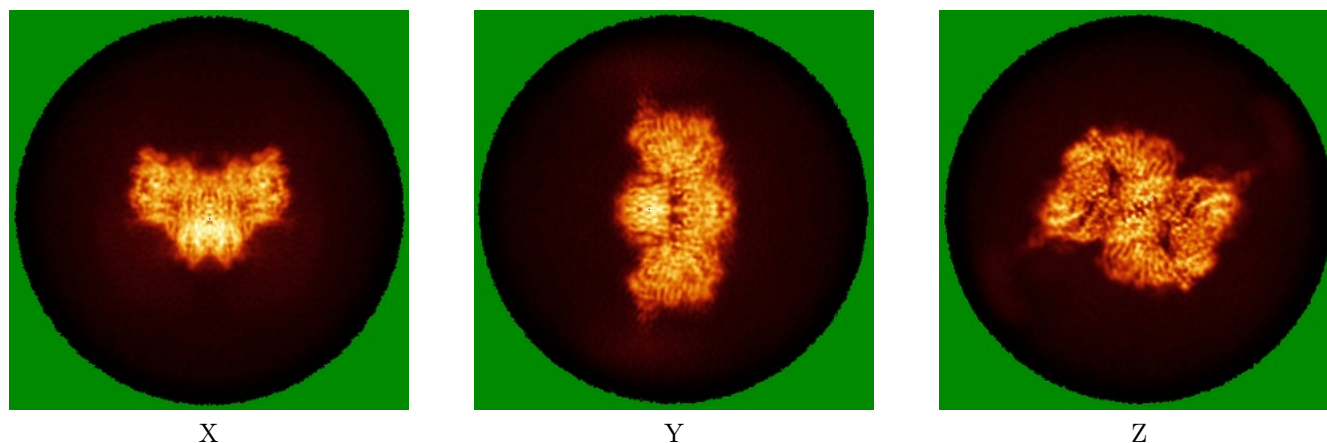


Z Index: 351

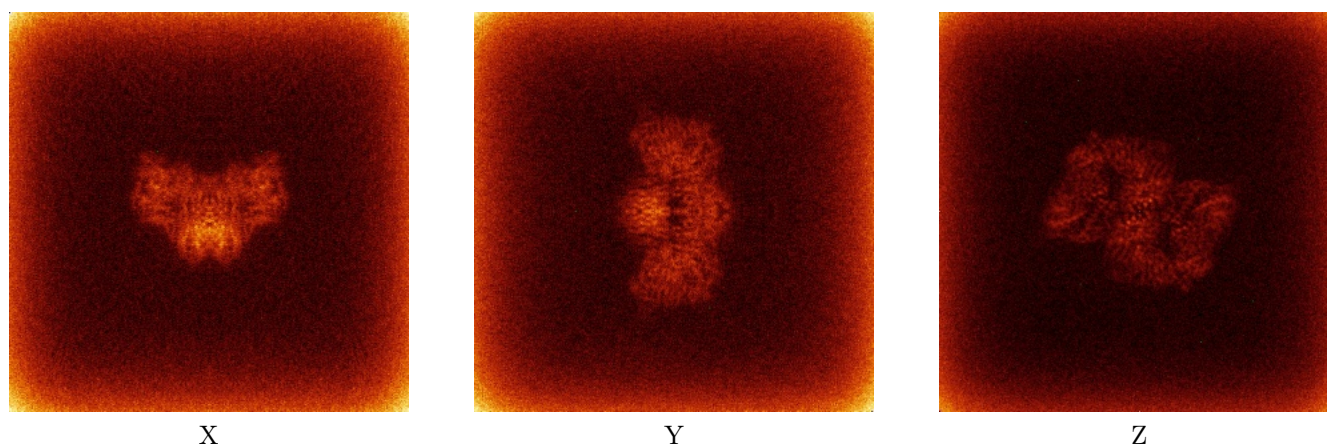
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

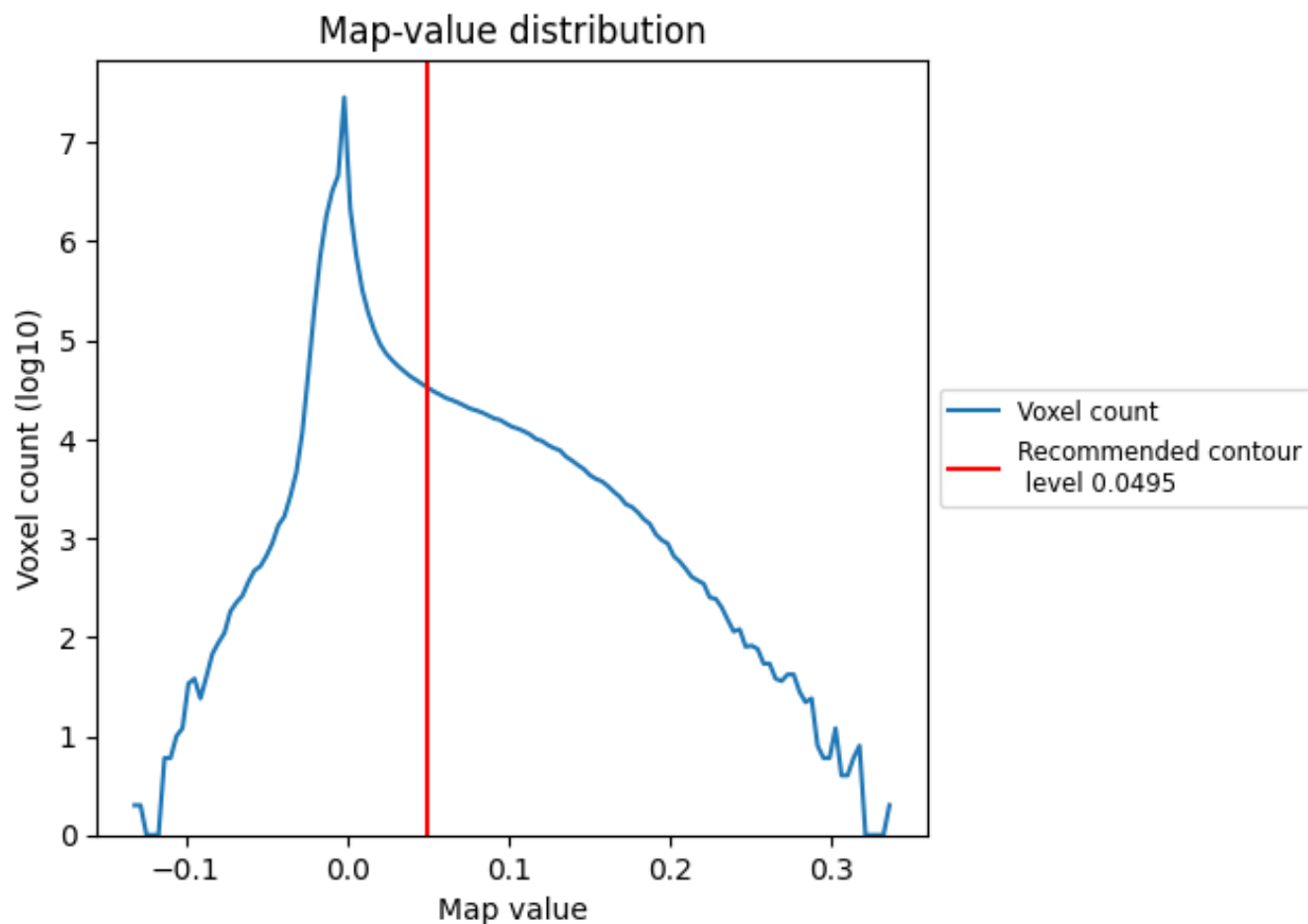
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

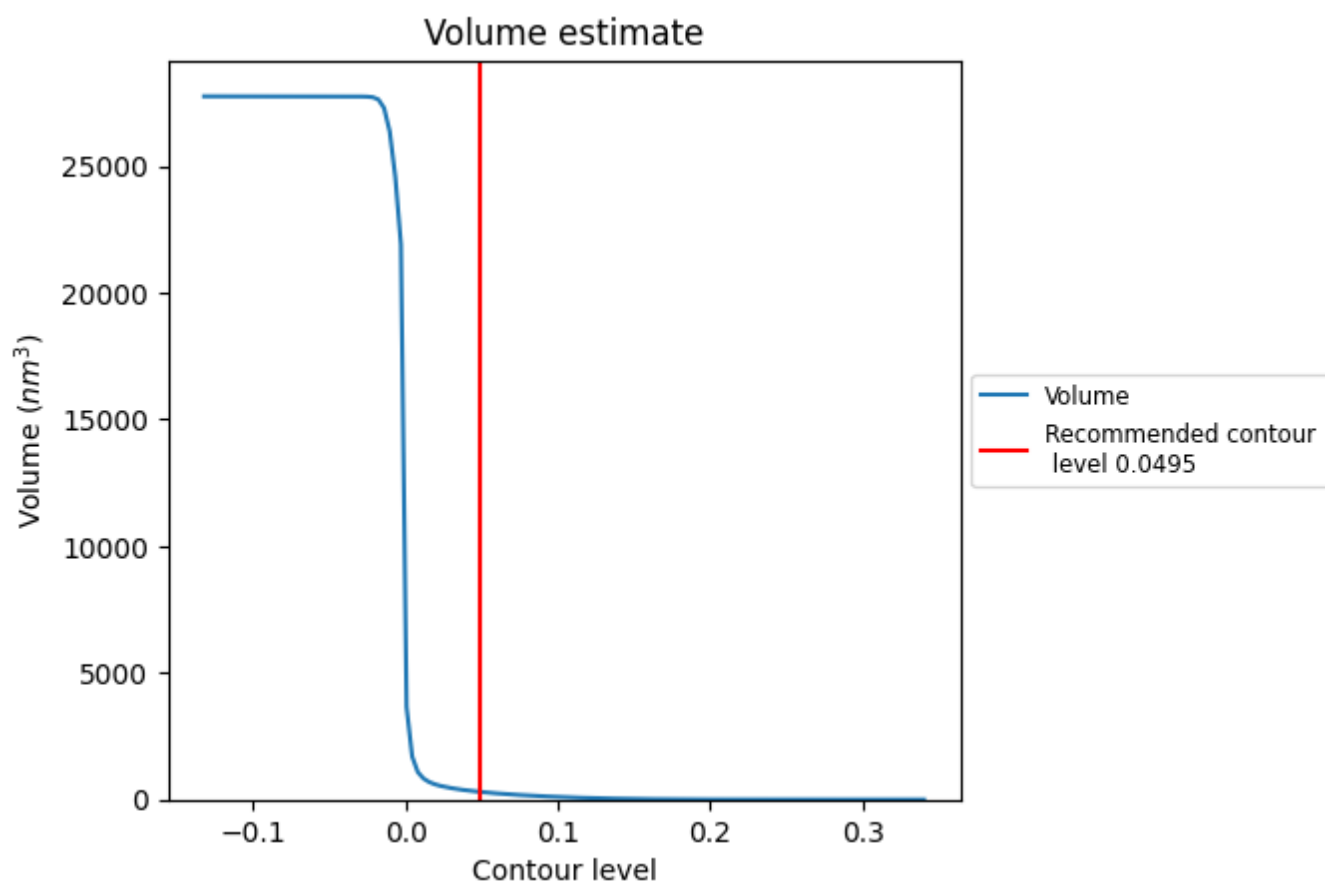
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

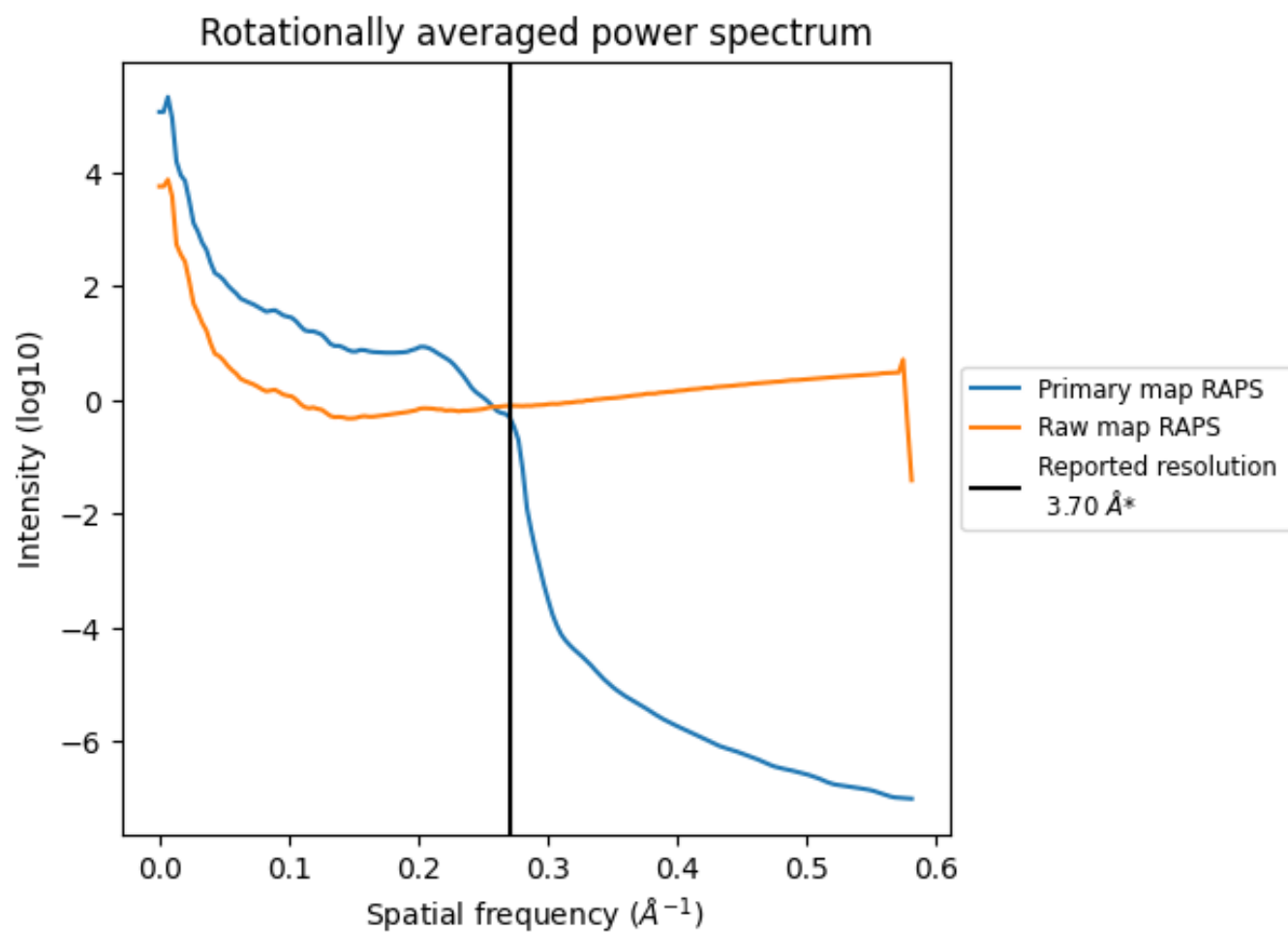
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm^3 ; this corresponds to an approximate mass of 271 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

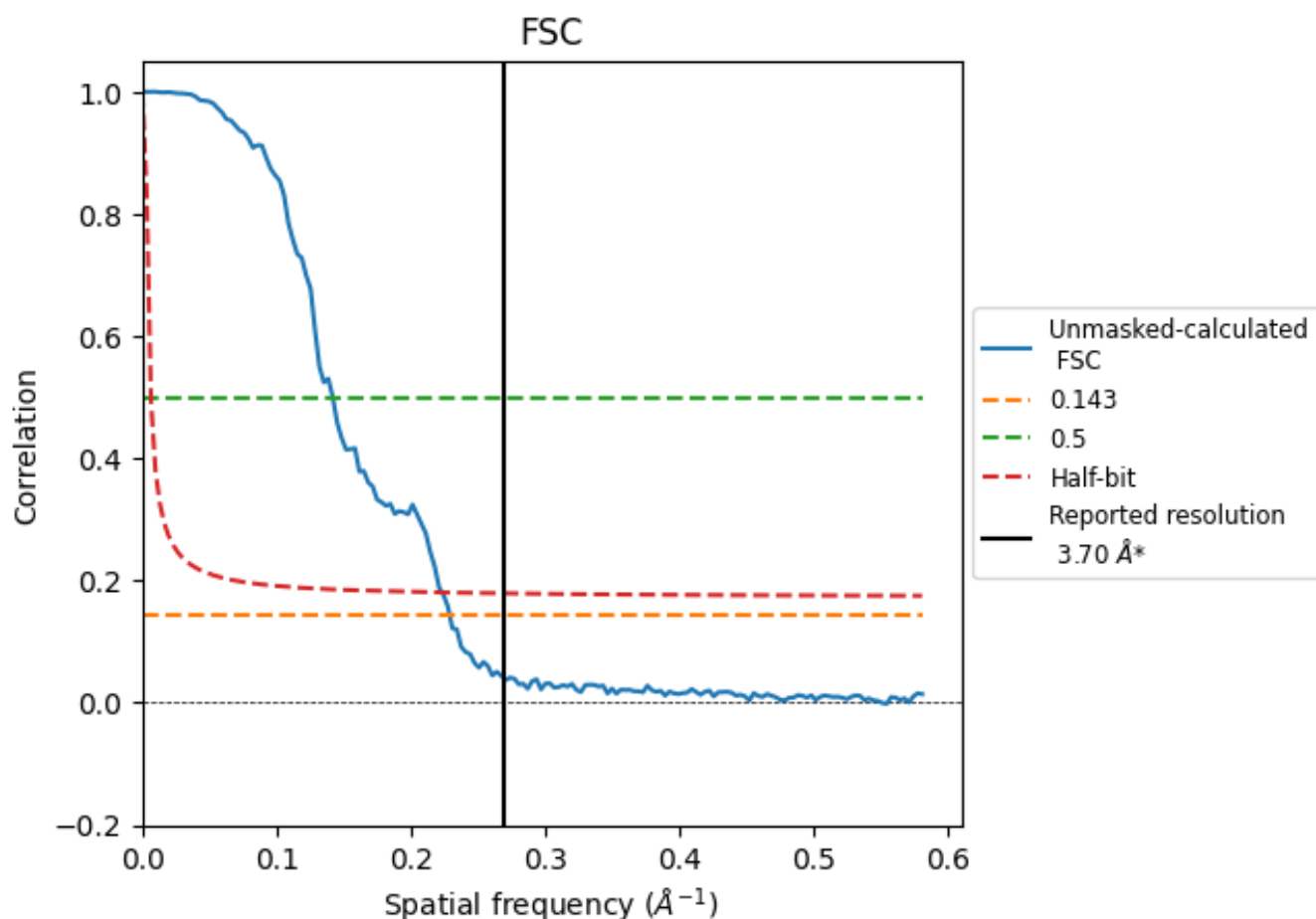


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	7.04	4.47

*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 4.36 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19070 and PDB model 8RDE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

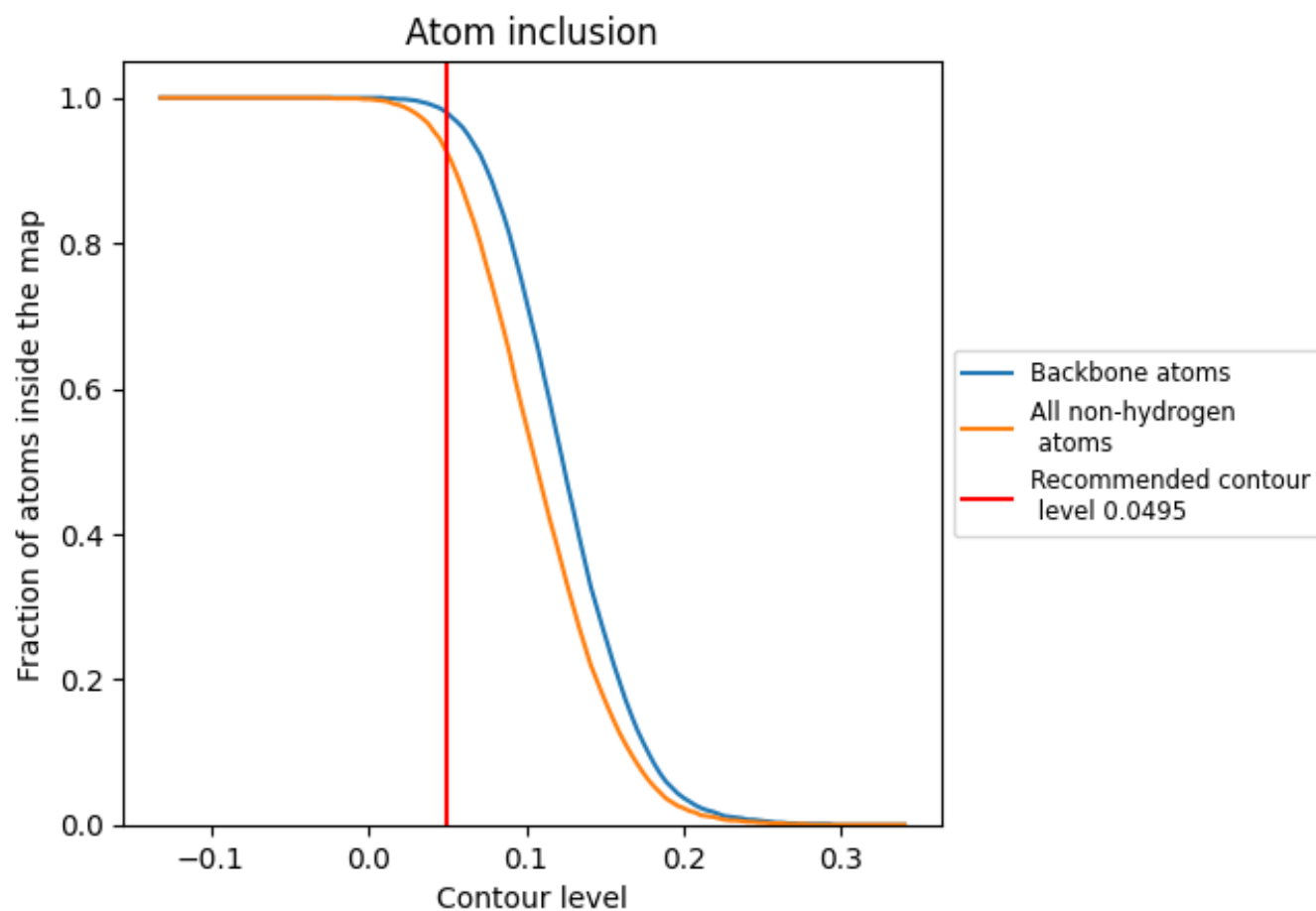


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.0495) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.3430
A	0.9230	0.3390
D	0.9290	0.3470

