



Full wwPDB EM Validation Report ⓘ

Feb 6, 2025 – 03:31 pm GMT

PDB ID : 8R0T
EMDB ID : EMD-18803
Title : STRUCTURE OF THE MOUSE FCGBP DIMER PROTEIN IN ITS SEMIEXTENDED CONFORMATION
Authors : Gallego, P.; Hansson, G.C.; Johansson, M.E.V.
Deposited on : 2023-10-31
Resolution : 3.90 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

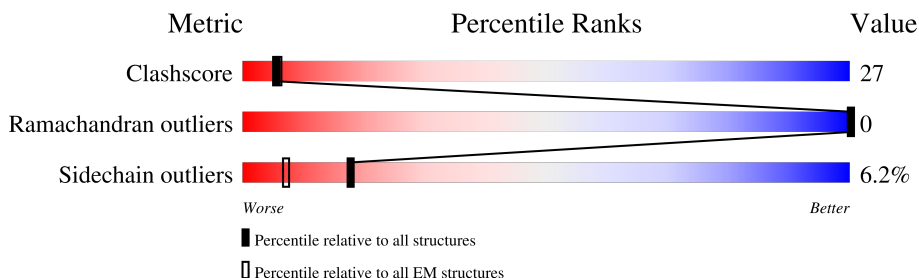
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1232	 99%
2	B	399	 55% 43%
3	C	930	 58% 39%
3	F	930	 12% 8% 79%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11461 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	13	Total	C	N	O	S	0	0
			110	71	17	21	1		

- Molecule 2 is a protein called Fc fragment of IgG binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			2946	1835	498	576	37		

- Molecule 3 is a protein called Fc fragment of IgG binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	927	Total	C	N	O	S	1	0
			6854	4252	1197	1322	83		
3	F	195	Total	C	N	O	S	0	0
			1449	901	259	276	13		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2584	THR	-	expression tag	UNP E9Q9C6
C	2585	ARG	-	expression tag	UNP E9Q9C6
C	2586	THR	-	expression tag	UNP E9Q9C6
C	2587	ARG	-	expression tag	UNP E9Q9C6
F	2584	THR	-	expression tag	UNP E9Q9C6
F	2585	ARG	-	expression tag	UNP E9Q9C6
F	2586	THR	-	expression tag	UNP E9Q9C6
F	2587	ARG	-	expression tag	UNP E9Q9C6

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Ca	0
			1	1	
5	C	2	Total	Ca	0
			2	2	
5	F	1	Total	Ca	0
			1	1	



F2553	I2468	CYS	ALA	MET
D2556	V2469	SER	LEU	CYS
Q2557	S2470	PRO	SER	ALA
T2558	K2471	ASN	GLY	HIS
N2559	V2472	ASN	LEU	LYS
	H2473	GLY	THR	GLY
	I2474	LEU	GLY	ASP
		THR	CYS	LYS
Q2565			CYS	ALA
G2566	D2478	HIS	THR	TYR
K2567	G2479	GLU	ARG	LEU
T2568	L2480	CYS	CYS	GLN
P2569	V2481	ALA	PHE	MET
	T2482	GLU	SER	SER
K2572	V2483	GLY	ILE	PRO
	I2484	CYS	VAL	VAL
Q2576	P2485	GLU	ALA	SER
D2577	S2486	CYS	TYR	LEU
F2578	K2487	ASP	ALA	PHE
S2579	G2488	ASP	ALA	ARG
P2580	A2489	HIS	GLU	GLY
C2581	W2490	PHE	GLN	ARG
	V2491	LEU	ALA	CYS
	N2492	ALA	TYR	GLY
	G2493	SER	ALA	GLY
	L2494	GLY	CYS	LEU
	R2495	VAL	ASN	CYS
	V2496	VAL	PHE	ASN
	D2497	PRO	GLY	ASN
	V2502	ILE	LYS	GLY
	L2503	PRO	TRP	ASN
		ALA	GLN	ASN
	R2509	ASP	THR	TRP
	R2510	CYS	ARG	SER
	N2511	GLY	ASP	ASP
	P2512	CYS	PRO	ASP
		CYS	VAL	PHE
	S2515	VAL	CYS	PHE
	N2516	HIS	PRO	VAL
		ASN	LEU	VAL
	V2524	GLN	CYS	ALA
	T2525	GLY	GLN	GLY
	V2526	TYR	ALA	GLY
	V2527	PRO	ALA	GLY
	L2528	MET	ALA	VAL
		PRO	HIS	VAL
	G2532	VAL	LYS	ALA
	L2533	ASN	VAL	PRO
	L2534	SER	LEU	ASN
	D2535	TYR	LEU	ASN
	V2536	SER	VAL	VAL
	V2537	LEU	GLU	GLU
	V2538	MET	ALA	ALA
		SER	THR	PHE
		ARG	TYR	GLY
		ASP	PHE	THR
	L2542	CYS	ALA	ALA
	A2543	SER	GLN	TRP
	A2544	GLU	CYS	ARG
	N2545	ARG	VAL	ALA
	L2546	CYS	TYR	PRO
		PHE	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167045	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	0.357	Depositor
Minimum map value	-0.141	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0267	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	0.23	0/115	0.43	0/158
2	B	0.29	0/3033	0.55	1/4150 (0.0%)
3	C	0.36	3/7026 (0.0%)	0.64	5/9580 (0.1%)
3	F	0.35	0/1479	0.64	1/2011 (0.0%)
All	All	0.34	3/11653 (0.0%)	0.61	7/15899 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2569	PRO	N-CD	8.02	1.59	1.47
3	C	1741	PRO	N-CD	7.04	1.57	1.47
3	C	2451	PRO	N-CD	-6.13	1.39	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1442	PRO	CA-N-CD	-8.51	99.58	111.50
3	C	1935	PRO	N-CA-C	-7.73	92.00	112.10
3	C	1986	TYR	N-CA-CB	7.44	124.00	110.60
3	F	2553	PHE	CB-CA-C	-6.25	97.90	110.40
3	C	2253	GLN	N-CA-CB	5.81	121.07	110.60
3	C	2558	THR	N-CA-C	5.58	126.06	111.00
3	C	2226	ASP	N-CA-CB	5.37	120.27	110.60

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	110	0	90	14	0
2	B	2946	0	2711	162	0
3	C	6854	0	6448	393	0
3	F	1449	0	1409	68	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	56	0	52	4	0
4	F	14	0	13	2	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	F	1	0	0	0	0
All	All	11461	0	10749	604	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 27.

All (604) 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)
3:C:2474:ILE:HD12	3:C:2476:PHE:CE2	1.39	1.56
2:B:1282:THR:OG1	2:B:1387:TYR:CE2	1.67	1.43
3:C:1979:TYR:HB3	3:C:1985:PHE:CE1	1.51	1.42
3:C:1700:HIS:CD2	3:C:2313:GLN:HG3	1.56	1.40
2:B:1282:THR:OG1	2:B:1387:TYR:HE2	0.96	1.30
3:C:1979:TYR:CB	3:C:1985:PHE:CZ	2.16	1.27
3:C:1979:TYR:HB3	3:C:1985:PHE:CZ	1.69	1.25
3:C:2044:THR:HG23	3:C:2050:TYR:CD2	1.75	1.20
3:C:2252:ARG:HA	3:C:2255:VAL:HG22	1.27	1.16
3:C:2044:THR:CG2	3:C:2050:TYR:CD2	2.30	1.15
3:C:2474:ILE:CD1	3:C:2476:PHE:CE2	2.29	1.15
3:C:2044:THR:HG23	3:C:2050:TYR:HD2	1.02	1.09
3:C:2268:LEU:HD11	3:C:2272:LEU:HD22	1.16	1.08
3:C:2268:LEU:CD1	3:C:2272:LEU:HD22	1.83	1.08
3:C:2471:LYS:HG2	3:C:2484:ILE:HG12	1.26	1.07
3:C:2474:ILE:HD12	3:C:2476:PHE:CD2	1.88	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2501:THR:HG23	3:C:2507:SER:HA	1.32	1.07
3:C:1979:TYR:HB2	3:C:1985:PHE:CZ	1.87	1.05
3:C:1979:TYR:CB	3:C:1985:PHE:CE1	2.39	1.04
3:C:1959:LEU:HD21	3:C:1980:VAL:HG13	1.36	1.03
1:A:1255:LEU:HB3	2:B:1379:VAL:HB	1.39	1.02
3:C:1972:CYS:SG	3:C:1985:PHE:CZ	2.53	1.01
3:C:2570:ILE:HG13	3:C:2574:ARG:CD	1.90	1.00
3:C:2570:ILE:HG13	3:C:2574:ARG:HD2	1.40	1.00
3:C:1795:ASN:O	3:C:1796:LYS:HG2	1.62	0.98
3:C:1972:CYS:SG	3:C:1985:PHE:HZ	1.86	0.97
3:C:1700:HIS:CD2	3:C:2313:GLN:CG	2.48	0.96
2:B:1295:PHE:HB2	2:B:1319:THR:HG22	1.48	0.95
3:C:1937:LEU:O	3:C:1937:LEU:HD12	1.65	0.95
3:C:2451:PRO:HD2	3:C:2453:TYR:CD2	2.01	0.94
3:C:2268:LEU:HD11	3:C:2272:LEU:CD2	1.98	0.94
3:C:2268:LEU:HD12	3:C:2272:LEU:HB2	1.46	0.94
3:C:2252:ARG:HA	3:C:2255:VAL:CG2	1.99	0.93
3:F:2577:ASP:OD1	3:F:2578:PHE:N	2.02	0.93
2:B:1362:VAL:HG22	2:B:1372:THR:HB	1.49	0.92
3:C:2225:ASN:HB3	3:C:2228:CYS:HB2	1.52	0.91
3:C:2044:THR:CG2	3:C:2050:TYR:HD2	1.73	0.91
3:C:2468:ILE:HB	3:C:2532:GLY:HA3	1.53	0.90
3:C:2571:GLU:OE2	3:C:2572:LYS:HG3	1.73	0.89
3:C:1700:HIS:NE2	3:C:2313:GLN:HG3	1.88	0.89
2:B:1278:LEU:O	2:B:1394:LEU:HG	1.73	0.87
3:C:2474:ILE:CG1	3:C:2481:VAL:HB	2.05	0.87
3:C:2520:GLN:HB3	3:C:2523:GLY:HA3	1.56	0.87
2:B:1361:ALA:O	2:B:1372:THR:HA	1.73	0.86
3:C:2044:THR:HG22	3:C:2050:TYR:CE2	2.09	0.86
3:C:2451:PRO:HD2	3:C:2453:TYR:CE2	2.10	0.86
2:B:1493:GLY:HA3	3:C:1968:GLY:HA3	1.59	0.85
3:C:2044:THR:CG2	3:C:2050:TYR:CE2	2.59	0.84
2:B:1458:CYS:H	2:B:1499:LEU:HD13	1.42	0.84
2:B:1282:THR:OG1	2:B:1387:TYR:CD2	2.30	0.83
2:B:1394:LEU:HD23	2:B:1420:TRP:HZ3	1.44	0.83
3:C:2231:ILE:CD1	3:C:2272:LEU:HD11	2.08	0.83
2:B:1362:VAL:HG12	2:B:1363:LEU:N	1.95	0.81
2:B:1394:LEU:HD23	2:B:1420:TRP:CZ3	2.15	0.81
3:C:2231:ILE:HD11	3:C:2272:LEU:HD11	1.62	0.81
2:B:1284:CYS:N	2:B:1392:CYS:SG	2.51	0.81
3:C:2289:TRP:CZ2	3:C:2297:LEU:HD11	2.17	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2289:TRP:HZ2	3:C:2297:LEU:HD11	1.47	0.80
3:C:2474:ILE:HD12	3:C:2476:PHE:HE2	1.41	0.79
2:B:1304:ARG:HB2	3:C:1936:SER:HB3	1.62	0.79
3:C:1713:THR:HG22	3:C:1722:THR:HG23	1.64	0.79
3:F:2446:LEU:HD23	3:F:2448:LYS:H	1.47	0.78
3:C:1688:GLY:O	3:C:1689:THR:HG23	1.81	0.78
3:C:2490:TRP:CD2	3:F:2577:ASP:HB3	2.18	0.78
3:C:1959:LEU:CD2	3:C:1980:VAL:HG13	2.14	0.78
3:C:2563:GLY:HA3	3:C:2568:THR:HG23	1.65	0.78
3:F:2411:GLY:HA3	3:F:2538:VAL:O	1.82	0.78
3:C:2544:ALA:HB2	3:C:2554:ASP:HB3	1.66	0.77
3:C:1983:ALA:HB3	3:C:1985:PHE:HE1	1.50	0.77
3:C:1972:CYS:SG	3:C:1985:PHE:CE2	2.77	0.77
2:B:1297:VAL:HA	2:B:1317:VAL:HA	1.64	0.76
3:C:1983:ALA:HB3	3:C:1985:PHE:CE1	2.20	0.76
2:B:1398:MET:O	2:B:1398:MET:HG2	1.85	0.76
3:C:1795:ASN:O	3:C:1796:LYS:CG	2.32	0.76
3:C:2415:ILE:HD12	3:C:2431:ILE:HD11	1.66	0.76
3:C:2469:VAL:HG22	3:C:2532:GLY:HA2	1.67	0.76
3:C:2471:LYS:HG2	3:C:2484:ILE:CG1	2.11	0.76
3:C:2044:THR:HG22	3:C:2050:TYR:CD2	2.19	0.76
3:C:1979:TYR:CD2	3:C:1985:PHE:CD2	2.75	0.75
3:F:2461:PRO:HB3	3:F:2465:ASN:HA	1.68	0.75
2:B:1373:TYR:CD1	2:B:1379:VAL:HG22	2.22	0.75
3:C:2415:ILE:HB	3:C:2534:LEU:HB3	1.67	0.75
3:C:2451:PRO:HD2	3:C:2453:TYR:HD2	1.52	0.75
3:C:2474:ILE:HG13	3:C:2481:VAL:HB	1.69	0.75
2:B:1325:SER:H	2:B:1334:VAL:HA	1.53	0.74
3:C:1985:PHE:HB2	3:C:1987:PRO:HD3	1.68	0.74
3:C:2340:LEU:HD13	3:C:2352:CYS:HB2	1.68	0.74
3:C:2410:ARG:HD2	3:C:2540:ASP:HB2	1.70	0.74
3:C:1695:THR:HG1	3:C:1713:THR:HG1	1.30	0.73
3:C:1979:TYR:HD2	3:C:1985:PHE:CD2	2.06	0.73
3:C:2398:GLU:HB3	3:C:2407:GLN:HE22	1.52	0.73
3:C:2527:TRP:HB3	3:C:2535:ASP:H	1.53	0.73
3:C:1700:HIS:HD2	3:C:2313:GLN:HG3	1.44	0.73
3:C:2436:VAL:HB	3:C:2456:LEU:HB3	1.71	0.72
3:C:2440:SER:HG	3:C:2453:TYR:HE1	1.34	0.72
2:B:1530:CYS:HB3	2:B:1534:SER:HB2	1.71	0.72
2:B:1469:PHE:HB3	2:B:1517:ILE:HG23	1.72	0.72
2:B:1589:CYS:HB2	2:B:1596:TYR:HB2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1777:LEU:CD2	3:C:1779:VAL:HG22	2.19	0.72
3:C:1850:THR:HG22	3:C:1865:PRO:HB2	1.71	0.71
3:C:1777:LEU:HD23	3:C:1779:VAL:CG2	2.21	0.71
2:B:1317:VAL:HG22	2:B:1324:ILE:HB	1.72	0.71
3:C:2440:SER:OG	3:C:2453:TYR:HE1	1.74	0.71
3:C:2493:GLY:O	3:F:2454:ARG:NH1	2.24	0.70
3:C:2468:ILE:HD12	3:C:2532:GLY:H	1.57	0.70
2:B:1281:GLY:O	2:B:1392:CYS:N	2.24	0.70
2:B:1324:ILE:HG23	2:B:1334:VAL:HB	1.72	0.70
2:B:1343:LEU:HG	2:B:1356:ASN:HB2	1.73	0.70
2:B:1279:LEU:HD12	2:B:1299:THR:HB	1.74	0.70
3:C:2268:LEU:CG	3:C:2272:LEU:HD22	2.21	0.69
3:F:2544:ALA:H	3:F:2553:PHE:HB3	1.57	0.69
3:C:1664:ASP:HA	3:C:1796:LYS:HA	1.75	0.69
2:B:1264:PHE:HB3	2:B:1398:MET:SD	2.31	0.69
3:C:1959:LEU:HD13	3:C:1965:VAL:HG11	1.73	0.69
3:F:2436:VAL:O	3:F:2436:VAL:HG13	1.93	0.69
3:C:2231:ILE:HD11	3:C:2272:LEU:CD1	2.23	0.69
3:F:2558:THR:HG22	3:F:2558:THR:O	1.92	0.69
3:C:2570:ILE:HG13	3:C:2574:ARG:HD3	1.72	0.68
2:B:1332:GLY:HA2	2:B:1341:MET:H	1.59	0.68
3:C:1688:GLY:O	3:C:1689:THR:CG2	2.42	0.68
3:C:2373:SER:OG	3:C:2509:ARG:NH2	2.27	0.67
3:C:2290:ARG:HH21	3:C:2296:PRO:HA	1.58	0.67
3:C:2225:ASN:CB	3:C:2228:CYS:HB2	2.24	0.67
3:C:1777:LEU:CD2	3:C:1779:VAL:CG2	2.73	0.67
3:C:2469:VAL:HG21	3:C:2528:LEU:HG	1.77	0.67
3:C:2335:CYS:HB3	3:C:2339:PHE:HB2	1.75	0.66
3:C:1979:TYR:HD2	3:C:1985:PHE:CE2	2.13	0.66
2:B:1332:GLY:HA3	2:B:1340:LEU:HB2	1.77	0.66
3:C:2399:ILE:HG23	3:C:2404:ARG:HH21	1.61	0.66
3:C:1843:PRO:HA	3:C:1847:GLY:HA3	1.78	0.66
3:C:2469:VAL:HG11	3:C:2534:LEU:HD12	1.78	0.66
3:C:2519:HIS:HD1	3:C:2525:THR:HG1	1.36	0.66
2:B:1406:GLN:HG3	2:B:1406:GLN:O	1.96	0.66
2:B:1606:THR:HA	2:B:1642:ILE:HG12	1.78	0.66
3:C:2340:LEU:HD12	3:C:2349:ALA:HA	1.78	0.66
3:C:2498:LEU:HD13	3:C:2510:ARG:HD2	1.76	0.66
2:B:1362:VAL:CG1	2:B:1363:LEU:N	2.60	0.65
3:C:2471:LYS:HD3	3:C:2484:ILE:HD11	1.77	0.65
3:F:2509:ARG:HH12	3:F:2512:PRO:HD3	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2044:THR:HG23	3:C:2050:TYR:CE2	2.27	0.65
3:C:2519:HIS:ND1	3:C:2525:THR:OG1	2.26	0.65
3:C:1663:LEU:HD11	3:C:1794:TYR:HA	1.79	0.65
3:C:1670:PHE:HB3	3:C:1809:PRO:HB2	1.78	0.65
3:C:1959:LEU:HB3	3:C:1965:VAL:CG2	2.26	0.65
2:B:1521:ARG:HB3	2:B:1527:GLU:HG2	1.79	0.65
3:C:2389:ALA:HA	3:C:2512:PRO:HG3	1.79	0.65
2:B:1343:LEU:HB3	2:B:1344:PRO:HD3	1.80	0.64
3:C:2225:ASN:HB3	3:C:2228:CYS:CB	2.26	0.64
3:C:2526:VAL:HG22	3:C:2536:VAL:HG22	1.79	0.64
2:B:1325:SER:OG	2:B:1333:LYS:O	2.14	0.64
2:B:1586:GLY:HA3	2:B:1616:PRO:HG2	1.78	0.64
3:C:1678:LEU:HD23	3:C:1696:VAL:HB	1.78	0.64
3:C:2139:LYS:HB2	3:C:2151:SER:HB3	1.80	0.64
3:C:2373:SER:HB3	3:C:2388:GLU:HG2	1.80	0.64
3:C:2435:GLY:N	3:C:2460:GLN:OE1	2.30	0.64
2:B:1333:LYS:HD3	2:B:1639:SER:HA	1.79	0.64
3:C:2574:ARG:NH1	3:C:2576:GLN:HE22	1.96	0.64
2:B:1591:VAL:HG21	2:B:1621:LEU:HD23	1.79	0.64
3:C:2319:LEU:HD12	3:C:2319:LEU:O	1.98	0.64
3:C:1856:LEU:HD21	3:C:1893:TYR:HE2	1.61	0.63
2:B:1333:LYS:H	2:B:1340:LEU:HA	1.62	0.63
2:B:1273:GLY:HA3	2:B:1277:TYR:HE2	1.63	0.63
2:B:1295:PHE:CB	2:B:1319:THR:HG22	2.26	0.63
3:C:2471:LYS:CG	3:C:2484:ILE:HG12	2.17	0.63
3:C:1713:THR:HG22	3:C:1722:THR:CG2	2.28	0.63
3:C:2218:GLU:HA	3:C:2223:GLU:HB2	1.81	0.62
2:B:1362:VAL:HG12	2:B:1363:LEU:H	1.62	0.62
3:C:2077:LEU:HD23	3:C:2086:GLN:HG3	1.81	0.62
3:F:2553:PHE:CG	3:F:2553:PHE:O	2.50	0.62
3:C:1676:TYR:O	3:C:1696:VAL:N	2.31	0.62
3:C:1856:LEU:HG	3:C:1856:LEU:O	1.99	0.62
3:C:1679:SER:HB3	3:C:1777:LEU:HD13	1.81	0.62
3:C:1777:LEU:HD23	3:C:1779:VAL:HG22	1.79	0.62
3:C:2097:VAL:HA	3:C:2109:GLY:HA2	1.80	0.62
3:C:2490:TRP:CE2	3:F:2577:ASP:HB3	2.34	0.62
3:C:1756:ASP:OD1	3:C:1948:ARG:NH2	2.33	0.62
3:C:1965:VAL:HG13	3:C:1966:PRO:HD2	1.81	0.62
3:C:2351:ASP:HB2	3:C:2363:VAL:HB	1.80	0.62
3:C:2570:ILE:CG1	3:C:2574:ARG:HD2	2.23	0.62
3:C:2490:TRP:CG	3:F:2577:ASP:HB3	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2442:ARG:CD	3:C:2450:VAL:HG23	2.30	0.62
2:B:1275:CYS:HA	2:B:1300:LYS:HE2	1.82	0.62
2:B:1370:GLN:HG3	2:B:1382:THR:HB	1.82	0.62
3:C:1677:LEU:HA	3:C:1695:THR:HA	1.82	0.62
3:C:2474:ILE:CD1	3:C:2481:VAL:HB	2.30	0.62
3:F:2434:PRO:HA	3:F:2459:VAL:HB	1.82	0.61
3:C:1856:LEU:HD12	3:C:1904:LEU:HD22	1.80	0.61
3:C:2415:ILE:CD1	3:C:2431:ILE:HD11	2.30	0.61
2:B:1656:GLY:HA3	3:C:1773:SER:HB3	1.82	0.61
3:C:2474:ILE:HD11	3:C:2481:VAL:HB	1.82	0.61
3:C:1849:ILE:HA	3:C:1856:LEU:HD23	1.83	0.61
3:F:2553:PHE:O	3:F:2553:PHE:CD2	2.54	0.61
3:C:2232:ARG:HH22	3:C:2272:LEU:HD12	1.65	0.61
3:C:2518:VAL:CG2	3:C:2526:VAL:HB	2.30	0.61
3:C:1908:ARG:HH21	3:C:1915:LEU:H	1.47	0.61
3:F:2436:VAL:HG22	3:F:2456:LEU:HD23	1.83	0.61
3:C:1849:ILE:HG13	3:C:1850:THR:HG23	1.83	0.61
3:F:2485:PRO:O	3:F:2510:ARG:NH2	2.34	0.61
3:F:2568:THR:HG22	3:F:2568:THR:O	2.01	0.61
3:C:2231:ILE:HD12	3:C:2272:LEU:HD11	1.82	0.60
3:C:2527:TRP:O	3:C:2534:LEU:HG	2.01	0.60
2:B:1548:PRO:HB2	2:B:1551:ALA:H	1.66	0.60
3:F:2509:ARG:NH2	3:F:2511:MET:SD	2.74	0.60
2:B:1541:PRO:O	2:B:1568:GLN:NE2	2.34	0.60
3:C:2211:CYS:SG	3:C:2212:PRO:HD3	2.42	0.60
2:B:1314:GLN:OE1	2:B:1327:HIS:NE2	2.35	0.60
3:F:2478:ASP:HB2	3:F:2503:LEU:HD21	1.83	0.60
2:B:1362:VAL:CG1	2:B:1363:LEU:H	2.15	0.60
2:B:1469:PHE:HB2	2:B:1472:CYS:HB2	1.84	0.60
3:C:2252:ARG:CA	3:C:2255:VAL:HG22	2.17	0.60
2:B:1591:VAL:O	2:B:1594:THR:OG1	2.12	0.59
3:C:1879:VAL:HG23	3:C:2349:ALA:HB1	1.84	0.59
3:C:1937:LEU:HD12	3:C:1937:LEU:C	2.22	0.59
2:B:1292:LEU:HG	2:B:1294:PRO:HD3	1.83	0.59
3:C:1979:TYR:CD2	3:C:1985:PHE:CE2	2.89	0.59
3:F:2424:PHE:HE2	3:F:2546:LEU:HD11	1.68	0.59
3:F:2576:GLN:HA	3:F:2579:SER:HB3	1.83	0.59
3:C:2268:LEU:CD1	3:C:2272:LEU:HB2	2.27	0.59
3:C:2372:CYS:SG	3:C:2406:CYS:HB3	2.43	0.59
3:C:1857:ALA:O	3:C:1860:HIS:HB2	2.03	0.58
3:C:2544:ALA:HA	3:C:2552:ASN:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2453:TYR:O	3:C:2453:TYR:CD1	2.56	0.58
3:C:2147:HIS:CG	3:C:2274:ALA:HB1	2.39	0.58
3:C:2374:GLU:HB3	3:C:2387:HIS:O	2.03	0.58
2:B:1371:VAL:HB	2:B:1381:VAL:HG13	1.86	0.58
3:C:2265:LYS:O	3:C:2270:ARG:NH1	2.37	0.58
3:C:2570:ILE:HA	3:C:2574:ARG:HB2	1.85	0.58
3:F:2436:VAL:CG2	3:F:2456:LEU:HB3	2.33	0.58
3:C:2511:MET:N	3:C:2515:SER:O	2.28	0.58
2:B:1396:GLY:HA3	2:B:1405:ASP:HB3	1.85	0.58
3:C:1849:ILE:HA	3:C:1856:LEU:CD2	2.34	0.58
3:C:2529:GLY:HA3	3:C:2533:LEU:HD12	1.86	0.57
3:C:2468:ILE:HD12	3:C:2532:GLY:N	2.19	0.57
3:C:2514:GLY:HA3	3:C:2530:LYS:HD3	1.86	0.57
2:B:1457:PHE:HA	2:B:1499:LEU:HD22	1.86	0.57
3:C:2474:ILE:HG13	3:C:2474:ILE:O	2.05	0.57
2:B:1581:VAL:HG22	2:B:1585:GLY:HA3	1.86	0.57
3:F:2472:VAL:HG11	3:F:2526:VAL:HG21	1.86	0.57
3:C:2563:GLY:CA	3:C:2568:THR:HG23	2.33	0.57
1:A:1253:CYS:O	2:B:1381:VAL:N	2.31	0.57
3:C:2424:PHE:HB3	3:C:2553:PHE:CD2	2.40	0.57
2:B:1298:THR:N	2:B:1316:THR:O	2.23	0.56
3:C:1937:LEU:O	3:C:1937:LEU:CD1	2.47	0.56
3:C:2529:GLY:H	3:C:2533:LEU:HB2	1.70	0.56
1:A:1255:LEU:HB3	2:B:1379:VAL:CB	2.24	0.56
3:F:2450:VAL:HG21	3:F:2542:LEU:HD11	1.87	0.56
3:C:2040:LEU:HB2	3:C:2053:HIS:HA	1.87	0.56
3:F:2446:LEU:CD1	3:F:2545:MET:HA	2.36	0.56
2:B:1463:PRO:HG2	3:F:2565:GLN:HB2	1.88	0.56
3:C:2484:ILE:HG22	3:C:2486:SER:H	1.71	0.56
3:C:1700:HIS:NE2	3:C:2313:GLN:CG	2.64	0.56
3:C:2268:LEU:CD1	3:C:2272:LEU:CD2	2.70	0.56
3:C:2110:GLU:HB3	3:C:2399:ILE:HG21	1.86	0.56
3:C:2290:ARG:HD2	3:C:2297:LEU:HG	1.88	0.56
3:C:2442:ARG:HD2	3:C:2450:VAL:HG23	1.86	0.56
2:B:1347:LEU:HD23	2:B:1349:GLY:H	1.71	0.55
2:B:1351:ARG:NH2	2:B:1554:THR:OG1	2.39	0.55
3:F:2428:HIS:CG	4:F:2601:NAG:H62	2.41	0.55
3:C:1856:LEU:HD12	3:C:1904:LEU:CD2	2.36	0.55
3:C:2458:ASP:OD2	3:C:2471:LYS:HE2	2.05	0.55
3:C:2520:GLN:HB3	3:C:2523:GLY:CA	2.34	0.55
3:C:2318:ALA:HB3	3:C:2355:VAL:HG11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2232:ARG:NH2	3:C:2272:LEU:HD12	2.22	0.55
3:C:2448:LYS:HE2	3:C:2542:LEU:HA	1.88	0.55
3:C:2376:CYS:HA	3:C:2386:CYS:HA	1.90	0.54
2:B:1365:THR:HG22	2:B:1369:LEU:H	1.72	0.54
3:F:2420:ASN:HB2	4:F:2601:NAG:H2	1.89	0.54
2:B:1649:ILE:HG12	3:C:1780:PRO:HA	1.89	0.54
3:C:1723:LEU:HD22	3:C:1757:VAL:HG21	1.88	0.54
3:F:2489:ALA:O	3:F:2495:ARG:HA	2.07	0.54
3:F:2509:ARG:NH1	3:F:2510:ARG:O	2.41	0.54
2:B:1259:PRO:HG3	2:B:1311:TYR:HA	1.90	0.54
2:B:1365:THR:OG1	2:B:1366:ASP:OD1	2.25	0.54
3:C:2442:ARG:HG3	3:C:2450:VAL:HG21	1.90	0.54
2:B:1296:THR:O	2:B:1318:THR:N	2.33	0.54
3:C:2304:HIS:CE1	3:C:2336:ASP:HB3	2.43	0.54
2:B:1270:ASP:O	2:B:1272:GLN:NE2	2.40	0.54
3:C:1714:LEU:CD2	3:C:1759:VAL:HG11	2.38	0.54
3:C:1979:TYR:HB2	3:C:1985:PHE:CE2	2.39	0.54
3:C:2304:HIS:HE1	3:C:2336:ASP:HB3	1.73	0.54
3:C:1688:GLY:C	3:C:1689:THR:HG23	2.28	0.54
2:B:1588:GLY:HA2	2:B:1596:TYR:O	2.08	0.53
1:A:1255:LEU:N	2:B:1379:VAL:O	2.34	0.53
2:B:1314:GLN:HA	2:B:1326:ILE:O	2.08	0.53
3:C:1995:CYS:HA	3:C:2005:CYS:HA	1.90	0.53
3:C:2253:GLN:NE2	3:C:2257:ASP:OD1	2.42	0.53
3:C:2443:CYS:H	3:C:2546:LEU:HA	1.72	0.53
3:C:2363:VAL:HG23	3:C:2380:PRO:HD3	1.91	0.53
3:F:2558:THR:O	3:F:2558:THR:CG2	2.56	0.53
2:B:1278:LEU:HB2	2:B:1424:TRP:HB3	1.91	0.53
2:B:1362:VAL:CG2	2:B:1372:THR:HB	2.31	0.53
3:C:1679:SER:CB	3:C:1777:LEU:HD13	2.39	0.53
3:C:2115:PRO:HB3	3:C:2343:HIS:HB3	1.90	0.53
3:C:2461:PRO:HA	3:C:2467:LYS:H	1.73	0.53
3:F:2511:MET:N	3:F:2515:SER:O	2.38	0.53
2:B:1323:ASN:HD21	2:B:1336:VAL:HG13	1.74	0.53
3:C:2448:LYS:NZ	3:C:2545:MET:SD	2.68	0.53
3:C:1676:TYR:N	3:C:1696:VAL:O	2.36	0.53
3:C:2112:VAL:HG13	3:C:2402:GLY:HA3	1.89	0.53
3:C:2410:ARG:CD	3:C:2540:ASP:HB2	2.37	0.53
2:B:1374:ASP:OD1	2:B:1375:TRP:N	2.42	0.53
3:C:2305:TYR:HA	3:C:2333:CYS:HA	1.90	0.53
3:C:2415:ILE:HD13	3:C:2421:LEU:HG	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2528:LEU:HA	3:C:2533:LEU:O	2.09	0.53
1:A:1255:LEU:CB	2:B:1379:VAL:HB	2.28	0.52
3:C:2174:ASP:HB2	4:C:2604:NAG:H82	1.90	0.52
3:C:2438:GLU:HA	3:C:2455:VAL:O	2.09	0.52
3:C:1777:LEU:HD23	3:C:1779:VAL:HG23	1.92	0.52
2:B:1407:VAL:N	2:B:1420:TRP:HE1	2.07	0.52
3:C:1959:LEU:HB3	3:C:1965:VAL:HG21	1.90	0.52
3:C:1682:CYS:HB2	3:C:1786:THR:HB	1.91	0.52
3:C:1743:HIS:NE2	3:C:1937:LEU:HD11	2.24	0.52
2:B:1323:ASN:H	2:B:1336:VAL:HG22	1.74	0.52
3:C:2451:PRO:HD2	3:C:2453:TYR:HE2	1.72	0.52
2:B:1374:ASP:HB3	2:B:1378:ARG:HB3	1.90	0.52
2:B:1469:PHE:N	2:B:1518:GLU:OE2	2.43	0.51
2:B:1549:PRO:HA	2:B:1590:TRP:CD1	2.45	0.51
3:C:2086:GLN:NE2	3:C:2146:ALA:O	2.43	0.51
1:A:1254:TRP:O	2:B:1262:ASN:N	2.44	0.51
2:B:1277:TYR:HA	2:B:1425:GLN:HA	1.91	0.51
3:C:1764:GLY:HA3	3:C:1780:PRO:HB3	1.91	0.51
3:C:1924:GLN:NE2	3:C:1926:CYS:O	2.44	0.51
3:C:2511:MET:HG3	3:C:2527:TRP:CH2	2.46	0.51
2:B:1368:GLY:C	2:B:1384:PRO:HB3	2.30	0.51
3:C:2177:LEU:HG	3:C:2178:PRO:HD2	1.93	0.51
2:B:1511:GLN:HE21	2:B:1563:CYS:HB3	1.75	0.51
3:C:1862:LEU:HD12	3:C:1902:ALA:HB2	1.93	0.51
3:C:2439:LEU:HD11	3:C:2457:ALA:HB2	1.92	0.51
3:C:2100:ALA:HB3	3:C:2142:PHE:HB3	1.92	0.51
2:B:1599:GLY:HA2	2:B:1614:CYS:HB3	1.93	0.51
3:C:1673:THR:HG22	3:C:1700:HIS:HB3	1.92	0.51
3:C:1986:TYR:CZ	3:C:1994:LEU:HD13	2.46	0.51
3:C:2567:LYS:HB2	3:C:2571:GLU:H	1.74	0.51
3:C:2194:ARG:HH22	3:C:2201:GLY:HA2	1.75	0.51
2:B:1278:LEU:O	2:B:1394:LEU:N	2.44	0.50
3:C:2098:GLY:H	3:C:2109:GLY:H	1.58	0.50
3:C:2497:ASP:N	3:C:2497:ASP:OD1	2.44	0.50
3:F:2567:LYS:HG3	3:F:2569:PRO:HG3	1.92	0.50
2:B:1511:GLN:OE1	2:B:1565:GLU:N	2.44	0.50
3:C:2099:LEU:HD23	3:C:2132:LEU:HB2	1.93	0.50
3:C:1795:ASN:C	3:C:1796:LYS:HG2	2.29	0.50
3:C:1849:ILE:HD11	3:C:1869:PHE:HA	1.92	0.50
3:C:2092:VAL:HG21	3:C:2134:THR:HG21	1.93	0.50
3:C:2396:VAL:HB	3:C:2537:MET:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1634:CYS:SG	2:B:1642:ILE:HG22	2.52	0.50
2:B:1654:ALA:HB3	3:C:1775:VAL:HG13	1.93	0.50
3:C:2525:THR:O	3:C:2536:VAL:HA	2.12	0.50
3:C:1924:GLN:O	3:C:1949:GLU:HA	2.11	0.50
3:F:2567:LYS:CG	3:F:2569:PRO:HG3	2.42	0.50
3:F:2398:GLU:OE2	3:F:2400:GLN:NE2	2.44	0.50
2:B:1398:MET:O	2:B:1398:MET:CG	2.57	0.50
3:C:1672:GLY:N	3:C:1707:SER:OG	2.45	0.50
3:C:2442:ARG:HG3	3:C:2450:VAL:CG2	2.42	0.50
3:C:1894:VAL:HG21	3:C:1907:TRP:CD1	2.47	0.49
3:C:1979:TYR:CD2	3:C:1985:PHE:CG	3.00	0.49
1:A:1254:TRP:HB3	2:B:1262:ASN:HB3	1.95	0.49
2:B:1369:LEU:HG	2:B:1384:PRO:HD3	1.93	0.49
3:C:2458:ASP:OD1	3:C:2470:SER:OG	2.30	0.49
3:C:2231:ILE:HA	3:C:2236:GLY:HA3	1.94	0.49
3:C:2411:GLY:HA3	3:C:2538:VAL:HG12	1.94	0.49
3:C:2501:THR:HG23	3:C:2507:SER:CA	2.23	0.49
3:F:2524:VAL:HG23	3:F:2538:VAL:HG22	1.93	0.49
1:A:1254:TRP:N	2:B:1262:ASN:O	2.40	0.49
3:C:1844:ASP:OD1	3:C:1844:ASP:N	2.45	0.49
3:C:1921:SER:HB3	3:C:1951:CYS:HB3	1.94	0.49
2:B:1409:PRO:HD3	2:B:1424:TRP:CD1	2.47	0.49
2:B:1460:PRO:HG3	2:B:1523:GLN:HE22	1.77	0.49
2:B:1416:SER:OG	2:B:1419:THR:OG1	2.30	0.49
3:C:1959:LEU:HB3	3:C:1965:VAL:HG23	1.94	0.49
3:C:2537:MET:SD	3:C:2537:MET:N	2.86	0.49
3:C:2453:TYR:HB2	3:C:2476:PHE:CD1	2.48	0.48
3:F:2411:GLY:CA	3:F:2538:VAL:O	2.57	0.48
2:B:1356:ASN:HA	2:B:1361:ALA:HA	1.95	0.48
3:C:2238:PHE:CD1	3:C:2289:TRP:HA	2.48	0.48
3:F:2472:VAL:HG23	3:F:2528:LEU:HD22	1.94	0.48
3:C:2453:TYR:HB2	3:C:2476:PHE:HD1	1.78	0.48
2:B:1452:TYR:OH	2:B:1494:GLY:O	2.30	0.48
3:C:2280:GLN:HE22	3:C:2331:GLU:H	1.61	0.48
3:C:2474:ILE:HD11	3:C:2481:VAL:CB	2.43	0.48
3:C:2454:ARG:HH12	3:F:2493:GLY:HA3	1.78	0.48
3:C:1784:ALA:HA	3:C:1794:TYR:HB3	1.95	0.48
3:C:1832:CYS:SG	3:C:1878:GLN:NE2	2.87	0.48
3:C:2054:GLY:HA3	3:C:2058:TYR:HE2	1.78	0.48
2:B:1583:LEU:H	2:B:1583:LEU:HD22	1.79	0.48
2:B:1632:GLU:HG3	2:B:1646:PRO:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2471:LYS:HD3	3:C:2484:ILE:CD1	2.42	0.48
3:C:2490:TRP:CD2	3:F:2577:ASP:CB	2.94	0.48
3:C:1962:ASP:OD1	3:C:1962:ASP:N	2.47	0.48
2:B:1417:ILE:N	2:B:1418:PRO:HD2	2.28	0.48
3:C:1826:GLU:HG3	3:C:1829:PRO:HG3	1.95	0.48
2:B:1366:ASP:OD1	2:B:1366:ASP:N	2.48	0.47
2:B:1377:TRP:HE1	2:B:1501:GLN:HG2	1.77	0.47
3:C:1774:PHE:CG	3:C:1892:THR:HG23	2.48	0.47
3:C:2045:LEU:HD22	3:C:2166:ASN:HA	1.96	0.47
3:F:2484:ILE:HD13	3:F:2490:TRP:HD1	1.79	0.47
2:B:1270:ASP:N	2:B:1270:ASP:OD1	2.47	0.47
3:C:2012[A]:GLU:HG2	3:C:2013:PRO:HD2	1.96	0.47
3:C:2218:GLU:HG2	3:C:2223:GLU:HB3	1.96	0.47
3:C:2400:GLN:O	3:C:2403:VAL:HG12	2.14	0.47
3:C:2525:THR:HB	3:C:2537:MET:HB2	1.96	0.47
3:F:2471:LYS:HG2	3:F:2484:ILE:HG13	1.95	0.47
2:B:1345:VAL:HG23	2:B:1594:THR:HA	1.95	0.47
2:B:1352:ILE:HA	2:B:1365:THR:HA	1.95	0.47
2:B:1655:TRP:HB3	3:C:1659:HIS:O	2.14	0.47
3:C:1678:LEU:HA	3:C:1790:LEU:HB3	1.97	0.47
3:C:1760:ASN:HD22	3:C:1941:VAL:HG21	1.79	0.47
3:C:2225:ASN:CB	3:C:2228:CYS:CB	2.90	0.47
2:B:1315:VAL:O	2:B:1325:SER:HA	2.15	0.47
2:B:1361:ALA:HB2	2:B:1375:TRP:CH2	2.50	0.47
3:C:1750:VAL:HG22	3:C:1759:VAL:HG13	1.96	0.47
3:C:1972:CYS:SG	3:C:1985:PHE:HE2	2.36	0.47
3:C:1744:LEU:HG	3:C:1745:ASP:H	1.80	0.47
3:C:2438:GLU:OE1	3:C:2573:TRP:HA	2.15	0.47
2:B:1283:LEU:HD23	2:B:1286:GLY:HA2	1.96	0.47
3:C:2451:PRO:HG3	3:C:2520:GLN:HE22	1.80	0.47
3:F:2469:VAL:HG21	3:F:2534:LEU:HD23	1.97	0.47
3:C:2060:LEU:HA	3:C:2163:LEU:HB2	1.96	0.47
3:F:2424:PHE:CE2	3:F:2546:LEU:HD11	2.49	0.47
1:A:1257:GLY:HA3	2:B:1377:TRP:HB2	1.96	0.47
3:C:2366:SER:HB3	3:C:2375:ARG:HD2	1.95	0.47
2:B:1345:VAL:O	2:B:1353:SER:HA	2.14	0.46
3:C:1979:TYR:CB	3:C:1985:PHE:CE2	2.91	0.46
3:C:2336:ASP:O	3:C:2339:PHE:HB3	2.15	0.46
2:B:1372:THR:N	2:B:1380:ASP:O	2.46	0.46
2:B:1540:GLY:N	2:B:1563:CYS:SG	2.89	0.46
3:C:2170:ASN:OD1	3:C:2170:ASN:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2440:SER:H	3:C:2455:VAL:HG22	1.81	0.46
3:F:2515:SER:OG	3:F:2516:MET:N	2.48	0.46
3:F:2572:LYS:HE3	3:F:2572:LYS:HB2	1.50	0.46
1:A:1258:ASP:O	2:B:1260:HIS:ND1	2.40	0.46
3:C:2356:HIS:NE2	3:C:2376:CYS:SG	2.88	0.46
4:A:1301:NAG:O6	2:B:1370:GLN:OE1	2.33	0.46
2:B:1273:GLY:HA3	2:B:1277:TYR:CE2	2.48	0.46
3:C:2100:ALA:HB3	3:C:2142:PHE:CD2	2.50	0.46
3:C:2319:LEU:HD12	3:C:2319:LEU:C	2.35	0.46
3:C:2351:ASP:HB3	4:C:2601:NAG:H82	1.97	0.46
3:C:1669:ASP:OD1	3:C:1670:PHE:N	2.49	0.46
3:C:1675:GLU:HA	3:C:1697:ALA:HA	1.97	0.46
3:C:1856:LEU:HD21	3:C:1893:TYR:CE2	2.48	0.46
2:B:1478:PRO:HB3	2:B:1506:TYR:CZ	2.50	0.46
2:B:1576:SER:HB3	2:B:1595:TYR:OH	2.16	0.46
2:B:1612:CYS:HA	2:B:1623:CYS:HA	1.98	0.46
3:C:2317:ALA:HB1	3:C:2319:LEU:HG	1.97	0.46
3:C:1660:TYR:HE1	3:C:1668:PHE:CZ	2.34	0.45
3:C:1887:CYS:N	3:C:1913:CYS:SG	2.89	0.45
3:C:1965:VAL:CG1	3:C:1966:PRO:HD2	2.47	0.45
1:A:1255:LEU:HD13	2:B:1261:TYR:CD2	2.51	0.45
2:B:1464:GLY:O	2:B:1467:SER:OG	2.28	0.45
2:B:1655:TRP:HB3	3:C:1660:TYR:HA	1.97	0.45
3:C:2414:SER:O	3:C:2421:LEU:HA	2.17	0.45
3:C:2421:LEU:HD12	3:C:2431:ILE:CD1	2.45	0.45
3:C:2458:ASP:HB3	3:C:2471:LYS:O	2.16	0.45
1:A:1256:TRP:CZ3	2:B:1481:PHE:HA	2.51	0.45
2:B:1328:LYS:HD2	2:B:1377:TRP:CE3	2.50	0.45
3:C:1721:LEU:HB3	3:C:1731:LEU:HD11	1.98	0.45
2:B:1365:THR:OG1	2:B:1366:ASP:N	2.49	0.45
3:C:2474:ILE:CD1	3:C:2476:PHE:HE2	2.06	0.45
3:C:2264:ASP:N	3:C:2264:ASP:OD1	2.50	0.45
2:B:1655:TRP:H	3:C:1660:TYR:HB3	1.82	0.45
3:C:1959:LEU:HD22	3:C:1965:VAL:HG21	1.99	0.45
3:F:2414:SER:HA	3:F:2535:ASP:HA	1.97	0.45
3:F:2491:VAL:HG21	3:F:2502:VAL:HG11	1.99	0.45
2:B:1372:THR:O	2:B:1372:THR:HG23	2.16	0.45
2:B:1550:PRO:O	2:B:1552:ARG:NH1	2.50	0.45
3:C:1676:TYR:HA	3:C:1813:LYS:HA	1.99	0.45
3:C:1740:LEU:CD2	3:C:1752:ILE:HB	2.47	0.45
3:C:2474:ILE:HD11	3:C:2481:VAL:CG1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2484:ILE:HG22	3:F:2487:LYS:H	1.82	0.45
3:C:1701:ARG:HH21	3:C:2318:ALA:HA	1.82	0.44
3:C:2450:VAL:CG1	3:C:2542:LEU:HD23	2.47	0.44
3:F:2436:VAL:CG2	3:F:2456:LEU:HD23	2.47	0.44
3:C:1863:VAL:HG21	3:C:1897:CYS:HA	1.97	0.44
3:C:1979:TYR:CG	3:C:1985:PHE:CE1	3.05	0.44
3:C:2075:ILE:HD12	3:C:2150:MET:SD	2.58	0.44
2:B:1384:PRO:HG2	2:B:1386:SER:OG	2.17	0.44
3:C:1897:CYS:SG	3:C:1904:LEU:HD11	2.56	0.44
3:C:2335:CYS:HB2	3:C:2341:LEU:HD21	1.99	0.44
3:C:1695:THR:O	3:C:1712:VAL:HA	2.18	0.44
3:C:2128:ARG:HB2	3:C:2331:GLU:OE1	2.16	0.44
2:B:1282:THR:CB	2:B:1387:TYR:CD2	3.01	0.44
3:C:1852:PRO:HA	3:C:1860:HIS:CD2	2.53	0.44
3:C:2423:THR:CG2	3:C:2551:GLY:H	2.31	0.44
3:C:2490:TRP:CD1	3:F:2577:ASP:HB3	2.53	0.44
3:F:2468:ILE:HD12	3:F:2532:GLY:HA3	1.99	0.44
3:C:2448:LYS:HG2	3:C:2449:ASN:H	1.81	0.44
3:C:2469:VAL:HG21	3:C:2528:LEU:CG	2.46	0.44
3:C:2206:CYS:HB2	3:C:2209:GLN:HA	2.00	0.44
2:B:1302:GLU:HB2	2:B:1313:ARG:HB2	1.99	0.43
2:B:1521:ARG:HD2	2:B:1536:TYR:CZ	2.53	0.43
3:C:1691:TYR:CE2	4:C:2603:NAG:H62	2.53	0.43
3:F:2452:TRP:HZ2	3:F:2454:ARG:HD2	1.82	0.43
3:C:1758:VAL:HA	3:C:1767:LEU:O	2.18	0.43
3:C:2040:LEU:HD12	3:C:2041:HIS:N	2.33	0.43
3:C:2105:VAL:HG12	3:C:2130:ILE:HG12	2.00	0.43
3:C:2268:LEU:O	3:C:2272:LEU:CB	2.66	0.43
3:C:2317:ALA:CB	3:C:2319:LEU:HG	2.49	0.43
3:C:2379:SER:HB3	3:C:2382:ASN:O	2.18	0.43
3:F:2543:ALA:HA	3:F:2553:PHE:HB3	2.00	0.43
3:C:1959:LEU:HD13	3:C:1965:VAL:HG21	2.00	0.43
2:B:1369:LEU:N	2:B:1384:PRO:HB3	2.33	0.43
3:C:1864:PRO:HA	3:C:1865:PRO:HD3	1.91	0.43
3:C:1923:TYR:HA	3:C:1950:GLY:O	2.18	0.43
3:C:2268:LEU:O	3:C:2272:LEU:HB3	2.19	0.43
3:C:2328:ARG:NH2	3:C:2329:CYS:SG	2.84	0.43
3:C:2391:CYS:SG	3:C:2395:HIS:HB2	2.59	0.43
3:C:2031:CYS:HA	3:C:2153:PRO:HA	2.00	0.43
3:C:2214:CYS:O	3:C:2218:GLU:HG3	2.18	0.43
3:C:2374:GLU:HB2	3:C:2389:ALA:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2423:THR:C	3:F:2425:ASP:H	2.21	0.43
3:F:2525:THR:HG23	3:F:2537:MET:HB2	2.00	0.43
2:B:1284:CYS:SG	2:B:1285:PRO:HD3	2.59	0.43
2:B:1573:PHE:HB2	2:B:1580:CYS:SG	2.59	0.43
3:C:2439:LEU:HA	3:C:2549:ALA:HB3	2.00	0.43
3:C:2458:ASP:HB2	3:C:2473:HIS:HD2	1.84	0.43
3:F:2436:VAL:O	3:F:2436:VAL:CG1	2.64	0.43
2:B:1374:ASP:CB	2:B:1378:ARG:HB3	2.48	0.43
3:C:2124:THR:HB	3:C:2131:VAL:HG12	2.01	0.43
3:F:2481:VAL:HG13	3:F:2491:VAL:HG13	2.01	0.43
3:F:2433:SER:HG	3:F:2437:TYR:HH	1.45	0.43
3:F:2473:HIS:HB3	3:F:2480:LEU:HD11	2.01	0.42
3:C:1790:LEU:HD13	3:C:1812:TRP:HD1	1.83	0.42
3:C:2506:VAL:HG23	3:C:2518:VAL:HB	2.00	0.42
3:F:2455:VAL:HG12	3:F:2474:ILE:HG23	2.01	0.42
2:B:1656:GLY:CA	3:C:1773:SER:HB3	2.49	0.42
3:C:2056:CYS:SG	3:C:2202:CYS:N	2.91	0.42
3:C:2469:VAL:HG21	3:C:2528:LEU:CD1	2.49	0.42
3:C:2483:VAL:HA	3:C:2489:ALA:HA	2.02	0.42
2:B:1367:PHE:HB3	2:B:1386:SER:HB3	2.00	0.42
3:C:1756:ASP:CG	3:C:1770:ASP:HB3	2.39	0.42
2:B:1298:THR:OG1	2:B:1316:THR:HB	2.20	0.42
3:C:2099:LEU:CD2	3:C:2132:LEU:HB2	2.49	0.42
3:C:2364:ASN:ND2	4:C:2601:NAG:H62	2.35	0.42
3:C:2438:GLU:HG3	3:C:2454:ARG:HG3	2.02	0.42
3:C:2570:ILE:HG23	3:C:2571:GLU:N	2.35	0.42
3:C:1986:TYR:N	3:C:1987:PRO:CD	2.82	0.42
2:B:1359:SER:O	2:B:1378:ARG:NH1	2.52	0.42
3:C:1694:VAL:HA	3:C:1713:THR:O	2.20	0.42
3:C:1922:HIS:O	3:C:1951:CYS:HA	2.20	0.42
3:C:2226:ASP:O	3:C:2230:LYS:HG2	2.19	0.42
3:C:2256:TYR:O	3:C:2256:TYR:CG	2.73	0.42
3:C:2317:ALA:HB2	3:C:2360:TYR:CD1	2.55	0.42
3:C:2317:ALA:HB2	3:C:2360:TYR:HB2	2.01	0.42
2:B:1642:ILE:H	2:B:1642:ILE:HD12	1.85	0.42
3:C:2065:HIS:HB2	3:C:2159:ARG:HG2	2.02	0.42
2:B:1323:ASN:ND2	2:B:1336:VAL:HG13	2.33	0.42
2:B:1573:PHE:HB3	2:B:1581:VAL:O	2.20	0.42
3:C:1717:TYR:CD2	3:C:1747:LYS:HD3	2.54	0.42
3:C:2268:LEU:HD11	3:C:2272:LEU:CG	2.48	0.42
3:C:2421:LEU:HD12	3:C:2431:ILE:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1595:TYR:HE1	2:B:1597:GLU:HB3	1.85	0.41
3:C:2371:ASP:OD2	3:C:2509:ARG:NE	2.38	0.41
3:F:2446:LEU:HD11	3:F:2545:MET:HA	1.99	0.41
3:C:2506:VAL:HG22	3:C:2508:VAL:HG23	2.02	0.41
2:B:1478:PRO:HB3	2:B:1506:TYR:CE1	2.54	0.41
3:C:2399:ILE:HA	3:C:2403:VAL:O	2.20	0.41
3:F:2483:VAL:HB	3:F:2516:MET:SD	2.60	0.41
2:B:1611:ARG:HH21	2:B:1627:SER:C	2.24	0.41
3:C:1732:GLN:OE1	3:C:1736:GLU:N	2.54	0.41
3:C:2480:LEU:HD22	3:F:2480:LEU:HD22	2.02	0.41
2:B:1279:LEU:O	2:B:1394:LEU:N	2.53	0.41
3:C:1756:ASP:CG	3:C:1776:ARG:HH22	2.23	0.41
3:C:1954:ASP:OD1	3:C:1954:ASP:N	2.51	0.41
3:C:2374:GLU:N	3:C:2389:ALA:O	2.53	0.41
3:C:2526:VAL:HG13	3:C:2534:LEU:HD21	2.03	0.41
2:B:1530:CYS:HA	2:B:1531:PRO:HD3	1.86	0.41
2:B:1576:SER:OG	2:B:1587:CYS:SG	2.67	0.41
3:C:1849:ILE:HD11	3:C:1869:PHE:HD1	1.86	0.41
3:C:1857:ALA:HA	3:C:1860:HIS:CD2	2.56	0.41
1:A:1254:TRP:HA	2:B:1380:ASP:HA	2.03	0.41
3:C:1679:SER:HA	3:C:1789:GLY:HA3	2.02	0.41
3:C:2567:LYS:O	3:C:2572:LYS:N	2.50	0.41
1:A:1249:TYR:HH	2:B:1388:HIS:CG	2.38	0.41
2:B:1549:PRO:HG2	2:B:1550:PRO:HD3	2.02	0.41
3:C:2340:LEU:HD23	3:C:2340:LEU:HA	1.86	0.41
3:C:2343:HIS:O	3:C:2343:HIS:ND1	2.53	0.41
3:C:2424:PHE:HB3	3:C:2553:PHE:CG	2.55	0.41
3:C:2440:SER:H	3:C:2455:VAL:CG2	2.33	0.41
3:C:2470:SER:O	3:C:2485:PRO:HD2	2.21	0.41
3:F:2556:ASP:HB3	3:F:2559:ASN:OD1	2.21	0.41
2:B:1328:LYS:HD2	2:B:1377:TRP:HE3	1.85	0.41
2:B:1333:LYS:HD2	2:B:1333:LYS:HA	1.90	0.41
3:C:2040:LEU:H	3:C:2040:LEU:HG	1.72	0.41
2:B:1447:ASP:OD1	2:B:1448:ARG:N	2.53	0.40
2:B:1607:THR:HG23	2:B:1609:SER:H	1.86	0.40
3:C:2212:PRO:HB3	3:C:2256:TYR:OH	2.21	0.40
3:C:2268:LEU:HD11	3:C:2272:LEU:HD13	2.02	0.40
3:C:2458:ASP:HB3	3:C:2471:LYS:C	2.40	0.40
2:B:1597:GLU:OE1	2:B:1597:GLU:N	2.54	0.40
3:C:1740:LEU:HD23	3:C:1752:ILE:HB	2.02	0.40
3:C:2141:LEU:HD23	3:C:2142:PHE:N	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2351:ASP:HB2	3:C:2363:VAL:CB	2.48	0.40
3:C:2469:VAL:HG22	3:C:2532:GLY:CA	2.43	0.40
3:F:2460:GLN:HG3	3:F:2462:CYS:H	1.87	0.40
3:F:2497:ASP:OD1	3:F:2497:ASP:N	2.55	0.40
2:B:1372:THR:CG2	2:B:1380:ASP:HB3	2.51	0.40
2:B:1651:GLU:OE2	3:C:1776:ARG:HD2	2.21	0.40
3:C:2085:PRO:HA	3:C:2146:ALA:HB2	2.03	0.40
3:C:2415:ILE:HB	3:C:2534:LEU:HD22	2.04	0.40
3:C:2112:VAL:HG22	3:C:2402:GLY:O	2.22	0.40
3:C:2134:THR:OG1	3:C:2136:LYS:O	2.37	0.40
3:C:2053:HIS:O	3:C:2053:HIS:ND1	2.54	0.40
3:C:2112:VAL:HG22	3:C:2402:GLY:HA3	2.02	0.40
3:C:2267:TYR:CG	3:C:2268:LEU:N	2.90	0.40
3:C:2307:ILE:H	3:C:2307:ILE:HG13	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	11/1232 (1%)	10 (91%)	1 (9%)	0	100	100
2	B	397/399 (100%)	366 (92%)	31 (8%)	0	100	100
3	C	926/930 (100%)	858 (93%)	68 (7%)	0	100	100
3	F	193/930 (21%)	177 (92%)	16 (8%)	0	100	100
All	All	1527/3491 (44%)	1411 (92%)	116 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	12/1023 (1%)	12 (100%)	0	100	100
2	B	322/322 (100%)	308 (96%)	14 (4%)	25	49
3	C	748/750 (100%)	694 (93%)	54 (7%)	12	36
3	F	159/750 (21%)	150 (94%)	9 (6%)	17	43
All	All	1241/2845 (44%)	1164 (94%)	77 (6%)	18	40

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1284	CYS
2	B	1317	VAL
2	B	1321	ASN
2	B	1369	LEU
2	B	1405	ASP
2	B	1472	CYS
2	B	1539	CYS
2	B	1547	CYS
2	B	1549	PRO
2	B	1563	CYS
2	B	1569	CYS
2	B	1574	VAL
2	B	1580	CYS
2	B	1589	CYS
3	C	1674	CYS
3	C	1723	LEU
3	C	1774	PHE
3	C	1775	VAL
3	C	1793	ASN
3	C	1799	ASN
3	C	1800	ASP
3	C	1802	LEU
3	C	1820	CYS
3	C	1828	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1832	CYS
3	C	1846	CYS
3	C	1872	CYS
3	C	1877	CYS
3	C	1882	HIS
3	C	1897	CYS
3	C	1911	ASP
3	C	1913	CYS
3	C	1926	CYS
3	C	1934	CYS
3	C	1970	CYS
3	C	1972	CYS
3	C	1973	LEU
3	C	2011	CYS
3	C	2040	LEU
3	C	2056	CYS
3	C	2064	CYS
3	C	2095	GLN
3	C	2099	LEU
3	C	2164	CYS
3	C	2170	ASN
3	C	2202	CYS
3	C	2220	GLN
3	C	2241	CYS
3	C	2279	CYS
3	C	2295	CYS
3	C	2305	TYR
3	C	2312	CYS
3	C	2313	GLN
3	C	2316	CYS
3	C	2322	LEU
3	C	2329	CYS
3	C	2336	ASP
3	C	2346	CYS
3	C	2384	LEU
3	C	2397	CYS
3	C	2436	VAL
3	C	2443	CYS
3	C	2524	VAL
3	C	2540	ASP
3	C	2546	LEU
3	C	2553	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	2562	TYR
3	C	2576	GLN
3	F	2395	HIS
3	F	2406	CYS
3	F	2415	ILE
3	F	2425	ASP
3	F	2542	LEU
3	F	2546	LEU
3	F	2559	ASN
3	F	2572	LYS
3	F	2581	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1523	GLN
3	C	1659	HIS
3	C	2147	HIS
3	C	2225	ASN
3	C	2280	GLN
3	C	2304	HIS
3	C	2400	GLN
3	C	2407	GLN
3	C	2520	GLN
3	C	2557	GLN
3	C	2576	GLN
3	F	2400	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

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	NAG	C	2602	3	14,14,15	0.22	0	17,19,21	0.36	0
4	NAG	A	1301	1	14,14,15	0.90	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	B	1701	2	14,14,15	0.27	0	17,19,21	1.10	1 (5%)
4	NAG	F	2601	3	14,14,15	0.54	0	17,19,21	0.81	0
4	NAG	C	2603	3	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	C	2601	3	14,14,15	0.97	1 (7%)	17,19,21	1.21	1 (5%)
4	NAG	C	2604	3	14,14,15	0.26	0	17,19,21	0.50	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
4	NAG	C	2602	3	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1701	2	-	2/6/23/26	0/1/1/1
4	NAG	F	2601	3	-	4/6/23/26	0/1/1/1
4	NAG	C	2603	3	-	2/6/23/26	0/1/1/1
4	NAG	C	2601	3	-	2/6/23/26	0/1/1/1
4	NAG	C	2604	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAG	O5-C1	3.41	1.49	1.43
4	A	1301	NAG	O5-C1	2.94	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2601	NAG	C1-O5-C5	4.75	118.62	112.19
4	A	1301	NAG	C1-O5-C5	3.96	117.55	112.19
4	B	1701	NAG	C1-O5-C5	3.13	116.43	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C4-C5-C6-O6
4	C	2604	NAG	C4-C5-C6-O6
4	C	2603	NAG	C4-C5-C6-O6
4	F	2601	NAG	C4-C5-C6-O6
4	B	1701	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	C	2604	NAG	O5-C5-C6-O6
4	F	2601	NAG	O5-C5-C6-O6
4	C	2601	NAG	O5-C5-C6-O6
4	C	2603	NAG	O5-C5-C6-O6
4	B	1701	NAG	O5-C5-C6-O6
4	C	2602	NAG	O5-C5-C6-O6
4	C	2604	NAG	C8-C7-N2-C2
4	C	2604	NAG	O7-C7-N2-C2
4	C	2601	NAG	C4-C5-C6-O6
4	C	2602	NAG	C4-C5-C6-O6
4	F	2601	NAG	C3-C2-N2-C7
4	F	2601	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	NAG	1	0
4	F	2601	NAG	2	0
4	C	2603	NAG	1	0
4	C	2601	NAG	2	0
4	C	2604	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

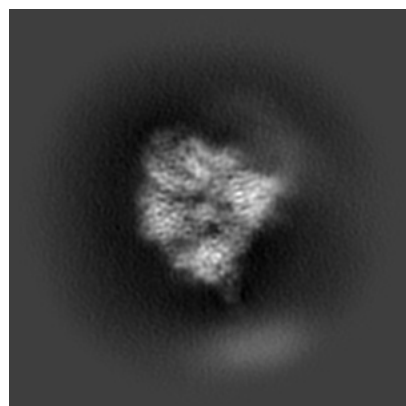
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18803. These allow visual inspection of the internal detail of the map and identification of artifacts.

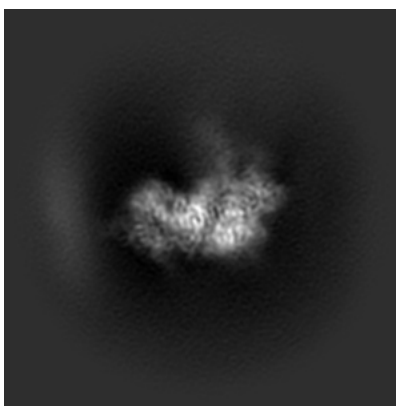
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

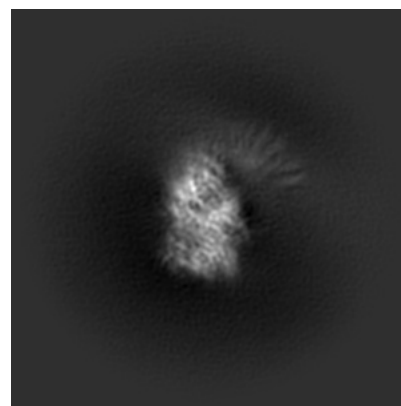
6.1.1 Primary map



X

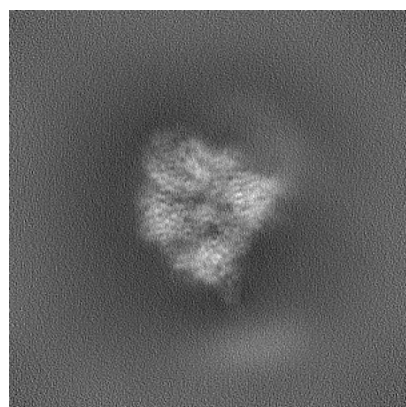


Y

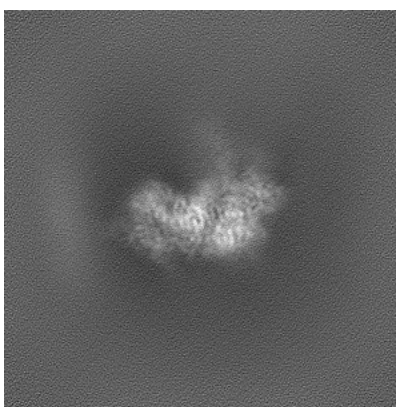


Z

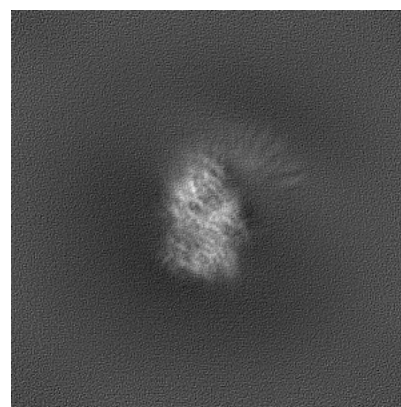
6.1.2 Raw map



X



Y

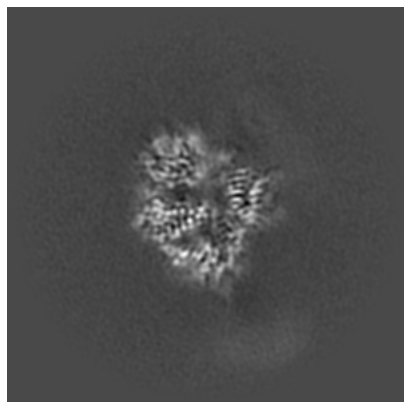


Z

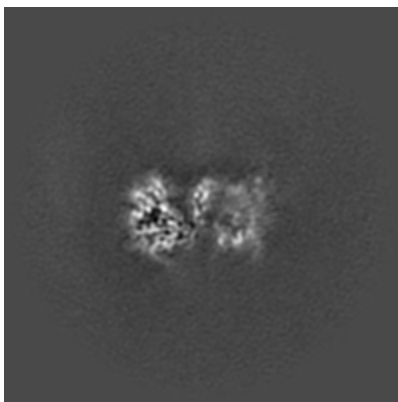
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

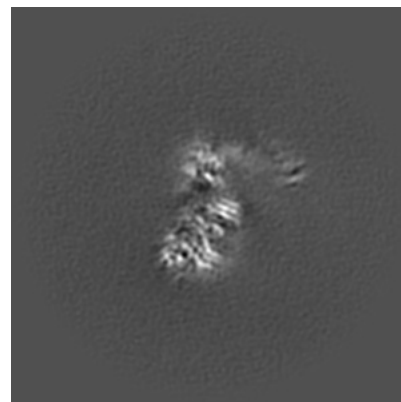
6.2.1 Primary map



X Index: 176

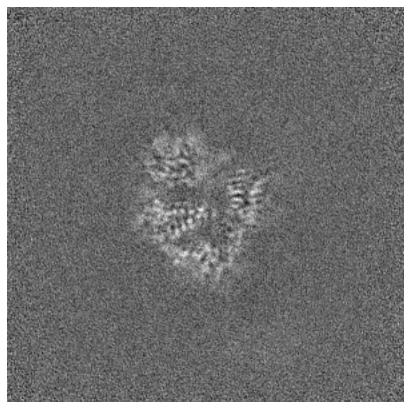


Y Index: 176

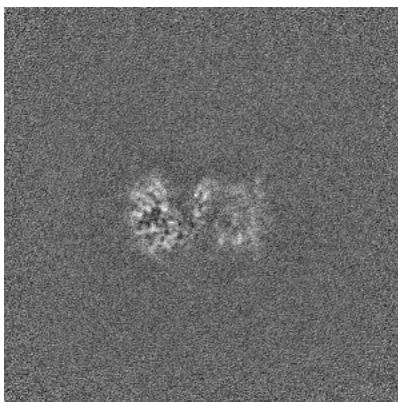


Z Index: 176

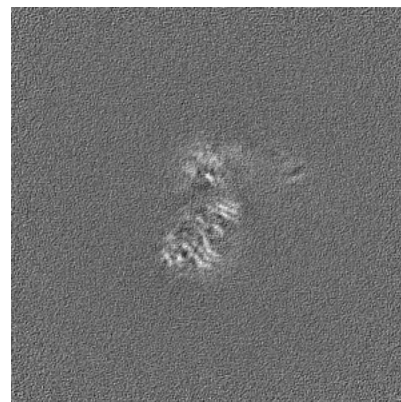
6.2.2 Raw map



X Index: 176



Y Index: 176

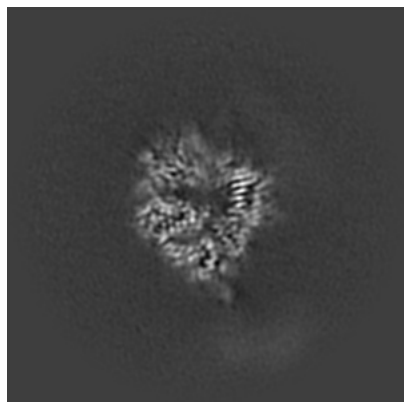


Z Index: 176

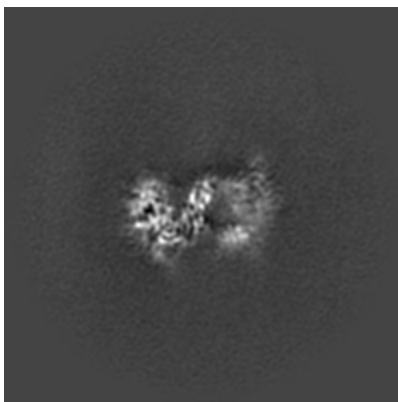
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

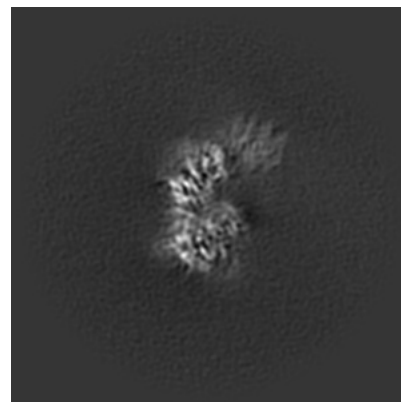
6.3.1 Primary map



X Index: 172

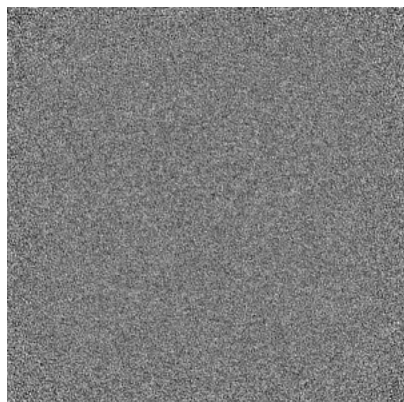


Y Index: 171

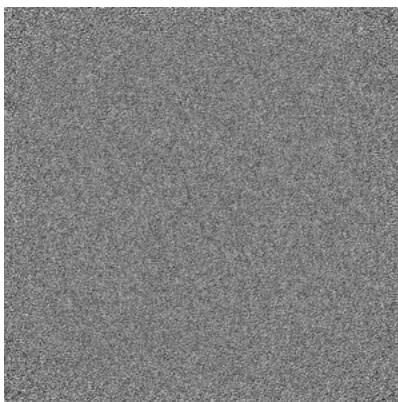


Z Index: 199

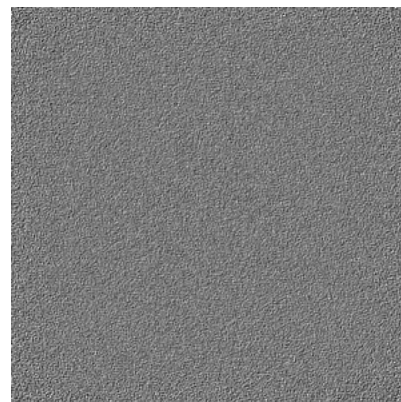
6.3.2 Raw map



X Index: 0



Y Index: 0

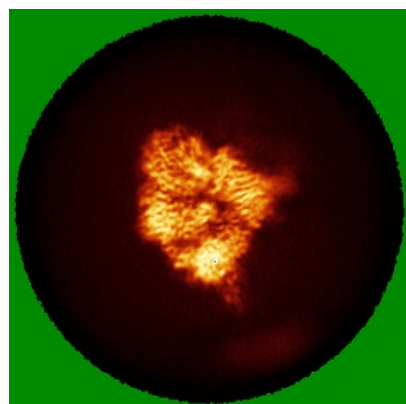


Z Index: 351

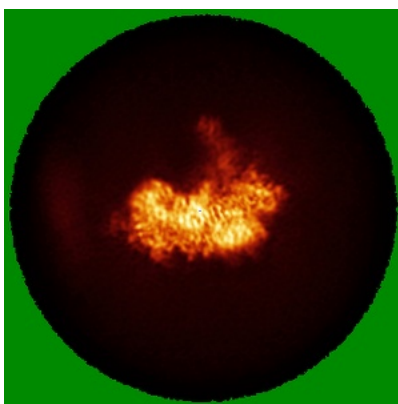
The images above show the largest variance slices of the map in three orthogonal directions.

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

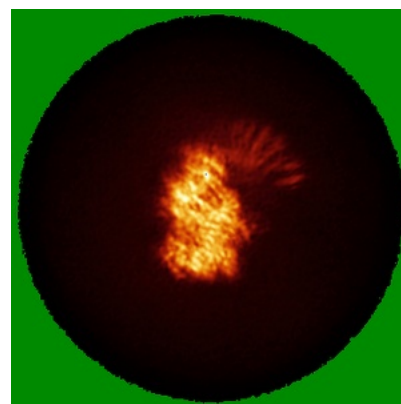
6.4.1 Primary map



X

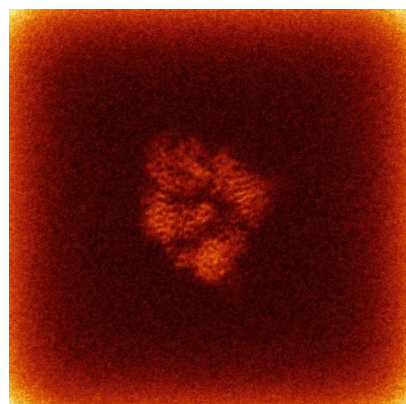


Y

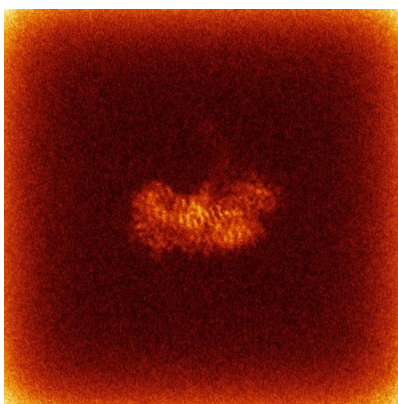


Z

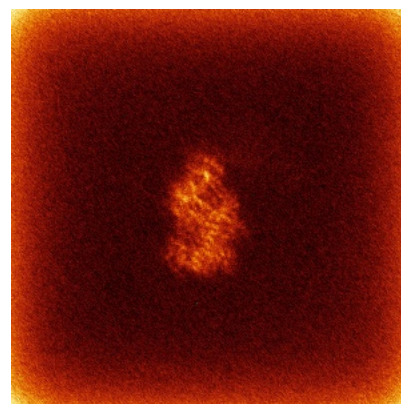
6.4.2 Raw map



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.

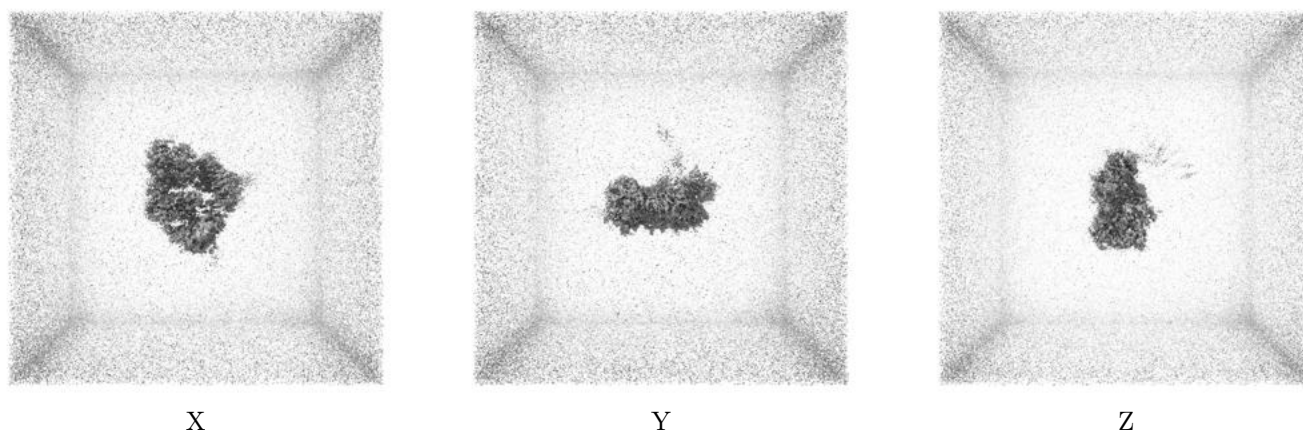
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

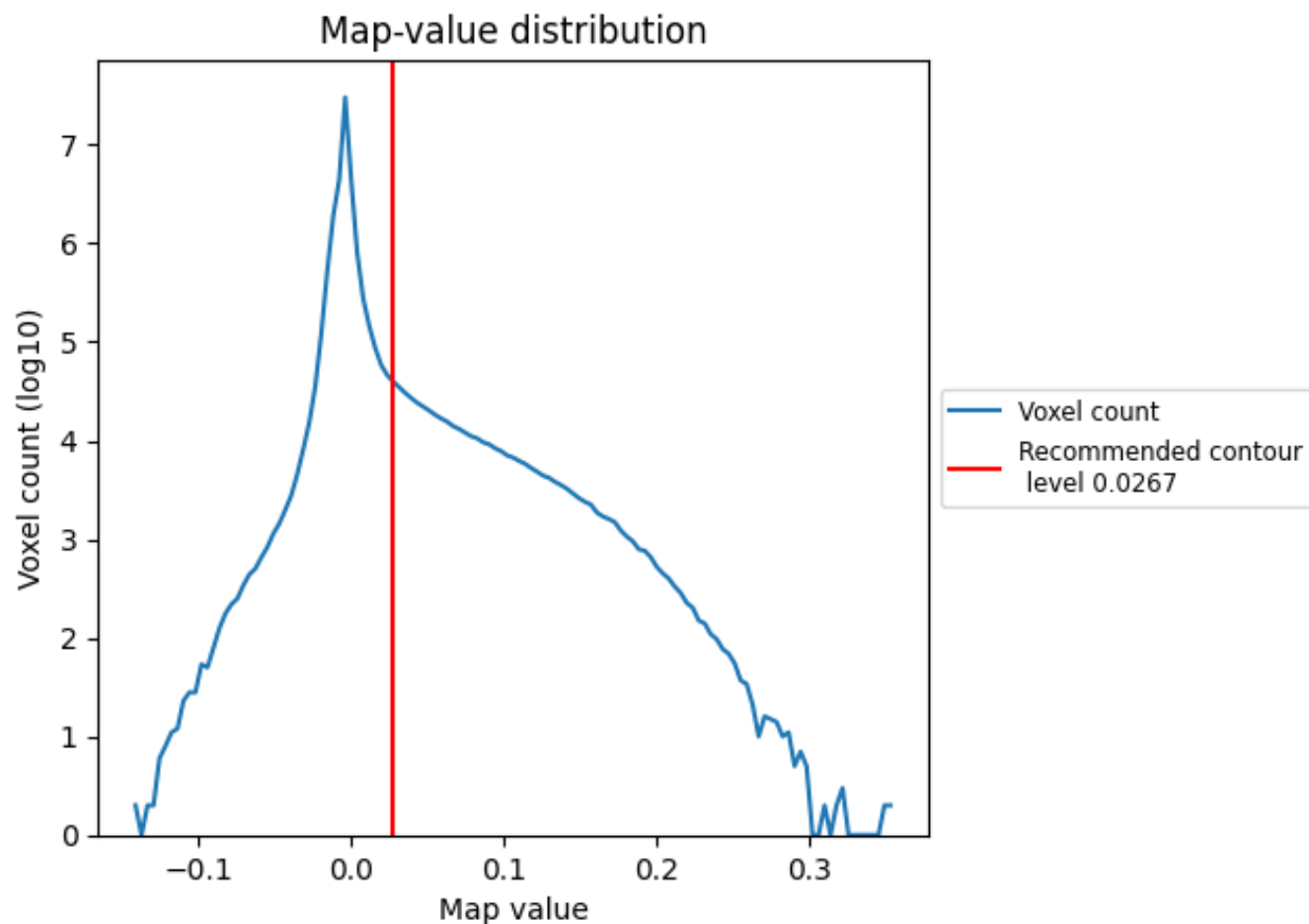
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

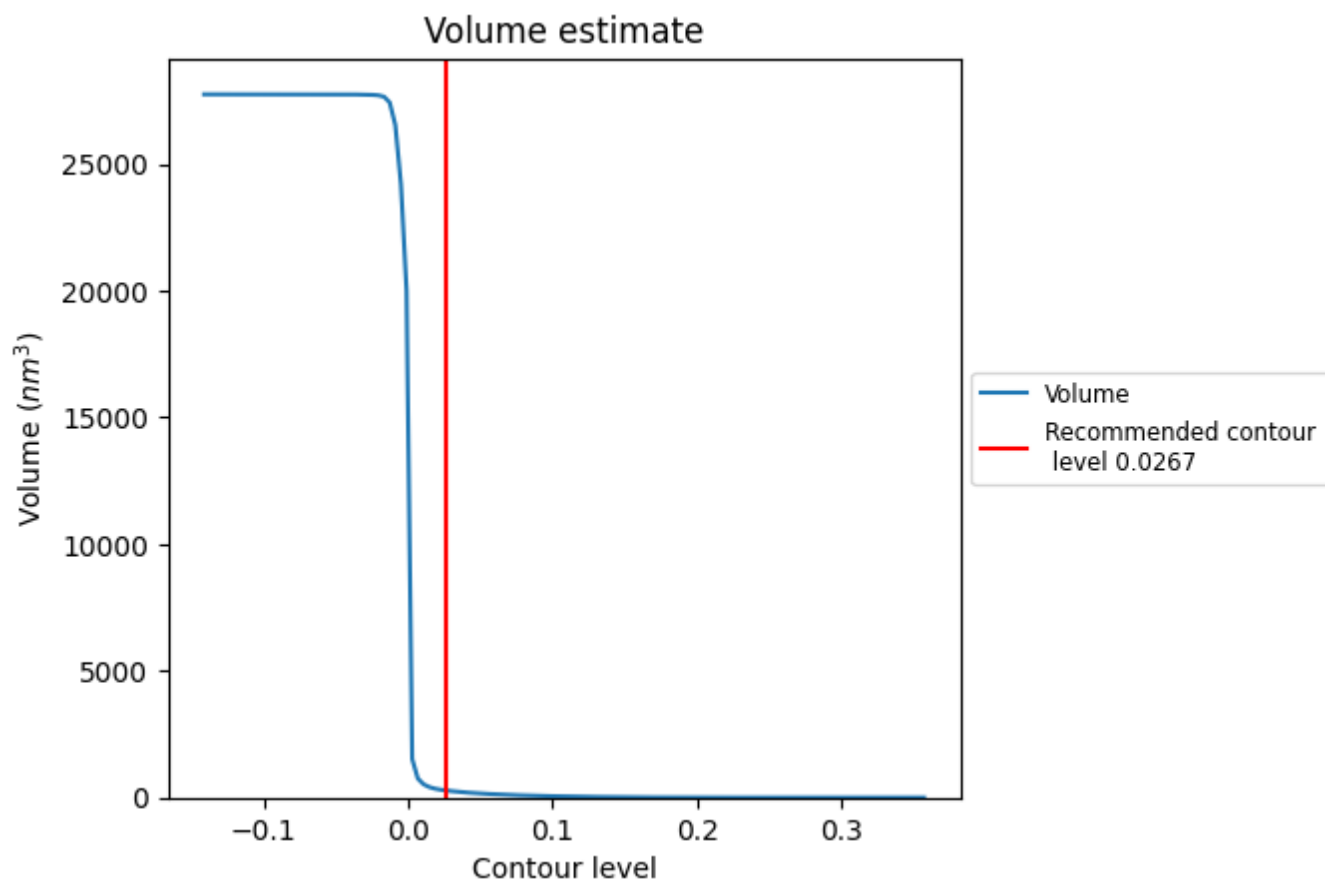
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

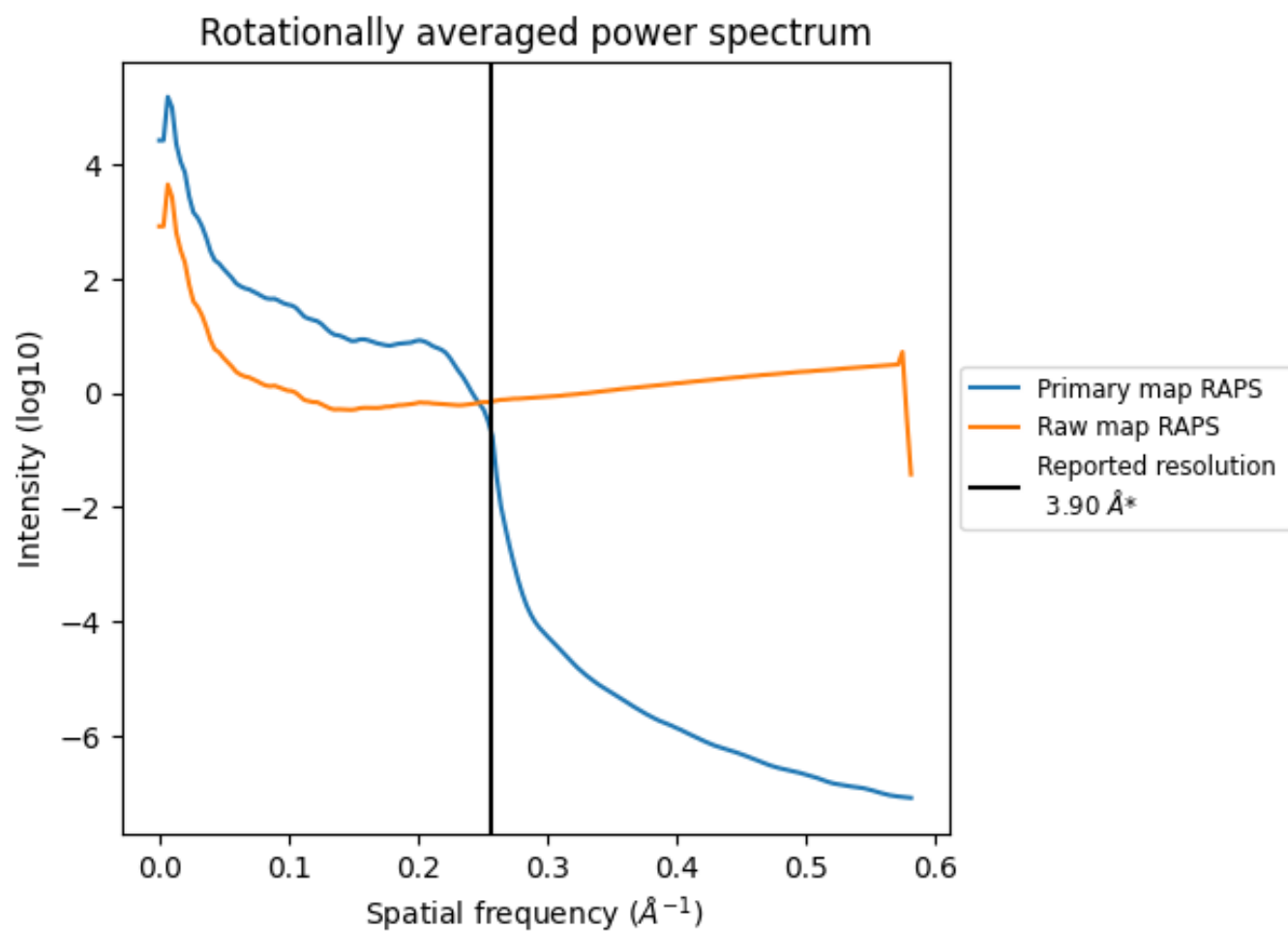
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm³; this corresponds to an approximate mass of 251 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 ⓘ

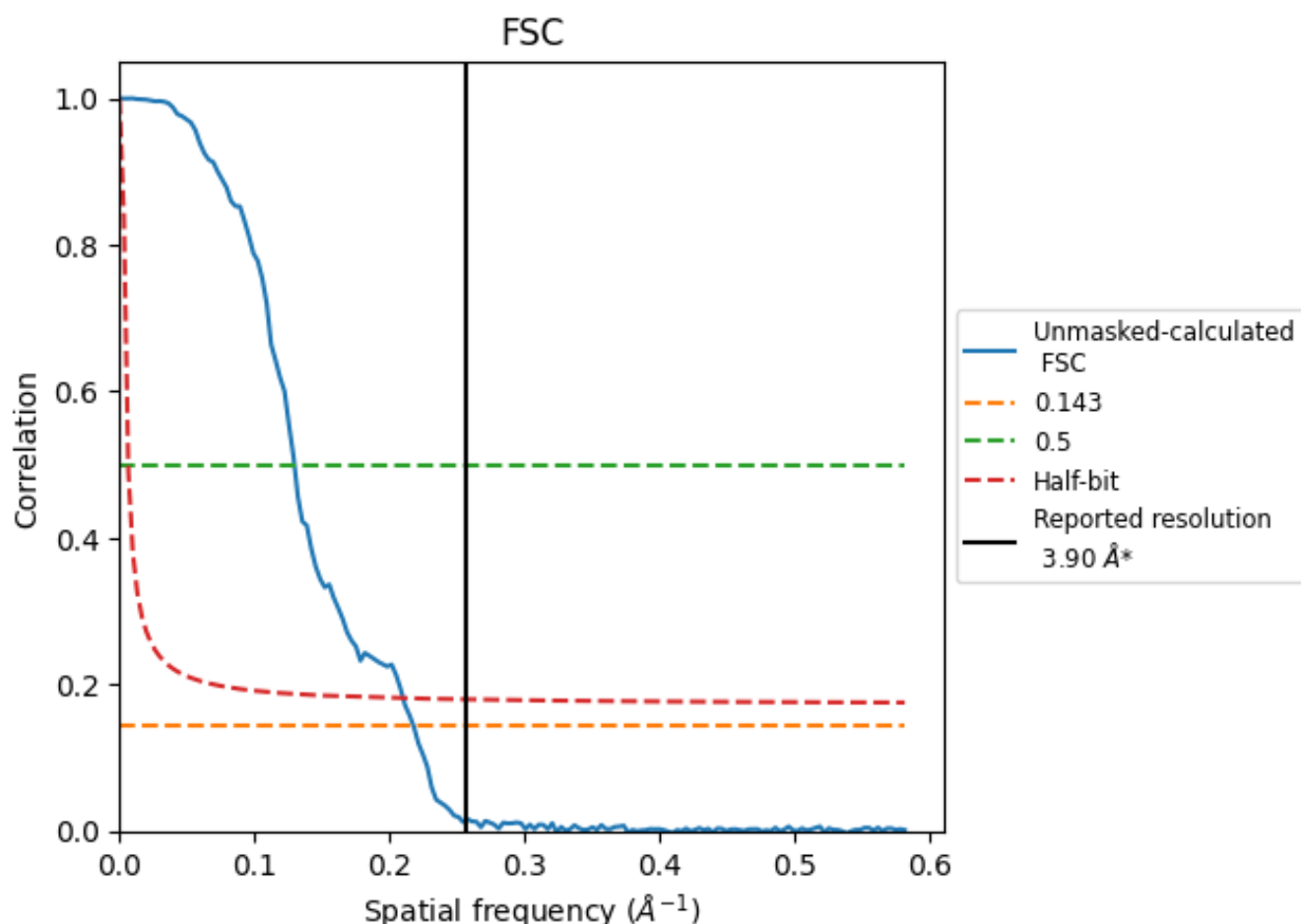


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

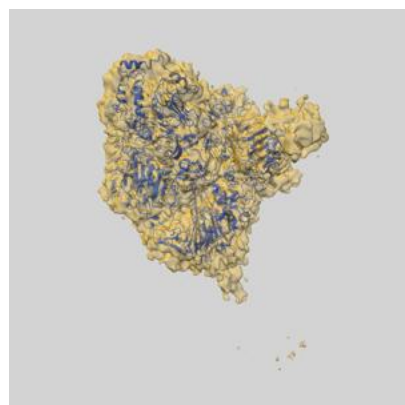
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.59	7.72	4.76

*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 4.59 differs from the reported value 3.9 by more than 10 %

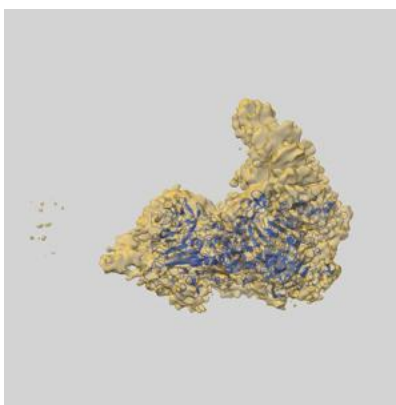
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18803 and PDB model 8R0T. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

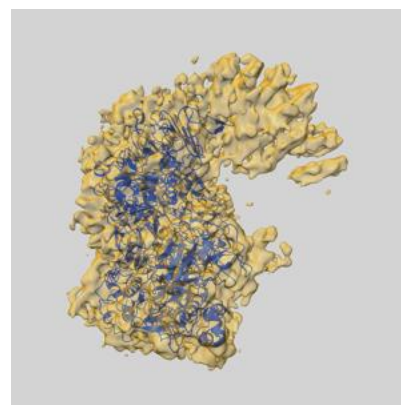
9.1 Map-model overlay [i](#)



X



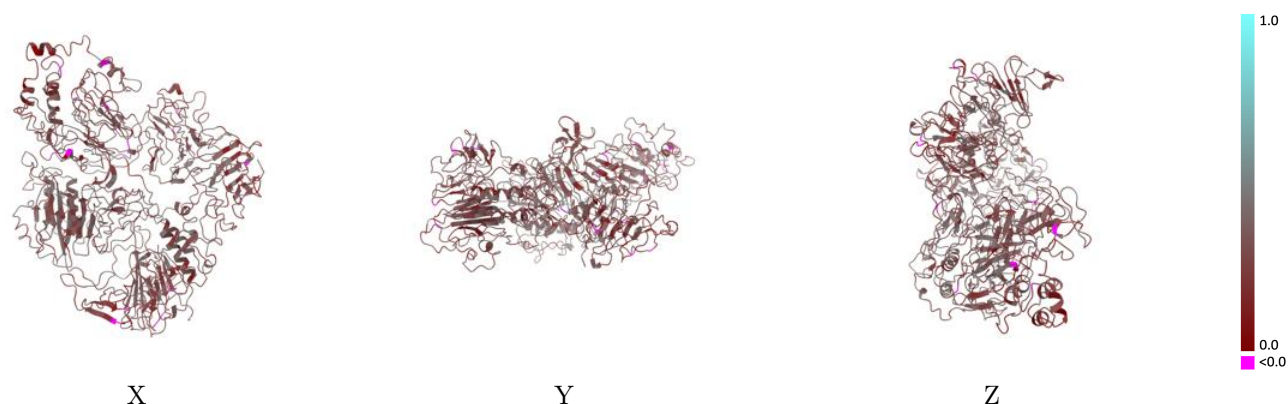
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0267 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](#)



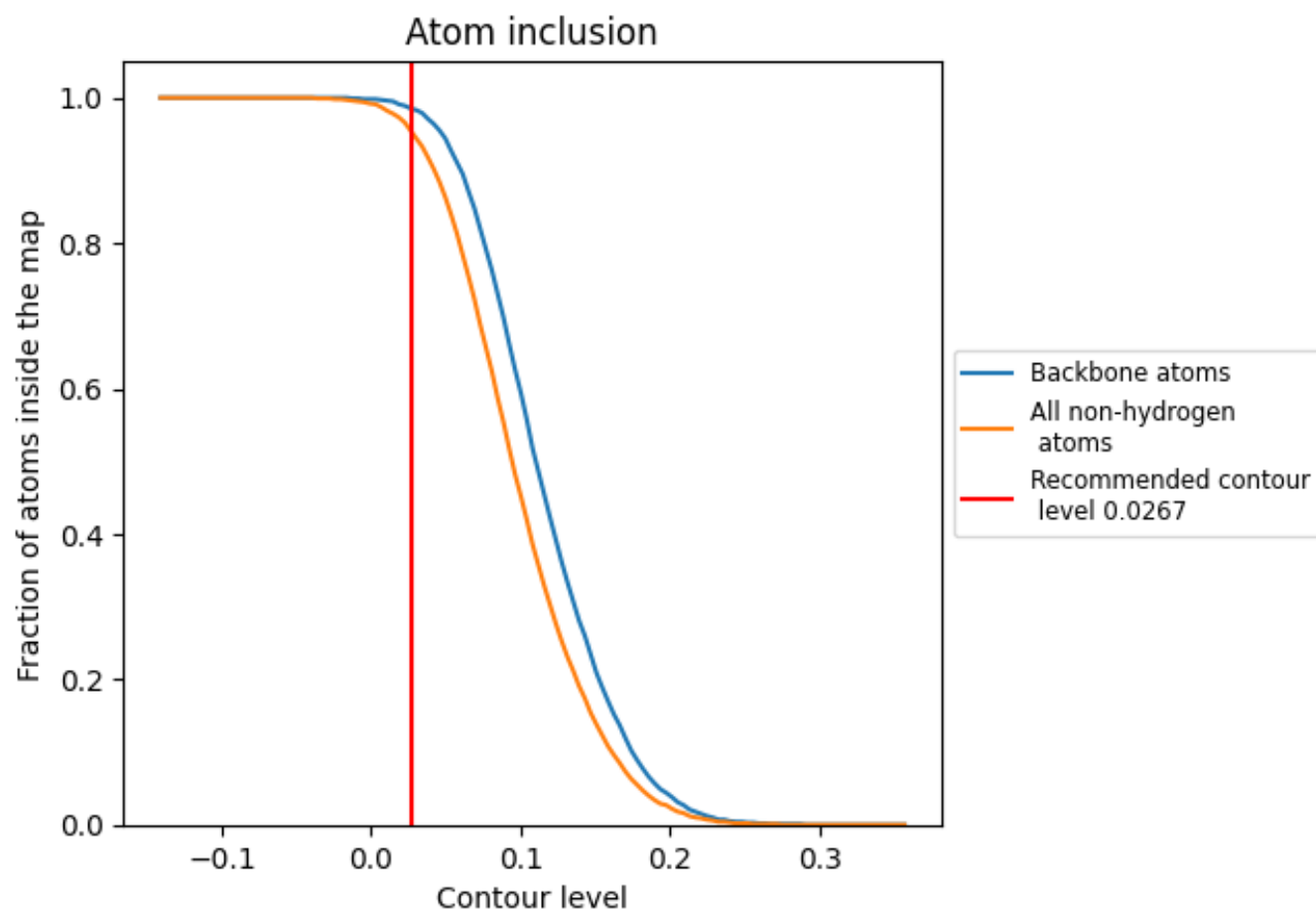
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0267).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9540	<div></div> 0.3050
A	<div></div> 0.9010	<div></div> 0.3230
B	<div></div> 0.9630	<div></div> 0.2920
C	<div></div> 0.9510	<div></div> 0.3110
F	<div></div> 0.9560	<div></div> 0.2980

