



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:17 AM UTC

PDB ID : 9JXR / pdb_00009jxr
EMDB ID : EMD-61877
Title : Cryo-EM structure of Drosophila melanogaster Pxo-G604A
Authors : Wang, X.; Bai, Z.; Wallis, C.; Wang, H.; Han, Y.; Jin, R.; Lei, M.; Gu, C.;
Jessen, H.; Shears, S.; Sun, Y.; Corry, B.; Zhang, Y.
Deposited on : 2024-10-11
Resolution : 3.53 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.dev132
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

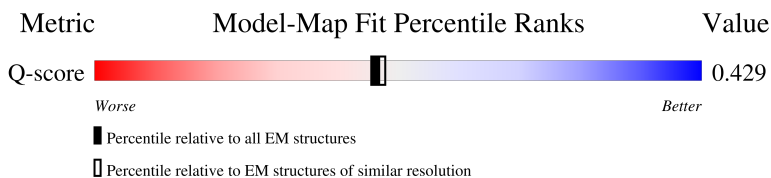
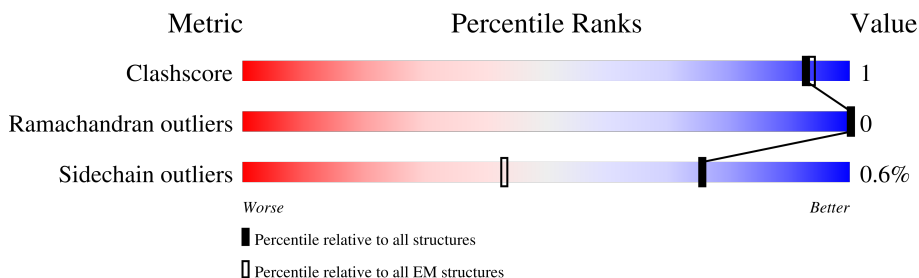
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	671	
1	B	671	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6350 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 Solute carrier family 53 member 1.

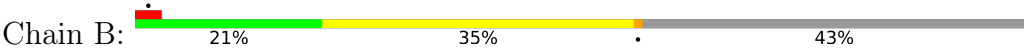
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	384	Total	C	N	O	S	0	0
			3175	2122	508	522	23		
1	B	384	Total	C	N	O	S	0	0
			3175	2122	508	522	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	ALA	GLY	engineered mutation	UNP Q9VRR2
B	604	ALA	GLY	engineered mutation	UNP Q9VRR2

LEU
GLN
GLY
GLU
ALA
SER
SER
ILE
GLU
ASP
LEU
CYS
SER

● Molecule 1: Solute carrier family 53 member 1



MET
LYS
PHE
ALA
GLU
HIS
LEU
THR
HIS
ASN
THR
ILE
THR
PRO
GLU
TRP
ARG
LYS
MET
GLN
TYR
ILE
TYR
GLY
MET
LYS
ALA
MET
SER
GLU
TYR
ALA
ILE
GLU
Gln
SER
PRO
SER
GLY
HIS
PRO
GLU
LEU
LYS
VAL
GLU
ARG
GLU
MET
VAL
THR
ARG
THR
TYR
PHE
LEU
ALA
LYS
PHE
ASN
GLU
VAL
PHE
PHE
ALA
HIS

TYR
CYS
ASP
LYS
LEU
LEU
ALA
LYS
ILE
ALA
SER
GLU
PHE
THR
PHE
TYR
SER
GLU
LYS
MET
ALA
GLU
TYR
ASN
THR
GLN
GLY
TYR
ASN
GLY
SER
ASN
SER
SER
LEU
PHE
ARG
MET
GLY
SER
GLU
TYR
LEU
ALA
THR
LYS
HIS
ASP
MET
GLY
HIS
PRO
GLU
LEU
LYS
VAL
LEU
PRO
ALA
TRP
LYS
VAL
THR
ARG
ARG
THR
TYR
PHE
LEU
ALA
LYS
PHE
ASN
GLU
VAL
PHE
PHE
ALA
HIS

LYS
ILE
GLN
ASP
LEU
LYS
LEU
ALA
PHE
SER
GLU
PHE
THR
PHE
TYR
LEU
GLY
ALA
GLU
LEU
TYR
ASN
GLY
SER
ASN
SER
SER
PHE
ARG
LYS
ILE
GLU
VAL
LEU
PRO
LYS
HIS
ASP
LYS
LEU
GLN
SER
VAL
ASP
TYR
GLY
ALA
THR
ARG
TRP
ARG
THR
PHE
LEU
ALA
LYS
PHE
VAL
GLU
ALA
ALA
HIS
PHE
TYR

THR
ASN
LYS
ASP
ILE
ASP
ARG
LEU
ILE
GLN
THR
THR
GLU
GLN
VAL
ALA
THR
GLY
GLY
ASP
ARG
GLN
ARG
ALA
MET
LYS
ARG
LEU
LEU
VAL
ARG
P223
W224
T225
T226
F227
K228
V229
G230
L231
F232
S233
G234
A235
L239
F240
I241
T242

V243
V244
I245
A246
F249
Y250
G251
F252
G253
F254
N255
W256
R257
A258
G259
N260
M261
M262
F263
R264
F267
L268
I269
L273
F274
L275
W276
G277
W283
R284
V288
N289
H290
V291
L292
I293
F294
E295
L296
D297
P298
R299
N300
H301
L302
S303
E304
Q305
N306
D384
F385
M308
E309

V310
A311
S312
V313
F314
G315
V316
I317
W318
A319
V322
L323
R324
Y325
D329
I333
P334
A338
P339
L340
C341
T344
L345
M346
L350
L351
N352
P353
T354
K355
H358
H359
E360
F363
I366
R367
R371
V372
A375
C378
F379
V380
N381
F382
A383
D384
F385
V386

L387
A388
Q389
D390
L391
N392
S393
H394
F398
L399
D400
I401
L404
F407
R410
S411
P412
T413
W414
H415
K416
A417
G418
K419
A420
H423
C424
V425
E426
Y427
V428
S429
L430
L431
H432
V435
H438
R443
F444
A445
Q446
C447
R450
Y451
R452
D453
F458
H459
A460

M463
S470
F471
V472
V473
V474
I475
F476
A477
H478
K479
Y480
H481
T482
T483
T484
D485
T486
Y487
L488
S490
K491
E492
M493
F494
W495
F496
Y497
C498
W499
I500
T501
A502
A503
I504
F505
C508
Y509
A510
Y511
T512
W513
D514
I515
K516
M517
D518
W519
G520
L521
F522
D523
S524
K525
A526
N529

R530
F531
L532
R533
E534
I535
E536
V537
Y538
T541
W542
F543
Y544
Y545
F546
L552
I553
L554
R555
F556
S557
W558
T559
L560
S561
M562
S563
L564
G568
Y569
I570
E571
O572
D573
W574
M575
M576
T577
I578
L579
S580
F581
L582
E583
V584
F585
R586
R587
F588
Y592
F593
R594
N597
L600

M601
M602
K605
F606
ARG
ALA
VAL
ARG
ASP
ILE
SER
VAL
F543
ALA
PRO
MET
MET
ASP
CYS
SER
SER
ASP
GLN
THR
THR
ILE
LEU
LEU
MET
MET
ASP
GLU
THR
ASP
GLY
VAL
LEU
ASN
ARG
ARG
GLY
LYS
ALA
ALA
GLY
LYS
SER
SER
ALA
THR
LYS
LYS
ASN
LYS
GLN
GLU
GLN
ARG
ARG
LEU
LEU
LEU

GLN
GLY
GLU
SER
ILE
GLU
ASP
LEU
CYS
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	4.794	Depositor
Minimum map value	-2.483	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	337.59998, 337.59998, 337.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

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	2.61	200/3291 (6.1%)	2.32	208/4483 (4.6%)
1	B	2.61	202/3291 (6.1%)	2.32	209/4483 (4.7%)
All	All	2.61	402/6582 (6.1%)	2.32	417/8966 (4.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
All	All	0	12

All (402) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	511	TYR	CA-C	-8.95	1.41	1.52
1	A	511	TYR	CA-C	-8.91	1.41	1.52
1	B	393	SER	CA-C	-8.85	1.41	1.52
1	A	393	SER	CA-C	-8.84	1.41	1.52
1	B	574	VAL	CA-C	8.64	1.63	1.52
1	A	413	THR	CA-C	-8.62	1.41	1.53
1	A	523	ASP	CA-C	8.62	1.63	1.52
1	B	413	THR	CA-C	-8.61	1.41	1.53
1	A	574	VAL	CA-C	8.60	1.63	1.52
1	B	523	ASP	CA-C	8.59	1.63	1.52
1	A	478	HIS	CE1-NE2	8.59	1.41	1.32
1	B	478	HIS	CE1-NE2	8.58	1.41	1.32
1	B	293	ILE	CA-C	8.42	1.63	1.52
1	A	293	ILE	CA-C	8.39	1.63	1.52
1	B	493	ASN	CA-C	8.15	1.63	1.52
1	A	493	ASN	CA-C	8.14	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	THR	CA-C	-8.07	1.42	1.52
1	B	225	THR	CA-C	-8.07	1.42	1.52
1	B	290	HIS	ND1-CE1	8.06	1.40	1.32
1	A	290	HIS	ND1-CE1	8.04	1.40	1.32
1	B	279	ASN	CA-C	-7.93	1.42	1.52
1	A	279	ASN	CA-C	-7.90	1.42	1.52
1	B	359	HIS	CE1-NE2	7.61	1.40	1.32
1	A	359	HIS	CE1-NE2	7.55	1.40	1.32
1	A	411	SER	CA-C	7.53	1.58	1.52
1	B	411	SER	CA-C	7.53	1.58	1.52
1	B	490	SER	CA-C	-7.51	1.43	1.52
1	B	372	VAL	CA-C	-7.51	1.43	1.52
1	A	490	SER	CA-C	-7.50	1.43	1.52
1	A	372	VAL	CA-C	-7.47	1.43	1.52
1	B	288	VAL	CA-C	-7.46	1.43	1.52
1	B	558	TRP	CA-C	7.44	1.62	1.52
1	A	288	VAL	CA-C	-7.44	1.43	1.52
1	A	558	TRP	CA-C	7.42	1.62	1.52
1	B	283	TRP	N-CA	7.40	1.55	1.46
1	A	318	TRP	CA-C	-7.39	1.43	1.52
1	B	318	TRP	CA-C	-7.37	1.43	1.52
1	A	283	TRP	N-CA	7.36	1.55	1.46
1	B	381	ASN	CA-C	-7.30	1.42	1.53
1	A	381	ASN	CA-C	-7.29	1.42	1.53
1	A	504	ILE	C-O	-7.18	1.15	1.24
1	B	504	ILE	C-O	-7.18	1.15	1.24
1	B	426	GLU	CA-C	-7.17	1.42	1.52
1	A	426	GLU	CA-C	-7.17	1.42	1.52
1	B	580	SER	CA-C	7.16	1.61	1.52
1	A	580	SER	CA-C	7.15	1.61	1.52
1	A	446	GLN	CA-C	-7.12	1.43	1.52
1	B	496	PHE	CA-C	-7.12	1.43	1.52
1	A	500	ILE	CA-C	-7.12	1.44	1.52
1	B	500	ILE	CA-C	-7.12	1.44	1.52
1	B	446	GLN	CA-C	-7.10	1.43	1.52
1	A	496	PHE	CA-C	-7.08	1.43	1.52
1	A	262	MET	C-O	-7.05	1.15	1.24
1	B	304	GLU	C-O	-7.04	1.15	1.24
1	A	304	GLU	C-O	-7.04	1.15	1.24
1	B	541	THR	CA-C	7.03	1.61	1.52
1	A	438	MET	SD-CE	7.00	1.97	1.79
1	B	438	MET	SD-CE	7.00	1.97	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	THR	CA-C	6.99	1.61	1.52
1	A	463	ASN	CA-C	6.99	1.62	1.52
1	B	463	ASN	CA-C	6.99	1.62	1.52
1	B	262	MET	C-O	-6.98	1.15	1.24
1	A	483	THR	C-O	-6.95	1.16	1.23
1	B	483	THR	C-O	-6.94	1.16	1.23
1	B	477	ALA	CA-C	-6.94	1.42	1.52
1	A	477	ALA	CA-C	-6.91	1.42	1.52
1	A	508	CYS	CA-C	6.91	1.61	1.52
1	B	246	ALA	CA-C	-6.89	1.44	1.52
1	B	508	CYS	CA-C	6.87	1.61	1.52
1	B	470	SER	CA-C	6.87	1.61	1.52
1	A	246	ALA	CA-C	-6.85	1.44	1.52
1	A	597	ASN	CA-C	6.85	1.61	1.52
1	B	597	ASN	CA-C	6.84	1.61	1.52
1	A	470	SER	CA-C	6.83	1.61	1.52
1	B	431	LEU	C-O	-6.80	1.15	1.24
1	A	447	CYS	CA-C	-6.78	1.44	1.52
1	B	447	CYS	CA-C	-6.76	1.44	1.52
1	A	431	LEU	C-O	-6.76	1.15	1.24
1	B	410	ARG	N-CA	-6.76	1.38	1.46
1	B	363	PHE	CA-C	6.74	1.61	1.52
1	B	514	ASP	CA-C	6.73	1.61	1.52
1	A	514	ASP	CA-C	6.73	1.61	1.52
1	A	410	ARG	N-CA	-6.72	1.38	1.46
1	A	363	PHE	CA-C	6.71	1.61	1.52
1	B	303	SER	CA-C	-6.69	1.44	1.52
1	A	319	ALA	CA-C	6.67	1.61	1.52
1	A	303	SER	CA-C	-6.67	1.44	1.52
1	A	481	HIS	CG-ND1	-6.65	1.30	1.38
1	B	319	ALA	CA-C	6.64	1.61	1.52
1	B	474	VAL	CA-C	-6.63	1.44	1.52
1	A	260	MET	C-O	-6.62	1.16	1.24
1	A	478	HIS	N-CA	-6.62	1.38	1.46
1	A	474	VAL	CA-C	-6.61	1.44	1.52
1	A	536	ILE	CA-CB	6.60	1.62	1.53
1	B	481	HIS	CG-ND1	-6.60	1.30	1.38
1	B	260	MET	C-O	-6.58	1.16	1.24
1	B	478	HIS	N-CA	-6.57	1.38	1.46
1	B	384	ASP	CA-C	-6.56	1.44	1.52
1	A	384	ASP	CA-C	-6.56	1.44	1.52
1	B	562	MET	N-CA	6.55	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	ILE	CA-CB	6.55	1.62	1.53
1	B	250	TYR	CA-C	6.52	1.61	1.52
1	A	250	TYR	CA-C	6.51	1.61	1.52
1	A	562	MET	N-CA	6.48	1.54	1.46
1	A	242	THR	CA-C	6.47	1.61	1.52
1	A	314	PHE	CA-C	-6.46	1.44	1.52
1	B	472	PHE	CA-C	-6.44	1.44	1.52
1	A	472	PHE	CA-C	-6.43	1.44	1.52
1	B	242	THR	CA-C	6.43	1.61	1.52
1	A	592	TYR	N-CA	-6.36	1.38	1.46
1	B	314	PHE	CA-C	-6.36	1.44	1.52
1	B	592	TYR	N-CA	-6.36	1.38	1.46
1	B	487	TYR	C-N	6.32	1.40	1.33
1	A	487	TYR	C-N	6.32	1.40	1.33
1	A	344	THR	N-CA	6.28	1.53	1.46
1	B	487	TYR	CA-CB	6.26	1.63	1.53
1	B	491	LYS	CA-C	6.26	1.61	1.52
1	B	344	THR	N-CA	6.26	1.53	1.46
1	A	240	PHE	CA-C	6.25	1.60	1.52
1	A	491	LYS	CA-C	6.24	1.61	1.52
1	B	310	VAL	N-CA	-6.24	1.39	1.46
1	A	359	HIS	CD2-NE2	6.24	1.44	1.37
1	A	487	TYR	CA-CB	6.24	1.63	1.53
1	B	415	HIS	N-CA	-6.22	1.38	1.45
1	A	310	VAL	N-CA	-6.21	1.39	1.46
1	B	359	HIS	CD2-NE2	6.21	1.44	1.37
1	B	240	PHE	CA-C	6.21	1.60	1.52
1	B	490	SER	N-CA	-6.19	1.39	1.46
1	A	415	HIS	N-CA	-6.19	1.38	1.45
1	B	435	VAL	CA-C	-6.17	1.45	1.52
1	A	379	PHE	C-O	-6.14	1.16	1.23
1	A	435	VAL	CA-C	-6.13	1.45	1.52
1	A	490	SER	N-CA	-6.13	1.39	1.46
1	B	379	PHE	C-O	-6.10	1.16	1.23
1	A	605	LYS	N-CA	-6.09	1.38	1.46
1	B	605	LYS	N-CA	-6.08	1.38	1.46
1	A	488	PRO	CA-CB	-6.06	1.45	1.53
1	A	516	LYS	CA-C	-6.06	1.44	1.52
1	B	488	PRO	CA-CB	-6.05	1.45	1.53
1	B	516	LYS	CA-C	-6.03	1.44	1.52
1	B	481	HIS	CE1-NE2	-6.03	1.26	1.32
1	A	531	PHE	N-CA	-6.03	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	LEU	CA-C	-6.03	1.45	1.52
1	A	353	PRO	CA-C	5.99	1.60	1.52
1	A	497	TYR	N-CA	5.99	1.53	1.46
1	B	353	PRO	CA-C	5.98	1.60	1.52
1	B	531	PHE	N-CA	-5.98	1.38	1.46
1	A	481	HIS	CE1-NE2	-5.97	1.26	1.32
1	A	463	ASN	C-O	-5.97	1.16	1.24
1	B	538	TYR	C-O	-5.97	1.16	1.23
1	A	323	LEU	CA-C	-5.97	1.45	1.52
1	A	392	ASN	N-CA	5.97	1.53	1.46
1	B	463	ASN	C-O	-5.96	1.16	1.24
1	B	378	CYS	N-CA	5.96	1.53	1.45
1	A	296	LEU	CA-C	-5.95	1.45	1.52
1	B	323	LEU	CA-C	-5.95	1.45	1.52
1	A	378	CYS	N-CA	5.94	1.53	1.45
1	B	432	HIS	CG-CD2	-5.94	1.29	1.35
1	B	497	TYR	N-CA	5.94	1.53	1.46
1	B	392	ASN	N-CA	5.93	1.53	1.46
1	B	260	MET	SD-CE	5.92	1.94	1.79
1	B	278	VAL	CA-CB	-5.92	1.47	1.54
1	A	538	TYR	C-O	-5.92	1.16	1.23
1	A	260	MET	SD-CE	5.91	1.94	1.79
1	A	432	HIS	CG-CD2	-5.91	1.29	1.35
1	B	522	PHE	CA-C	-5.89	1.44	1.52
1	A	487	TYR	C-O	-5.89	1.16	1.24
1	B	487	TYR	C-O	-5.89	1.16	1.24
1	A	278	VAL	CA-CB	-5.88	1.47	1.54
1	A	390	GLN	N-CA	-5.88	1.39	1.46
1	B	390	GLN	N-CA	-5.88	1.39	1.46
1	A	334	PRO	CA-CB	-5.88	1.45	1.53
1	A	452	ARG	N-CA	5.88	1.53	1.46
1	A	411	SER	C-N	5.86	1.40	1.33
1	B	452	ARG	N-CA	5.86	1.53	1.46
1	B	334	PRO	CA-CB	-5.86	1.45	1.53
1	B	536	ILE	CA-C	-5.86	1.45	1.52
1	A	489	LEU	CA-CB	5.85	1.63	1.53
1	A	576	MET	C-N	5.85	1.41	1.33
1	B	576	MET	C-N	5.85	1.41	1.33
1	A	522	PHE	CA-C	-5.85	1.45	1.52
1	B	489	LEU	CA-CB	5.85	1.63	1.53
1	A	503	ALA	N-CA	-5.84	1.39	1.46
1	B	503	ALA	N-CA	-5.84	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	SER	C-N	5.84	1.40	1.33
1	A	536	ILE	CA-C	-5.83	1.45	1.52
1	B	428	VAL	CA-CB	5.82	1.62	1.54
1	A	399	LEU	CA-CB	-5.82	1.44	1.53
1	A	488	PRO	C-O	-5.81	1.16	1.23
1	B	399	LEU	CA-CB	-5.81	1.44	1.53
1	A	307	ILE	N-CA	-5.79	1.39	1.46
1	B	488	PRO	C-O	-5.79	1.16	1.23
1	A	473	VAL	CA-C	-5.79	1.45	1.52
1	A	428	VAL	CA-CB	5.78	1.62	1.54
1	A	556	PHE	CA-C	-5.78	1.44	1.52
1	B	473	VAL	CA-C	-5.78	1.45	1.52
1	B	416	LYS	C-O	-5.78	1.16	1.24
1	B	556	PHE	CA-C	-5.77	1.44	1.52
1	B	307	ILE	N-CA	-5.76	1.39	1.46
1	B	302	LEU	C-O	-5.75	1.16	1.23
1	A	250	TYR	C-N	5.75	1.41	1.33
1	A	416	LYS	C-O	-5.74	1.16	1.24
1	B	250	TYR	C-N	5.74	1.41	1.33
1	A	411	SER	C-O	-5.74	1.16	1.24
1	B	577	THR	CA-CB	5.73	1.62	1.53
1	A	577	THR	CA-CB	5.73	1.62	1.53
1	A	302	LEU	C-O	-5.73	1.16	1.23
1	A	485	ASP	N-CA	5.72	1.53	1.46
1	A	495	TRP	C-O	-5.72	1.17	1.24
1	B	411	SER	C-O	-5.72	1.16	1.24
1	A	543	PHE	CA-CB	5.71	1.62	1.53
1	A	587	ARG	C-O	-5.71	1.17	1.24
1	A	235	ALA	N-CA	-5.70	1.39	1.46
1	B	587	ARG	C-O	-5.70	1.17	1.24
1	B	495	TRP	C-O	-5.69	1.17	1.24
1	B	543	PHE	CA-CB	5.69	1.62	1.53
1	A	484	THR	CA-C	5.68	1.60	1.52
1	B	235	ALA	N-CA	-5.68	1.39	1.46
1	B	485	ASP	N-CA	5.67	1.53	1.46
1	B	381	ASN	CA-CB	5.67	1.61	1.53
1	A	352	ASN	C-O	-5.66	1.17	1.24
1	A	381	ASN	CA-CB	5.65	1.61	1.53
1	A	311	ALA	CA-CB	-5.65	1.44	1.53
1	B	239	LEU	N-CA	-5.65	1.39	1.46
1	B	352	ASN	C-O	-5.64	1.17	1.24
1	B	553	ILE	CA-CB	5.61	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	THR	C-O	5.61	1.30	1.24
1	B	484	THR	CA-C	5.61	1.60	1.52
1	B	311	ALA	CA-CB	-5.61	1.44	1.53
1	B	512	THR	C-O	5.61	1.30	1.24
1	A	553	ILE	CA-CB	5.60	1.61	1.54
1	A	239	LEU	N-CA	-5.60	1.39	1.46
1	B	570	ILE	CB-CG1	5.58	1.64	1.53
1	A	233	SER	CA-C	-5.57	1.45	1.52
1	A	290	HIS	CD2-NE2	5.56	1.44	1.37
1	A	570	ILE	CB-CG1	5.56	1.64	1.53
1	A	305	GLN	C-O	-5.55	1.17	1.23
1	A	428	VAL	C-O	-5.54	1.17	1.24
1	B	233	SER	CA-C	-5.53	1.45	1.52
1	B	428	VAL	C-O	-5.53	1.17	1.24
1	B	290	HIS	CD2-NE2	5.51	1.44	1.37
1	B	305	GLN	C-O	-5.50	1.17	1.23
1	B	561	SER	C-O	-5.49	1.17	1.24
1	B	304	GLU	C-N	5.49	1.41	1.33
1	B	588	PHE	C-N	-5.49	1.26	1.33
1	A	352	ASN	C-N	5.48	1.39	1.33
1	B	245	ILE	CA-CB	-5.47	1.48	1.54
1	B	389	ASP	N-CA	5.47	1.52	1.46
1	B	398	PHE	CA-C	5.47	1.60	1.52
1	B	526	ALA	N-CA	-5.47	1.38	1.46
1	A	273	LEU	CB-CG	-5.47	1.42	1.53
1	A	389	ASP	N-CA	5.46	1.52	1.46
1	A	304	GLU	C-N	5.46	1.41	1.33
1	A	400	ASP	C-O	-5.46	1.17	1.24
1	A	398	PHE	CA-C	5.45	1.60	1.52
1	A	481	HIS	ND1-CE1	5.45	1.38	1.32
1	B	519	TRP	CA-C	5.45	1.59	1.52
1	B	273	LEU	CB-CG	-5.45	1.42	1.53
1	A	526	ALA	N-CA	-5.45	1.38	1.46
1	A	561	SER	C-O	-5.45	1.17	1.24
1	B	481	HIS	ND1-CE1	5.45	1.38	1.32
1	A	283	TRP	C-O	-5.45	1.17	1.24
1	A	588	PHE	C-N	-5.44	1.26	1.33
1	B	429	SER	N-CA	-5.43	1.38	1.46
1	A	429	SER	N-CA	-5.43	1.38	1.46
1	A	432	HIS	ND1-CE1	-5.42	1.27	1.32
1	B	225	THR	C-O	5.42	1.30	1.24
1	A	427	TYR	N-CA	-5.42	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	HIS	ND1-CE1	-5.42	1.27	1.32
1	B	352	ASN	C-N	5.42	1.39	1.33
1	A	245	ILE	CA-CB	-5.41	1.48	1.54
1	B	427	TYR	N-CA	-5.41	1.39	1.46
1	B	283	TRP	C-O	-5.41	1.17	1.24
1	B	295	GLU	N-CA	-5.41	1.38	1.46
1	A	519	TRP	CA-C	5.41	1.59	1.52
1	B	438	MET	CA-C	5.41	1.59	1.52
1	A	412	PRO	C-N	5.41	1.40	1.33
1	B	400	ASP	C-O	-5.41	1.17	1.24
1	A	295	GLU	N-CA	-5.40	1.38	1.46
1	A	225	THR	C-O	5.39	1.30	1.24
1	A	309	GLU	CA-C	5.39	1.60	1.52
1	A	582	LEU	N-CA	-5.39	1.39	1.46
1	A	438	MET	CA-C	5.38	1.59	1.52
1	A	371	ARG	CA-CB	-5.37	1.45	1.53
1	B	412	PRO	C-N	5.37	1.40	1.33
1	A	478	HIS	ND1-CE1	5.37	1.38	1.32
1	A	498	CYS	N-CA	5.37	1.52	1.46
1	B	554	LEU	CA-C	-5.36	1.45	1.52
1	B	582	LEU	N-CA	-5.36	1.39	1.46
1	B	371	ARG	CA-CB	-5.35	1.45	1.53
1	B	309	GLU	CA-C	5.35	1.60	1.52
1	A	554	LEU	CA-C	-5.35	1.45	1.52
1	B	329	ASP	CA-C	5.34	1.58	1.52
1	B	498	CYS	N-CA	5.34	1.52	1.46
1	A	329	ASP	CA-C	5.33	1.58	1.52
1	B	478	HIS	ND1-CE1	5.33	1.37	1.32
1	A	333	ILE	CA-CB	5.32	1.61	1.54
1	A	424	CYS	CA-C	-5.32	1.46	1.52
1	B	333	ILE	CA-CB	5.30	1.61	1.54
1	B	530	ARG	N-CA	-5.30	1.39	1.46
1	A	588	PHE	N-CA	-5.30	1.39	1.46
1	A	552	LEU	CA-C	-5.29	1.45	1.52
1	B	552	LEU	CA-C	-5.29	1.45	1.52
1	A	496	PHE	CA-CB	-5.28	1.45	1.53
1	B	496	PHE	CA-CB	-5.28	1.45	1.53
1	A	519	TRP	N-CA	-5.27	1.38	1.45
1	A	530	ARG	N-CA	-5.27	1.39	1.46
1	B	517	MET	N-CA	5.27	1.52	1.46
1	B	424	CYS	CA-C	-5.27	1.46	1.52
1	B	224	TRP	CA-C	-5.26	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	PHE	C-N	5.26	1.41	1.33
1	B	416	LYS	N-CA	5.26	1.52	1.46
1	B	519	TRP	N-CA	-5.25	1.38	1.45
1	A	249	PHE	C-N	5.25	1.41	1.33
1	A	263	PHE	CA-C	-5.25	1.45	1.52
1	A	451	TYR	CA-CB	5.25	1.61	1.53
1	B	588	PHE	N-CA	-5.25	1.39	1.46
1	B	554	LEU	CA-CB	5.25	1.61	1.53
1	A	554	LEU	CA-CB	5.24	1.61	1.53
1	A	224	TRP	CA-C	-5.24	1.46	1.52
1	A	509	TYR	C-N	-5.24	1.26	1.34
1	B	263	PHE	CA-C	-5.24	1.45	1.52
1	B	509	TYR	C-N	-5.24	1.26	1.34
1	A	416	LYS	N-CA	5.22	1.52	1.46
1	A	559	THR	C-N	-5.22	1.26	1.33
1	A	517	MET	N-CA	5.22	1.52	1.46
1	B	451	TYR	CA-CB	5.22	1.61	1.53
1	A	289	ASN	N-CA	-5.20	1.40	1.46
1	B	600	LEU	CA-C	5.20	1.59	1.52
1	A	600	LEU	CA-C	5.20	1.59	1.52
1	A	490	SER	C-N	-5.19	1.27	1.33
1	B	559	THR	C-N	-5.19	1.26	1.33
1	A	294	PHE	N-CA	5.18	1.53	1.46
1	B	490	SER	C-N	-5.18	1.27	1.33
1	B	366	ILE	N-CA	-5.18	1.40	1.46
1	B	420	ALA	C-N	-5.18	1.27	1.34
1	A	502	ALA	C-O	5.17	1.30	1.24
1	A	350	LEU	N-CA	5.17	1.52	1.46
1	A	420	ALA	C-N	-5.17	1.27	1.34
1	A	533	ARG	CA-C	-5.16	1.46	1.53
1	B	294	PHE	N-CA	5.16	1.53	1.46
1	B	350	LEU	N-CA	5.16	1.52	1.46
1	B	289	ASN	N-CA	-5.16	1.40	1.46
1	A	322	VAL	C-N	-5.16	1.27	1.33
1	B	533	ARG	CA-C	-5.16	1.46	1.53
1	A	480	TYR	CA-C	-5.14	1.45	1.52
1	B	502	ALA	C-O	5.14	1.30	1.24
1	A	346	MET	N-CA	-5.14	1.40	1.46
1	B	346	MET	N-CA	-5.14	1.40	1.46
1	A	366	ILE	N-CA	-5.14	1.40	1.46
1	A	244	VAL	CA-CB	5.13	1.60	1.54
1	A	417	ALA	N-CA	-5.13	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	VAL	C-N	-5.13	1.27	1.33
1	A	300	ASN	CA-CB	-5.13	1.46	1.53
1	A	387	LEU	CA-C	-5.13	1.46	1.52
1	A	532	LEU	N-CA	-5.12	1.38	1.46
1	B	417	ALA	N-CA	-5.12	1.39	1.46
1	B	532	LEU	N-CA	-5.11	1.38	1.46
1	A	290	HIS	C-O	-5.11	1.18	1.24
1	B	244	VAL	CA-CB	5.10	1.60	1.54
1	B	269	ILE	CA-CB	5.10	1.60	1.54
1	B	480	TYR	CA-C	-5.10	1.46	1.52
1	A	229	VAL	CA-C	5.09	1.59	1.52
1	B	443	ARG	CA-C	-5.09	1.46	1.52
1	B	530	ARG	C-N	-5.09	1.27	1.33
1	B	387	LEU	CA-C	-5.08	1.46	1.52
1	A	407	PHE	CA-C	5.08	1.59	1.52
1	B	229	VAL	CA-C	5.08	1.59	1.52
1	B	505	PHE	CA-C	-5.08	1.46	1.52
1	A	443	ARG	CA-C	-5.08	1.46	1.52
1	A	471	PHE	N-CA	5.07	1.52	1.46
1	B	300	ASN	CA-CB	-5.07	1.46	1.53
1	A	428	VAL	CA-C	-5.07	1.46	1.52
1	B	264	ARG	CA-CB	-5.06	1.45	1.53
1	A	264	ARG	CA-CB	-5.06	1.45	1.53
1	A	521	LEU	C-O	5.06	1.30	1.23
1	B	324	SER	N-CA	5.05	1.52	1.46
1	B	471	PHE	N-CA	5.05	1.52	1.46
1	B	545	TYR	N-CA	5.05	1.52	1.46
1	B	290	HIS	C-O	-5.04	1.18	1.24
1	A	505	PHE	CA-C	-5.04	1.46	1.52
1	B	407	PHE	CA-C	5.04	1.59	1.52
1	A	269	ILE	CA-CB	5.04	1.60	1.54
1	A	358	HIS	ND1-CE1	5.04	1.37	1.32
1	A	324	SER	N-CA	5.04	1.52	1.46
1	B	445	ALA	CA-CB	-5.04	1.45	1.53
1	A	530	ARG	C-N	-5.03	1.27	1.33
1	B	428	VAL	CA-C	-5.03	1.46	1.52
1	B	460	HIS	ND1-CE1	5.03	1.37	1.32
1	A	288	VAL	CA-CB	5.02	1.60	1.54
1	A	321	CYS	N-CA	5.02	1.52	1.46
1	B	307	ILE	CB-CG1	-5.02	1.43	1.53
1	A	307	ILE	CB-CG1	-5.02	1.43	1.53
1	B	489	LEU	C-N	5.02	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	521	LEU	C-O	5.02	1.30	1.23
1	A	445	ALA	CA-CB	-5.02	1.45	1.53
1	B	288	VAL	CA-CB	5.01	1.60	1.54
1	B	394	MET	C-O	5.01	1.29	1.23
1	B	316	VAL	CA-C	5.01	1.59	1.52
1	B	261	ARG	NE-CZ	5.01	1.38	1.33
1	A	316	VAL	CA-C	5.00	1.59	1.52
1	A	394	MET	C-O	5.00	1.29	1.23

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	VAL	N-CA-C	-11.42	99.18	110.72
1	A	229	VAL	N-CA-C	-11.40	99.20	110.72
1	B	544	TYR	N-CA-C	-10.15	100.30	111.36
1	A	544	TYR	N-CA-C	-10.14	100.31	111.36
1	B	542	TRP	N-CA-C	-10.11	100.09	111.82
1	A	542	TRP	N-CA-C	-10.10	100.11	111.82
1	A	250	TYR	N-CA-C	-10.05	99.73	112.90
1	B	250	TYR	N-CA-C	-10.05	99.73	112.90
1	A	597	ASN	N-CA-C	-9.88	99.53	111.69
1	B	597	ASN	N-CA-C	-9.87	99.56	111.69
1	A	525	LYS	N-CA-C	-9.79	101.35	113.20
1	B	525	LYS	N-CA-C	-9.79	101.35	113.20
1	A	602	ASN	OD1-CG-ND2	-9.68	112.92	122.60
1	B	519	TRP	N-CA-C	-9.64	100.71	114.12
1	A	399	LEU	N-CA-C	-9.64	100.27	112.90
1	A	519	TRP	N-CA-C	-9.64	100.72	114.12
1	B	602	ASN	OD1-CG-ND2	-9.64	112.96	122.60
1	B	279	ASN	N-CA-C	9.63	121.38	111.07
1	A	279	ASN	N-CA-C	9.63	121.37	111.07
1	B	399	LEU	N-CA-C	-9.61	100.31	112.90
1	B	514	ASP	CA-CB-CG	9.61	122.20	112.60
1	A	514	ASP	CA-CB-CG	9.59	122.19	112.60
1	B	600	LEU	N-CA-C	-9.41	100.57	112.90
1	A	600	LEU	N-CA-C	-9.41	100.57	112.90
1	A	293	ILE	N-CA-C	-9.26	101.84	110.82
1	B	293	ILE	N-CA-C	-9.26	101.84	110.82
1	B	490	SER	N-CA-C	9.19	122.14	111.11
1	A	490	SER	N-CA-C	9.19	122.13	111.11
1	A	518	ASP	CA-CB-CG	9.16	121.76	112.60
1	B	518	ASP	CA-CB-CG	9.15	121.75	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	TYR	N-CA-C	9.13	122.16	111.02
1	A	385	PHE	CA-CB-CG	9.12	122.92	113.80
1	B	511	TYR	N-CA-C	9.12	122.14	111.02
1	B	393	SER	N-CA-C	9.11	120.82	111.07
1	B	385	PHE	CA-CB-CG	9.10	122.90	113.80
1	A	393	SER	N-CA-C	9.08	120.79	111.07
1	B	505	PHE	N-CA-C	9.06	120.77	111.07
1	A	463	ASN	N-CA-C	-9.05	99.86	112.45
1	B	463	ASN	N-CA-C	-9.05	99.86	112.45
1	A	505	PHE	N-CA-C	9.05	120.75	111.07
1	A	472	PHE	CA-CB-CG	8.96	122.76	113.80
1	B	472	PHE	CA-CB-CG	8.93	122.73	113.80
1	B	251	GLY	CA-C-O	-8.86	116.11	122.23
1	A	251	GLY	CA-C-O	-8.86	116.12	122.23
1	B	306	ASN	N-CA-C	8.74	121.60	111.11
1	A	306	ASN	N-CA-C	8.74	121.60	111.11
1	B	541	THR	N-CA-C	-8.66	102.46	113.72
1	A	541	THR	N-CA-C	-8.64	102.49	113.72
1	A	605	LYS	N-CA-C	-8.58	101.14	111.69
1	B	605	LYS	N-CA-C	-8.55	101.17	111.69
1	B	472	PHE	N-CA-C	8.54	121.36	111.11
1	A	472	PHE	N-CA-C	8.52	121.34	111.11
1	B	575	MET	N-CA-C	-8.49	101.98	111.82
1	A	575	MET	N-CA-C	-8.47	102.00	111.82
1	B	381	ASN	N-CA-C	8.38	122.82	110.17
1	A	381	ASN	N-CA-C	8.36	122.80	110.17
1	B	413	THR	CA-C-O	-8.25	112.59	121.99
1	A	413	THR	CA-C-O	-8.25	112.59	121.99
1	A	302	LEU	N-CA-C	-8.22	99.17	110.35
1	B	302	LEU	N-CA-C	-8.22	99.17	110.35
1	A	273	LEU	N-CA-C	8.18	120.92	111.11
1	A	429	SER	N-CA-C	-8.16	100.13	111.39
1	B	273	LEU	N-CA-C	8.16	120.90	111.11
1	B	522	PHE	CA-CB-CG	8.15	121.95	113.80
1	B	503	ALA	N-CA-C	8.14	119.78	111.07
1	B	340	LEU	N-CA-C	-8.13	102.24	112.90
1	B	429	SER	N-CA-C	-8.13	100.17	111.39
1	A	503	ALA	N-CA-C	8.12	119.76	111.07
1	A	340	LEU	N-CA-C	-8.12	102.26	112.90
1	A	522	PHE	CA-CB-CG	8.09	121.89	113.80
1	B	534	GLU	N-CA-C	-8.06	102.47	111.82
1	A	294	PHE	CA-CB-CG	8.04	121.84	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	GLU	N-CA-C	-8.04	102.50	111.82
1	B	294	PHE	CA-CB-CG	8.02	121.82	113.80
1	B	496	PHE	N-CA-C	8.01	120.72	111.11
1	A	496	PHE	N-CA-C	8.00	120.71	111.11
1	B	514	ASP	N-CA-C	-7.96	102.20	112.23
1	A	514	ASP	N-CA-C	-7.96	102.20	112.23
1	A	606	PHE	CA-CB-CG	-7.96	105.84	113.80
1	B	308	MET	N-CA-C	7.94	119.93	111.28
1	B	606	PHE	CA-CB-CG	-7.93	105.87	113.80
1	A	432	HIS	N-CA-C	-7.93	103.30	113.77
1	A	308	MET	N-CA-C	7.93	119.92	111.28
1	B	432	HIS	N-CA-C	-7.92	103.31	113.77
1	A	530	ARG	CA-C-O	-7.79	111.54	120.58
1	B	530	ARG	CA-C-O	-7.79	111.55	120.58
1	A	478	HIS	ND1-CE1-NE2	-7.75	100.65	108.40
1	B	478	HIS	ND1-CE1-NE2	-7.75	100.65	108.40
1	B	252	PHE	N-CA-C	-7.71	102.96	113.30
1	A	252	PHE	N-CA-C	-7.71	102.97	113.30
1	A	470	SER	N-CA-C	-7.65	102.28	111.69
1	B	470	SER	N-CA-C	-7.65	102.28	111.69
1	B	280	VAL	N-CA-C	7.63	118.16	110.23
1	A	280	VAL	N-CA-C	7.60	118.14	110.23
1	A	264	ARG	N-CA-C	7.57	120.25	111.02
1	B	264	ARG	N-CA-C	7.55	120.23	111.02
1	A	407	PHE	N-CA-C	-7.53	102.74	112.23
1	B	407	PHE	N-CA-C	-7.53	102.75	112.23
1	B	481	HIS	ND1-CE1-NE2	7.41	115.81	108.40
1	A	481	HIS	ND1-CE1-NE2	7.39	115.79	108.40
1	B	490	SER	CA-C-O	7.39	128.81	120.90
1	A	490	SER	CA-C-O	7.36	128.78	120.90
1	A	602	ASN	N-CA-C	-7.32	103.31	112.90
1	B	602	ASN	N-CA-C	-7.31	103.32	112.90
1	B	530	ARG	N-CA-C	7.23	120.22	109.59
1	B	536	ILE	N-CA-CB	-7.23	102.79	111.90
1	A	536	ILE	N-CA-CB	-7.21	102.81	111.90
1	A	530	ARG	N-CA-C	7.20	120.17	109.59
1	A	354	THR	N-CA-C	-7.18	101.27	110.53
1	B	354	THR	N-CA-C	-7.17	101.28	110.53
1	B	555	ARG	N-CA-C	7.17	119.17	111.36
1	A	298	PRO	N-CA-C	-7.12	104.03	113.65
1	A	555	ARG	N-CA-C	7.11	119.11	111.36
1	B	298	PRO	N-CA-C	-7.11	104.05	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	LYS	N-CA-C	-7.10	102.59	111.11
1	B	243	VAL	N-CA-C	7.09	117.81	110.36
1	A	491	LYS	N-CA-C	-7.09	102.60	111.11
1	A	243	VAL	N-CA-C	7.08	117.80	110.36
1	A	306	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	B	504	ILE	N-CA-C	-7.05	103.42	110.62
1	A	504	ILE	N-CA-C	-7.05	103.43	110.62
1	B	306	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	B	381	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	381	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	557	SER	CA-C-O	-7.01	113.11	120.55
1	A	294	PHE	N-CA-C	7.00	121.27	112.87
1	B	557	SER	CA-C-O	-7.00	113.13	120.55
1	B	294	PHE	N-CA-C	7.00	121.27	112.87
1	A	588	PHE	N-CA-C	6.98	122.88	111.37
1	B	492	GLU	CA-C-O	-6.97	114.20	121.87
1	B	588	PHE	N-CA-C	6.95	122.84	111.37
1	B	239	LEU	N-CA-C	6.95	119.70	111.71
1	A	492	GLU	CA-C-O	-6.93	114.24	121.87
1	A	239	LEU	N-CA-C	6.91	119.66	111.71
1	B	398	PHE	CA-CB-CG	-6.90	106.90	113.80
1	A	398	PHE	CA-CB-CG	-6.89	106.91	113.80
1	B	276	TRP	N-CA-C	-6.88	103.56	112.23
1	B	345	LEU	CA-C-O	-6.86	113.61	120.82
1	A	276	TRP	N-CA-C	-6.86	103.59	112.23
1	A	345	LEU	CA-C-O	-6.86	113.62	120.82
1	B	279	ASN	CA-CB-CG	-6.78	105.82	112.60
1	A	279	ASN	CA-CB-CG	-6.77	105.83	112.60
1	B	484	THR	N-CA-C	-6.76	104.90	113.01
1	A	484	THR	N-CA-C	-6.75	104.91	113.01
1	A	292	LEU	N-CA-C	6.70	118.66	111.36
1	B	450	ARG	N-CA-C	6.69	118.23	111.07
1	A	450	ARG	N-CA-C	6.69	118.22	111.07
1	B	292	LEU	N-CA-C	6.68	118.65	111.36
1	A	289	ASN	CA-CB-CG	-6.68	105.92	112.60
1	A	430	LEU	N-CA-C	-6.64	104.04	111.28
1	B	289	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	430	LEU	N-CA-C	-6.63	104.05	111.28
1	A	255	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	367	ARG	N-CA-C	-6.58	103.94	112.23
1	B	554	LEU	N-CA-C	6.58	120.52	112.23
1	B	255	ASN	OD1-CG-ND2	-6.57	116.03	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	N-CA-C	-6.56	103.96	112.23
1	B	413	THR	N-CA-C	6.56	118.48	110.41
1	A	413	THR	N-CA-C	6.56	118.48	110.41
1	A	554	LEU	N-CA-C	6.55	120.48	112.23
1	A	284	ARG	N-CA-C	6.55	118.97	111.11
1	B	443	ARG	N-CA-C	6.54	122.10	111.37
1	A	569	TYR	CA-C-O	-6.54	113.33	121.50
1	B	569	TYR	CA-C-O	-6.53	113.34	121.50
1	A	443	ARG	N-CA-C	6.53	122.07	111.37
1	B	284	ARG	N-CA-C	6.52	118.93	111.11
1	B	490	SER	CA-C-N	6.51	129.33	120.54
1	B	490	SER	C-N-CA	6.51	129.33	120.54
1	A	490	SER	CA-C-N	6.50	129.32	120.54
1	A	490	SER	C-N-CA	6.50	129.32	120.54
1	A	290	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	B	290	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	585	PHE	N-CA-C	6.46	117.99	111.07
1	B	312	SER	N-CA-C	6.46	117.98	111.07
1	A	257	ARG	N-CA-C	-6.46	103.53	111.40
1	B	585	PHE	N-CA-C	6.45	117.97	111.07
1	B	355	LYS	N-CA-C	6.44	119.84	112.57
1	B	257	ARG	N-CA-C	-6.43	103.55	111.40
1	A	355	LYS	N-CA-C	6.43	119.83	112.57
1	A	392	ASN	N-CA-C	-6.42	104.37	111.82
1	A	312	SER	N-CA-C	6.42	117.94	111.07
1	B	392	ASN	N-CA-C	-6.40	104.39	111.82
1	B	432	HIS	CB-CG-ND1	-6.38	113.13	122.70
1	A	432	HIS	CB-CG-ND1	-6.37	113.14	122.70
1	B	269	ILE	O-C-N	6.37	128.05	121.87
1	A	269	ILE	O-C-N	6.36	128.04	121.87
1	B	432	HIS	O-C-N	6.34	126.40	120.51
1	A	432	HIS	O-C-N	6.31	126.38	120.51
1	B	420	ALA	N-CA-C	-6.31	104.28	112.23
1	A	556	PHE	N-CA-C	6.30	120.43	112.87
1	B	556	PHE	N-CA-C	6.29	120.42	112.87
1	B	267	PHE	CA-CB-CG	-6.28	107.52	113.80
1	A	401	ILE	N-CA-CB	6.28	114.72	110.52
1	B	401	ILE	N-CA-CB	6.28	114.72	110.52
1	A	420	ALA	N-CA-C	-6.27	104.33	112.23
1	A	267	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	258	ALA	CA-C-N	6.21	126.83	119.94
1	A	258	ALA	C-N-CA	6.21	126.83	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	501	THR	N-CA-C	-6.21	104.59	111.36
1	B	258	ALA	CA-C-N	6.21	126.83	119.94
1	B	258	ALA	C-N-CA	6.21	126.83	119.94
1	B	496	PHE	CA-C-O	-6.21	114.26	120.90
1	A	501	THR	N-CA-C	-6.20	104.60	111.36
1	A	300	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	497	TYR	N-CA-C	-6.18	104.54	111.28
1	A	496	PHE	CA-C-O	-6.18	114.29	120.90
1	B	300	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	497	TYR	N-CA-C	-6.17	104.55	111.28
1	B	346	MET	N-CA-C	6.14	117.64	111.07
1	A	259	GLY	O-C-N	6.14	128.08	122.18
1	A	392	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	392	ASN	CA-C-O	-6.13	112.92	119.97
1	B	392	ASN	CA-C-O	-6.12	112.93	119.97
1	B	392	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	346	MET	N-CA-C	6.12	117.61	111.07
1	B	259	GLY	O-C-N	6.11	128.05	122.18
1	A	227	PHE	N-CA-C	-6.10	103.96	111.40
1	B	227	PHE	N-CA-C	-6.10	103.96	111.40
1	A	446	GLN	N-CA-C	6.04	117.54	111.07
1	B	446	GLN	N-CA-C	6.03	117.53	111.07
1	B	536	ILE	N-CA-C	6.03	116.87	107.28
1	A	573	ASP	N-CA-C	-6.03	104.62	111.07
1	A	536	ILE	N-CA-C	6.02	116.86	107.28
1	B	573	ASP	N-CA-C	-6.01	104.63	111.07
1	A	316	VAL	N-CA-C	-5.96	104.70	110.72
1	B	316	VAL	N-CA-C	-5.96	104.70	110.72
1	A	420	ALA	CA-C-O	-5.92	112.81	119.79
1	A	352	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	420	ALA	CA-C-O	-5.91	112.82	119.79
1	A	602	ASN	CB-CG-ND2	5.90	125.25	116.40
1	B	482	THR	CB-CA-C	-5.89	100.83	110.85
1	A	594	ARG	N-CA-C	5.89	118.46	111.33
1	A	391	LEU	N-CA-C	-5.89	104.99	111.82
1	B	352	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	419	LYS	N-CA-C	-5.87	104.79	113.72
1	B	419	LYS	N-CA-C	-5.87	104.80	113.72
1	A	482	THR	CB-CA-C	-5.87	100.88	110.85
1	B	594	ARG	N-CA-C	5.86	118.42	111.33
1	B	602	ASN	CB-CG-ND2	5.86	125.18	116.40
1	B	391	LEU	N-CA-C	-5.85	105.03	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	LEU	CA-C-O	-5.84	112.42	119.49
1	A	518	ASP	N-CA-C	5.84	121.02	111.37
1	B	431	LEU	CA-C-O	-5.84	112.42	119.49
1	B	518	ASP	N-CA-C	5.84	121.01	111.37
1	B	477	ALA	N-CA-C	5.83	121.00	111.37
1	A	323	LEU	N-CA-C	5.83	117.64	111.28
1	B	323	LEU	N-CA-C	5.83	117.64	111.28
1	A	477	ALA	N-CA-C	5.82	120.98	111.37
1	B	546	PHE	N-CA-C	5.81	118.36	111.33
1	A	499	TRP	N-CA-C	5.80	120.88	111.37
1	B	499	TRP	N-CA-C	5.79	120.87	111.37
1	A	546	PHE	N-CA-C	5.79	118.34	111.33
1	B	574	VAL	CB-CA-C	-5.78	104.47	112.04
1	B	299	ARG	N-CA-C	5.78	117.25	111.07
1	A	351	LEU	CD1-CG-CD2	5.76	123.47	110.80
1	A	346	MET	N-CA-CB	5.76	118.36	110.01
1	B	346	MET	N-CA-CB	5.75	118.35	110.01
1	A	227	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	574	VAL	CB-CA-C	-5.75	104.50	112.04
1	B	351	LEU	CD1-CG-CD2	5.75	123.45	110.80
1	A	299	ARG	N-CA-C	5.73	117.20	111.07
1	A	412	PRO	N-CA-C	5.72	120.00	111.41
1	A	390	GLN	N-CA-C	5.71	118.24	111.33
1	B	227	PHE	CA-CB-CG	-5.71	108.09	113.80
1	B	412	PRO	N-CA-C	5.71	119.97	111.41
1	B	390	GLN	N-CA-C	5.70	118.22	111.33
1	A	389	ASP	N-CA-C	5.69	117.48	111.28
1	B	389	ASP	N-CA-C	5.67	117.45	111.28
1	A	559	THR	CB-CA-C	5.62	120.41	110.85
1	B	559	THR	CB-CA-C	5.62	120.41	110.85
1	B	300	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	300	ASN	CB-CG-ND2	5.61	124.81	116.40
1	B	482	THR	CA-CB-OG1	-5.61	101.19	109.60
1	B	482	THR	N-CA-CB	5.59	118.43	110.16
1	A	482	THR	CA-CB-OG1	-5.58	101.22	109.60
1	A	482	THR	N-CA-CB	5.57	118.41	110.16
1	B	573	ASP	CA-C-O	-5.57	114.97	120.82
1	A	478	HIS	CB-CG-ND1	-5.57	114.35	122.70
1	B	478	HIS	CB-CG-ND1	-5.56	114.37	122.70
1	A	573	ASP	CA-C-O	-5.55	114.99	120.82
1	A	240	PHE	N-CA-C	-5.55	105.31	111.36
1	A	407	PHE	CA-CB-CG	-5.54	108.26	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	PHE	CA-CB-CG	-5.54	108.26	113.80
1	B	240	PHE	N-CA-C	-5.53	105.33	111.36
1	A	274	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	233	SER	N-CA-C	5.50	116.96	111.07
1	B	274	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	375	ALA	CA-C-O	-5.48	113.36	118.73
1	A	233	SER	N-CA-C	5.47	116.92	111.07
1	A	444	PHE	N-CA-C	5.47	117.67	111.11
1	B	444	PHE	N-CA-C	5.46	117.67	111.11
1	A	431	LEU	CA-C-N	5.46	130.19	121.62
1	A	431	LEU	C-N-CA	5.46	130.19	121.62
1	A	559	THR	N-CA-C	-5.44	105.43	111.36
1	A	522	PHE	CA-C-N	-5.44	115.21	122.72
1	A	522	PHE	C-N-CA	-5.44	115.21	122.72
1	B	338	ALA	N-CA-C	5.44	120.15	112.75
1	B	431	LEU	CA-C-N	5.44	130.16	121.62
1	B	431	LEU	C-N-CA	5.44	130.16	121.62
1	B	522	PHE	CA-C-N	-5.44	115.21	122.72
1	B	522	PHE	C-N-CA	-5.44	115.21	122.72
1	B	559	THR	N-CA-C	-5.44	105.43	111.36
1	B	476	PHE	N-CA-C	-5.43	104.39	111.02
1	A	476	PHE	N-CA-C	-5.43	104.40	111.02
1	B	375	ALA	CA-C-O	-5.42	113.41	118.73
1	A	338	ALA	N-CA-C	5.41	120.11	112.75
1	B	450	ARG	CA-C-O	5.40	126.49	120.82
1	A	450	ARG	CA-C-O	5.40	126.49	120.82
1	B	481	HIS	CB-CG-ND1	-5.37	114.64	122.70
1	A	584	VAL	N-CA-C	-5.37	105.30	110.72
1	B	584	VAL	N-CA-C	-5.36	105.31	110.72
1	A	481	HIS	CB-CG-ND1	-5.36	114.66	122.70
1	A	508	CYS	N-CA-C	-5.33	105.13	111.69
1	A	314	PHE	N-CA-C	5.29	117.73	111.33
1	B	508	CYS	N-CA-C	-5.29	105.18	111.69
1	B	487	TYR	N-CA-C	5.29	121.50	109.81
1	B	404	LEU	N-CA-C	-5.29	105.60	111.36
1	A	532	LEU	CD1-CG-CD2	5.28	122.41	110.80
1	A	404	LEU	N-CA-C	-5.28	105.61	111.36
1	A	423	HIS	N-CA-C	-5.27	108.11	114.75
1	A	471	PHE	N-CA-C	-5.27	105.71	111.82
1	A	308	MET	CB-CA-C	-5.27	102.05	110.79
1	A	487	TYR	N-CA-C	5.27	121.45	109.81
1	B	502	ALA	CA-C-N	-5.26	113.60	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	ALA	C-N-CA	-5.26	113.60	120.44
1	A	490	SER	CA-CB-OG	5.26	121.62	111.10
1	B	532	LEU	CD1-CG-CD2	5.26	122.37	110.80
1	A	410	ARG	N-CA-C	5.26	118.03	111.24
1	B	314	PHE	N-CA-C	5.26	117.69	111.33
1	B	490	SER	CA-CB-OG	5.26	121.62	111.10
1	B	308	MET	CB-CA-C	-5.25	102.07	110.79
1	A	231	LEU	N-CA-CB	5.25	117.63	110.01
1	A	418	GLY	O-C-N	5.25	128.47	122.33
1	B	471	PHE	N-CA-C	-5.25	105.73	111.82
1	A	502	ALA	CA-C-N	-5.25	113.62	120.44
1	A	502	ALA	C-N-CA	-5.25	113.62	120.44
1	B	410	ARG	N-CA-C	5.25	118.01	111.24
1	B	231	LEU	N-CA-CB	5.24	117.61	110.01
1	B	480	TYR	N-CA-C	5.24	119.97	111.37
1	B	423	HIS	N-CA-C	-5.24	108.15	114.75
1	B	447	CYS	N-CA-C	5.23	116.99	111.28
1	B	453	ASP	N-CA-C	-5.23	103.56	111.56
1	A	480	TYR	N-CA-C	5.23	119.95	111.37
1	A	570	ILE	CB-CG1-CD1	-5.22	102.83	113.80
1	A	552	LEU	N-CA-C	5.22	119.93	111.37
1	A	416	LYS	CA-C-O	-5.21	115.07	120.70
1	A	297	ASP	N-CA-C	-5.21	103.03	109.64
1	A	535	GLU	N-CA-C	-5.21	100.41	108.90
1	A	229	VAL	N-CA-CB	5.21	118.39	110.58
1	A	423	HIS	CB-CA-C	5.20	115.87	109.16
1	A	453	ASP	N-CA-C	-5.20	103.60	111.56
1	B	229	VAL	N-CA-CB	5.20	118.39	110.58
1	B	570	ILE	CB-CG1-CD1	-5.20	102.87	113.80
1	B	416	LYS	CA-C-O	-5.20	115.08	120.70
1	A	325	TYR	N-CA-CB	5.20	117.72	109.82
1	A	460	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	447	CYS	N-CA-C	5.20	116.94	111.28
1	A	475	ILE	N-CA-C	-5.20	105.34	111.00
1	B	297	ASP	N-CA-C	-5.20	103.04	109.64
1	B	418	GLY	O-C-N	5.19	128.41	122.33
1	B	535	GLU	N-CA-C	-5.19	100.43	108.90
1	A	306	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	325	TYR	N-CA-CB	5.19	117.71	109.82
1	B	552	LEU	N-CA-C	5.19	119.89	111.37
1	B	423	HIS	CB-CA-C	5.19	115.85	109.16
1	B	460	HIS	CB-CG-CD2	-5.18	124.46	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	ILE	N-CA-C	-5.18	105.35	111.00
1	A	529	ASN	N-CA-C	-5.17	102.73	110.23
1	B	372	VAL	CB-CA-C	5.17	118.50	111.88
1	B	534	GLU	CA-C-N	-5.16	115.72	122.99
1	B	534	GLU	C-N-CA	-5.16	115.72	122.99
1	A	534	GLU	CA-C-N	-5.16	115.72	122.99
1	A	534	GLU	C-N-CA	-5.16	115.72	122.99
1	A	372	VAL	CB-CA-C	5.15	118.47	111.88
1	B	529	ASN	N-CA-C	-5.15	102.76	110.23
1	B	306	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	246	ALA	CA-C-O	5.13	126.20	120.82
1	B	491	LYS	CB-CA-C	-5.12	102.61	110.81
1	A	491	LYS	CB-CA-C	-5.12	102.62	110.81
1	B	246	ALA	CA-C-O	5.12	126.19	120.82
1	A	481	HIS	CE1-NE2-CD2	-5.12	103.89	109.00
1	A	488	PRO	CB-CA-C	-5.11	105.06	111.71
1	B	488	PRO	CB-CA-C	-5.11	105.06	111.71
1	B	480	TYR	CA-C-N	-5.11	113.43	120.28
1	B	480	TYR	C-N-CA	-5.11	113.43	120.28
1	A	451	TYR	N-CA-C	5.10	117.50	111.33
1	B	341	CYS	N-CA-C	5.10	117.50	111.33
1	A	341	CYS	N-CA-C	5.10	117.50	111.33
1	A	500	ILE	N-CA-CB	5.09	116.16	110.51
1	B	586	ARG	N-CA-C	5.09	117.56	111.71
1	B	481	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
1	B	451	TYR	N-CA-C	5.08	117.48	111.33
1	A	480	TYR	CA-C-N	-5.08	113.47	120.28
1	A	480	TYR	C-N-CA	-5.08	113.47	120.28
1	B	458	PHE	CA-C-O	-5.08	113.21	120.16
1	B	475	ILE	CA-C-N	-5.08	113.74	120.79
1	B	475	ILE	C-N-CA	-5.08	113.74	120.79
1	B	382	PHE	CA-C-O	5.07	125.80	119.97
1	A	475	ILE	CA-C-N	-5.07	113.74	120.79
1	A	475	ILE	C-N-CA	-5.07	113.74	120.79
1	B	500	ILE	N-CA-CB	5.07	116.14	110.51
1	A	579	LEU	N-CA-CB	5.06	118.12	110.28
1	A	382	PHE	CA-C-O	5.06	125.79	119.97
1	A	537	VAL	N-CA-C	-5.06	105.46	110.62
1	A	543	PHE	N-CA-C	-5.06	105.76	111.28
1	B	537	VAL	N-CA-C	-5.06	105.46	110.62
1	B	543	PHE	N-CA-C	-5.06	105.77	111.28
1	A	471	PHE	CA-C-O	-5.05	114.16	119.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	579	LEU	N-CA-CB	5.04	118.10	110.28
1	A	458	PHE	CA-C-O	-5.04	113.25	120.16
1	A	586	ARG	N-CA-C	5.04	117.50	111.71
1	B	471	PHE	CA-C-O	-5.04	114.17	119.97
1	A	415	HIS	N-CA-C	-5.03	101.42	109.07
1	B	415	HIS	N-CA-C	-5.03	101.43	109.07
1	A	428	VAL	N-CA-CB	-5.01	102.96	111.23
1	B	227	PHE	CA-C-O	-5.01	115.19	120.55
1	B	428	VAL	N-CA-CB	-5.00	102.98	111.23

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	PHE	Sidechain
1	A	358	HIS	Sidechain
1	A	460	HIS	Sidechain
1	A	487	TYR	Sidechain
1	A	496	PHE	Sidechain
1	A	546	PHE	Sidechain
1	B	294	PHE	Sidechain
1	B	358	HIS	Sidechain
1	B	460	HIS	Sidechain
1	B	487	TYR	Sidechain
1	B	496	PHE	Sidechain
1	B	546	PHE	Sidechain

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	3175	0	3094	9	0
1	B	3175	0	3094	9	0
All	All	6350	0	6188	17	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 1.

All (17) 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:571:GLU:CD	1:A:572:GLY:N	2.42	0.77
1:B:571:GLU:CD	1:B:572:GLY:N	2.42	0.77
1:A:571:GLU:CG	1:A:572:GLY:N	2.73	0.52
1:B:571:GLU:CD	1:B:572:GLY:CA	2.84	0.51
1:B:571:GLU:CG	1:B:572:GLY:N	2.73	0.50
1:A:571:GLU:CD	1:A:572:GLY:CA	2.84	0.50
1:B:571:GLU:OE2	1:B:572:GLY:CA	2.61	0.49
1:B:475:ILE:O	1:B:476:PHE:C	2.54	0.49
1:A:475:ILE:O	1:A:476:PHE:C	2.54	0.49
1:A:571:GLU:OE2	1:A:572:GLY:CA	2.61	0.48
1:B:487:TYR:CE1	1:B:490:SER:HA	2.49	0.48
1:A:487:TYR:CE1	1:A:490:SER:HA	2.49	0.48
1:A:571:GLU:CD	1:A:571:GLU:C	2.84	0.45
1:A:230:GLY:C	1:B:230:GLY:C	2.85	0.45
1:B:571:GLU:CD	1:B:571:GLU:C	2.84	0.44
1:B:476:PHE:O	1:B:477:ALA:C	2.62	0.41
1:A:476:PHE:O	1:A:477:ALA:C	2.62	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	382/671 (57%)	369 (97%)	13 (3%)	0	100	100
1	B	382/671 (57%)	369 (97%)	13 (3%)	0	100	100
All	All	764/1342 (57%)	738 (97%)	26 (3%)	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	334/583 (57%)	332 (99%)	2 (1%)	78	80
1	B	334/583 (57%)	332 (99%)	2 (1%)	78	80
All	All	668/1166 (57%)	664 (99%)	4 (1%)	76	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
1	A	476	PHE
1	B	301	HIS
1	B	476	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	290	HIS
1	A	335	GLN
1	B	289	ASN
1	B	290	HIS
1	B	335	GLN
1	B	390	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

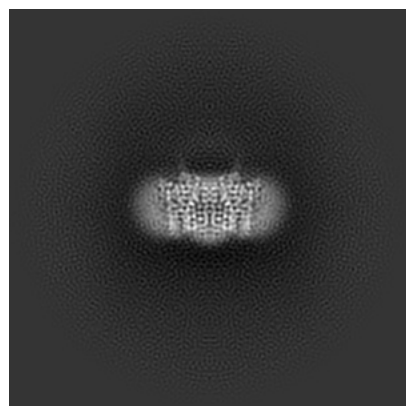
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61877. These allow visual inspection of the internal detail of the map and identification of artifacts.

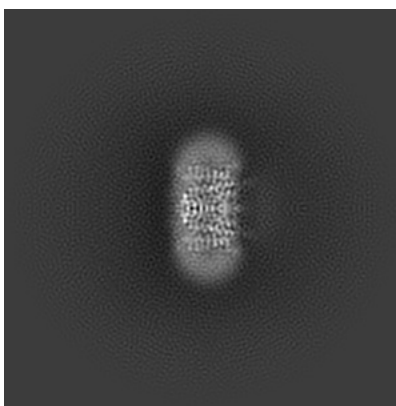
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

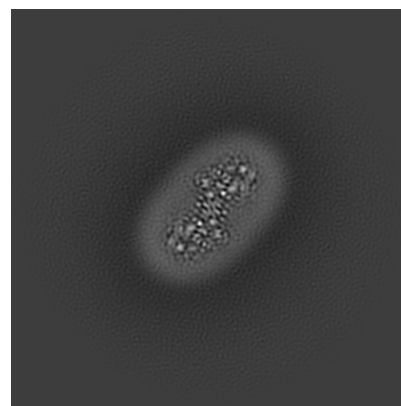
6.1.1 Primary map



X

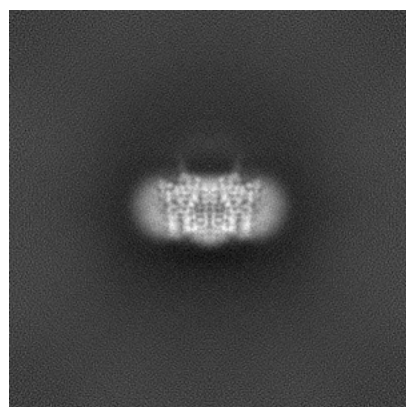


Y

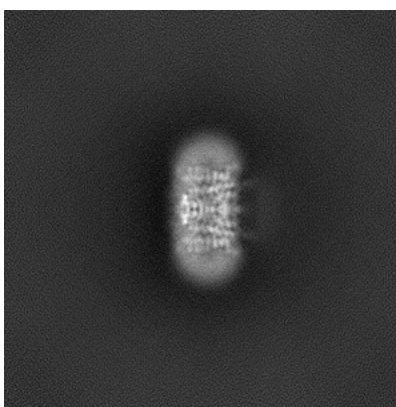


Z

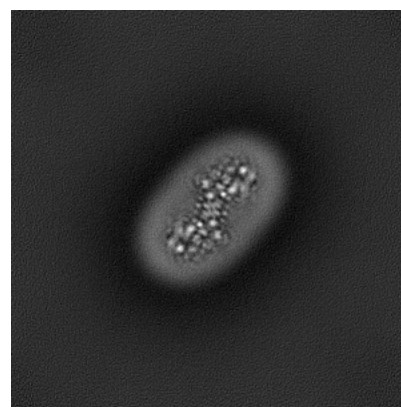
6.1.2 Raw map



X



Y

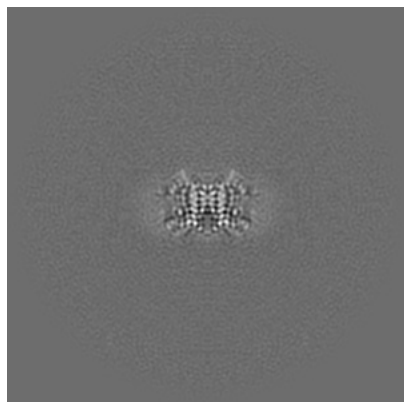


Z

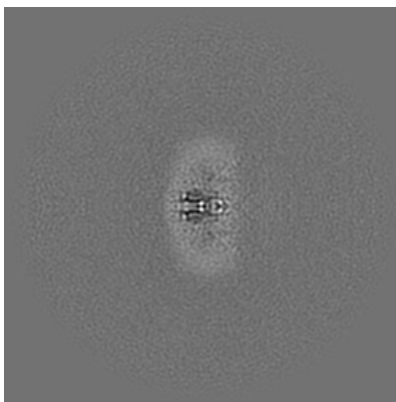
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

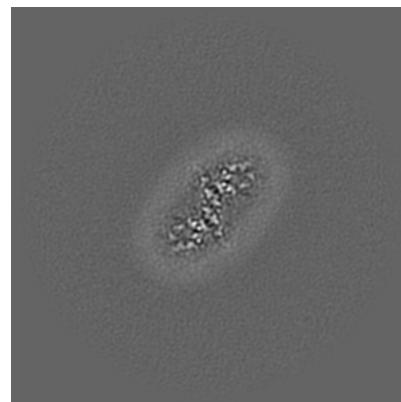
6.2.1 Primary map



X Index: 160

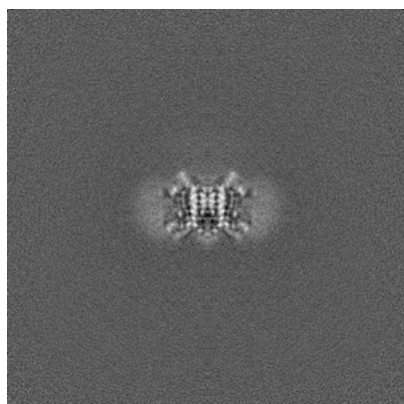


Y Index: 160

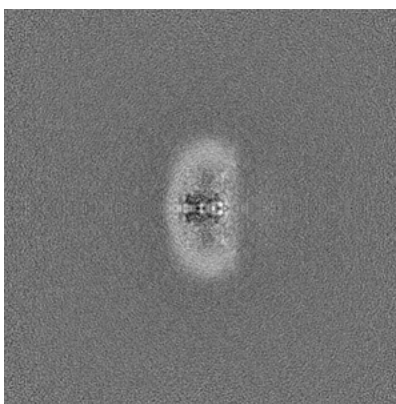


Z Index: 160

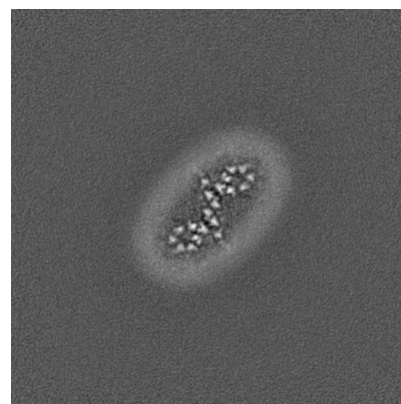
6.2.2 Raw map



X Index: 160



Y Index: 160

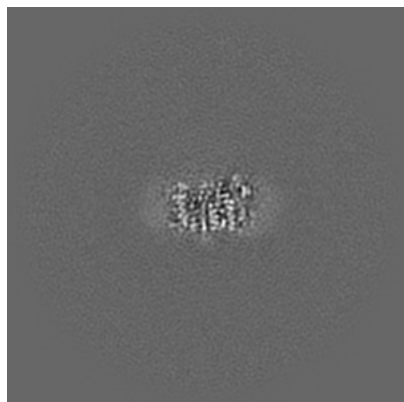


Z Index: 160

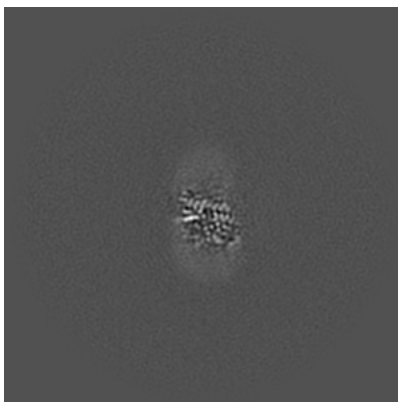
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

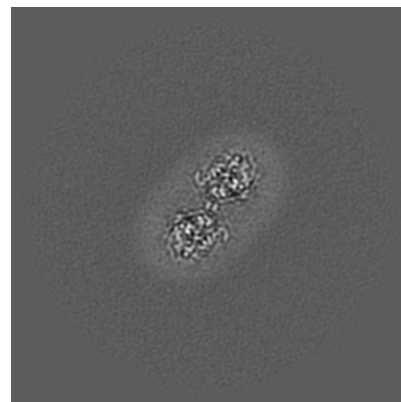
6.3.1 Primary map



X Index: 165

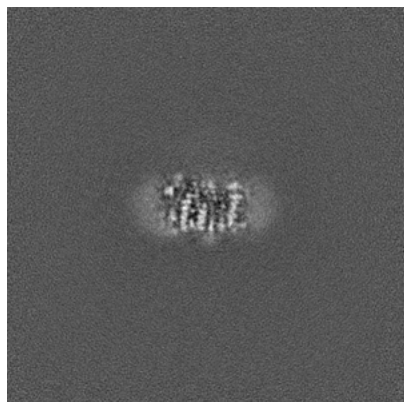


Y Index: 148

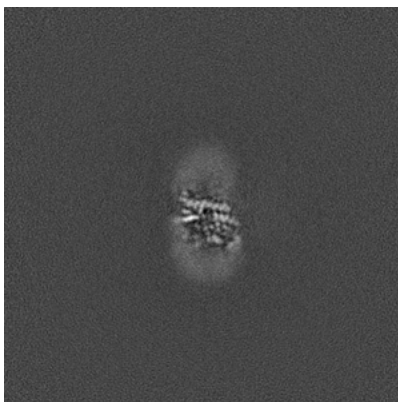


Z Index: 173

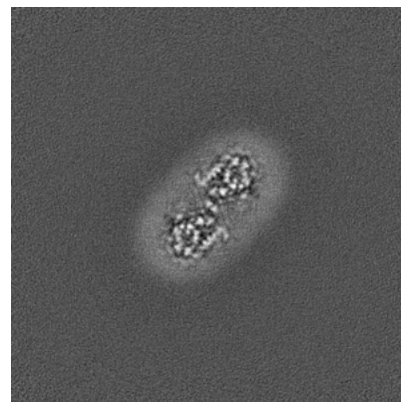
6.3.2 Raw map



X Index: 155



Y Index: 148

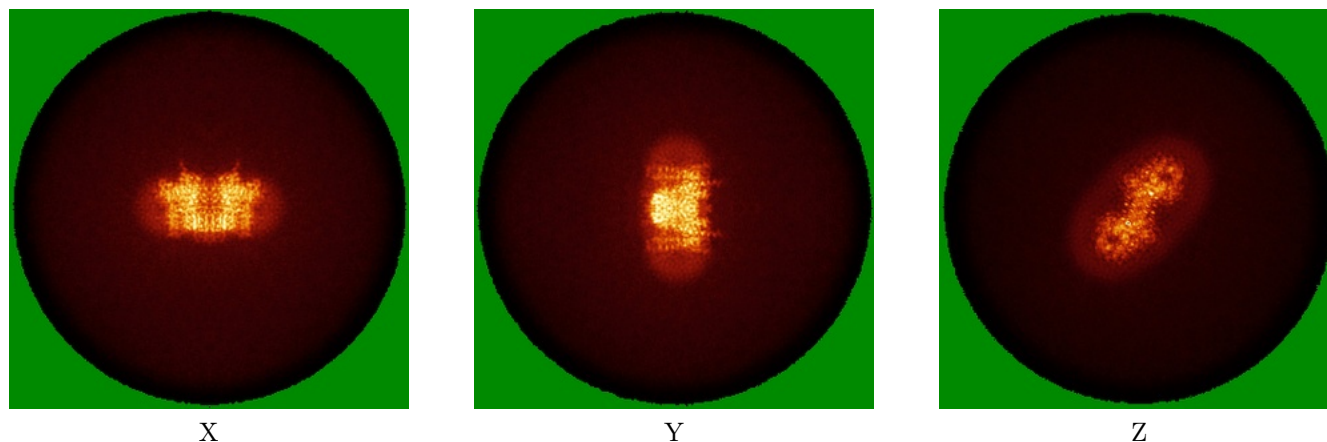


Z Index: 174

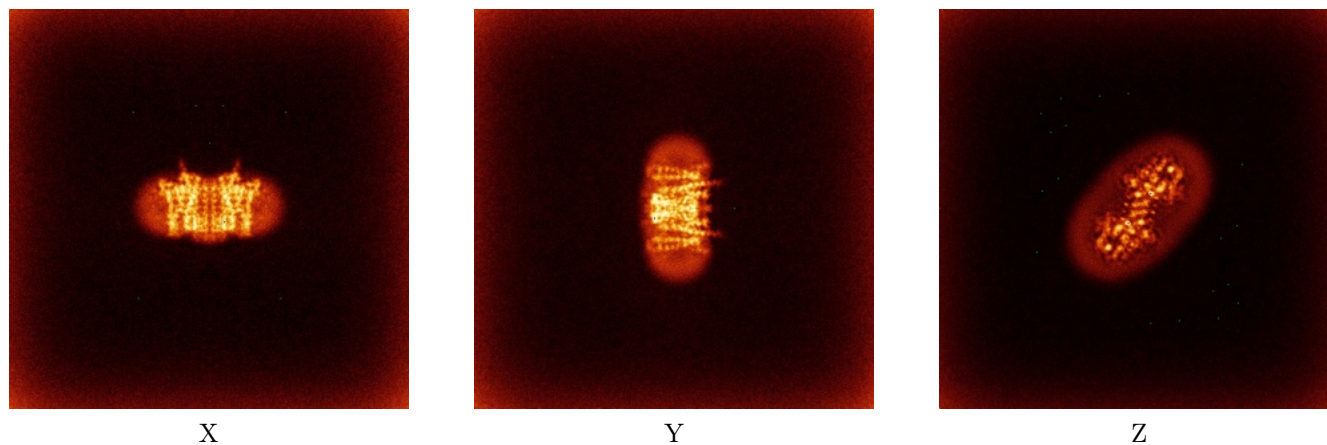
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

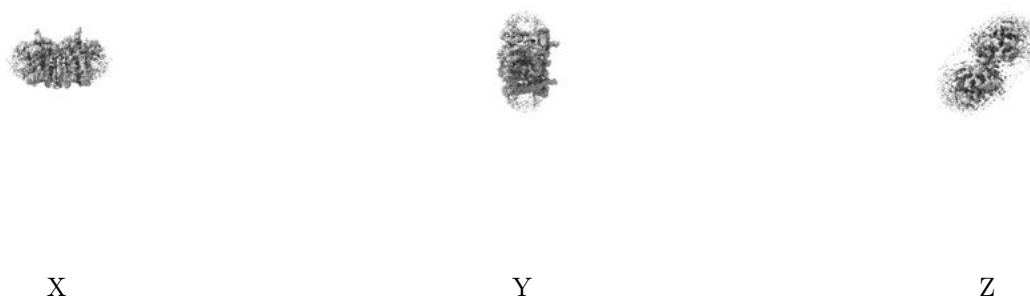
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

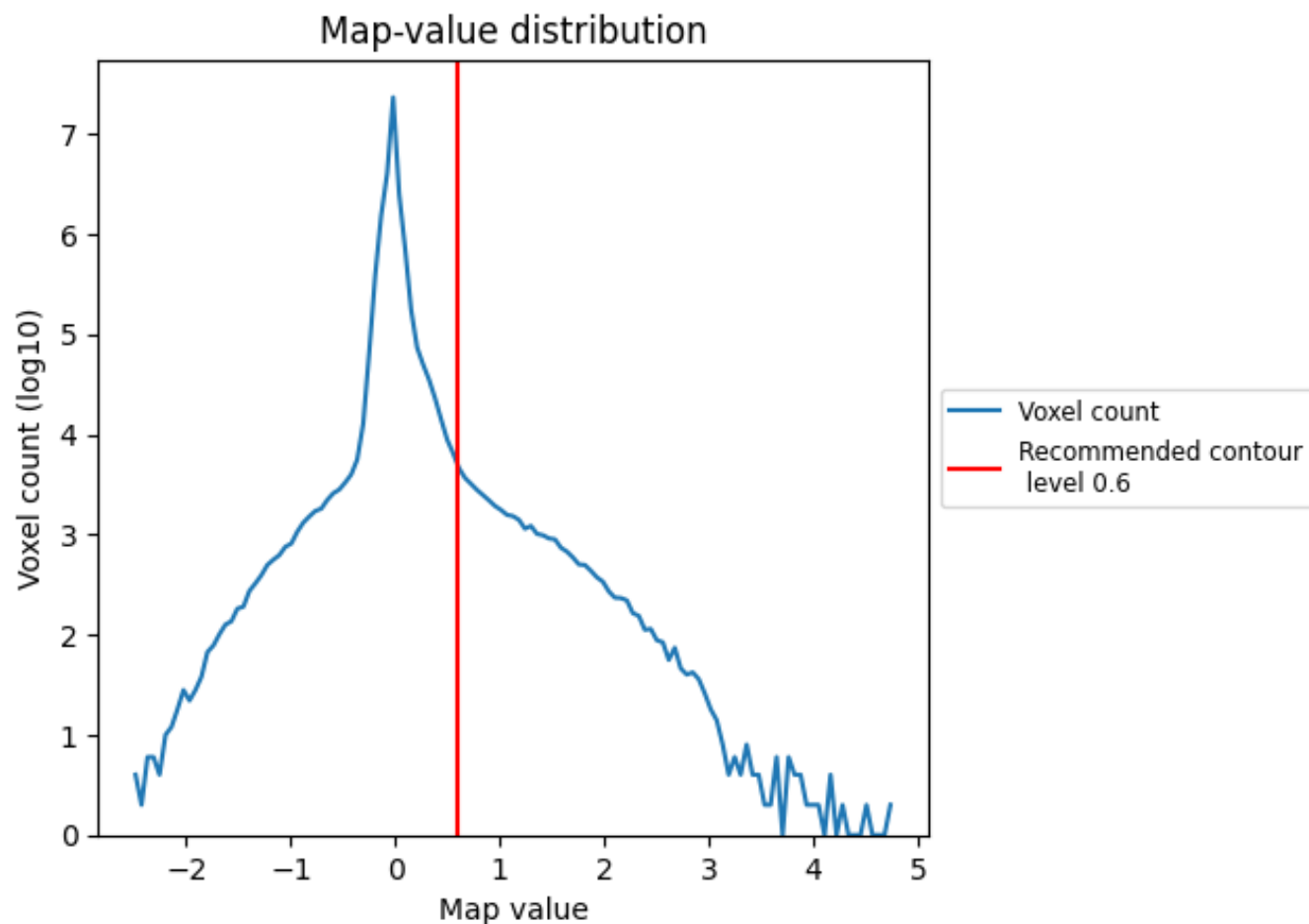
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

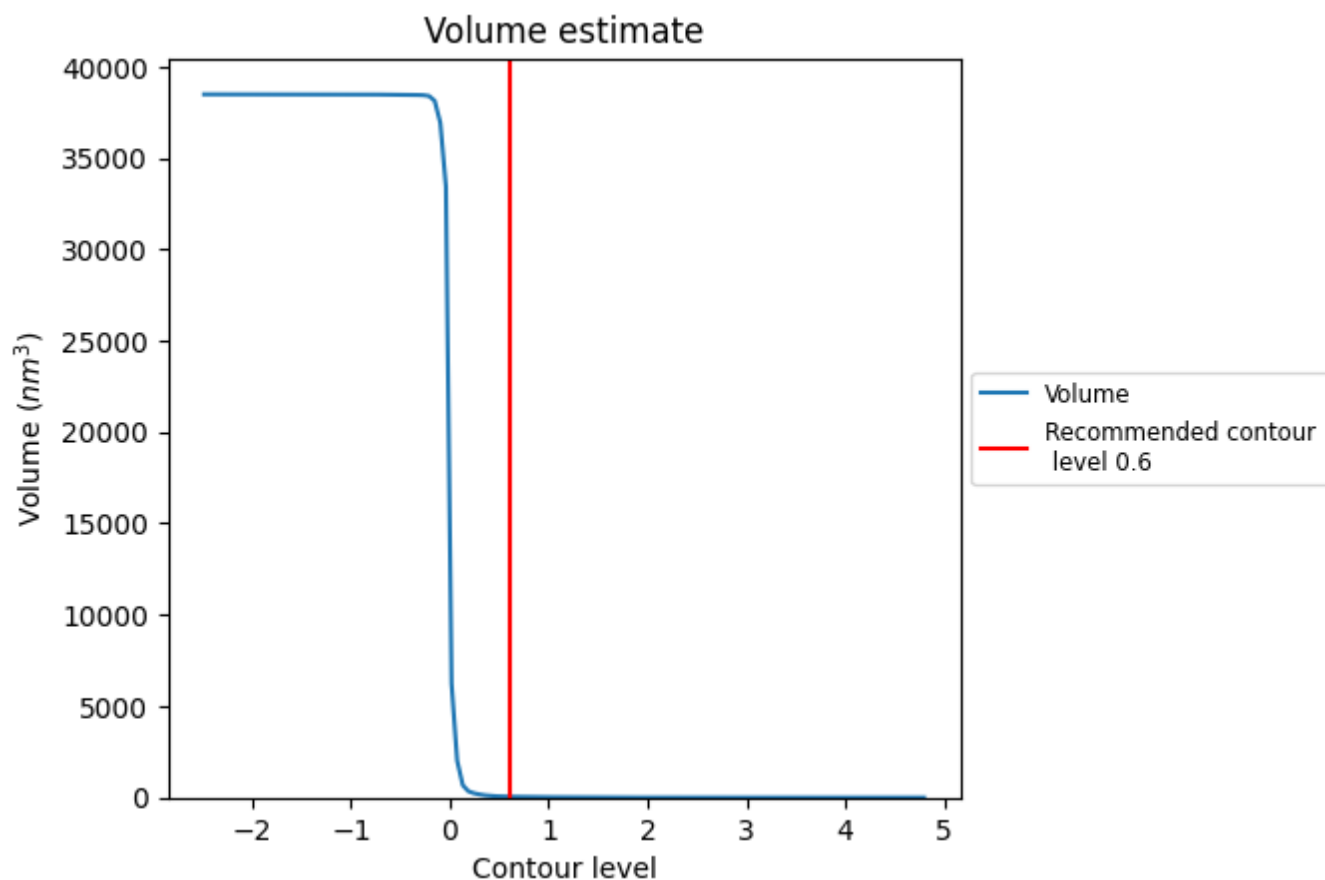
This section contains the results of statistical analysis of the map.

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.

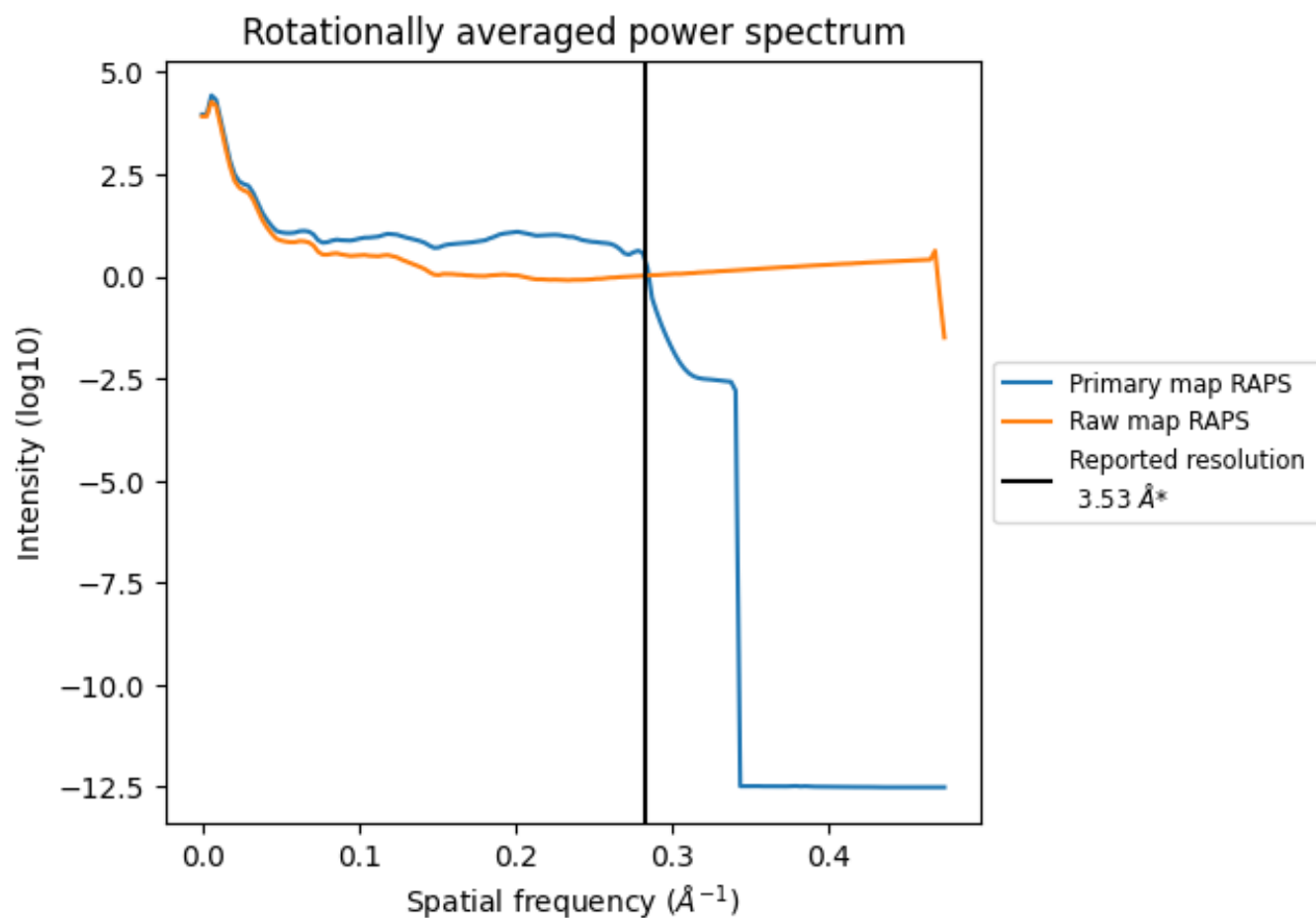
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm³; this corresponds to an approximate mass of 43 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 ⓘ

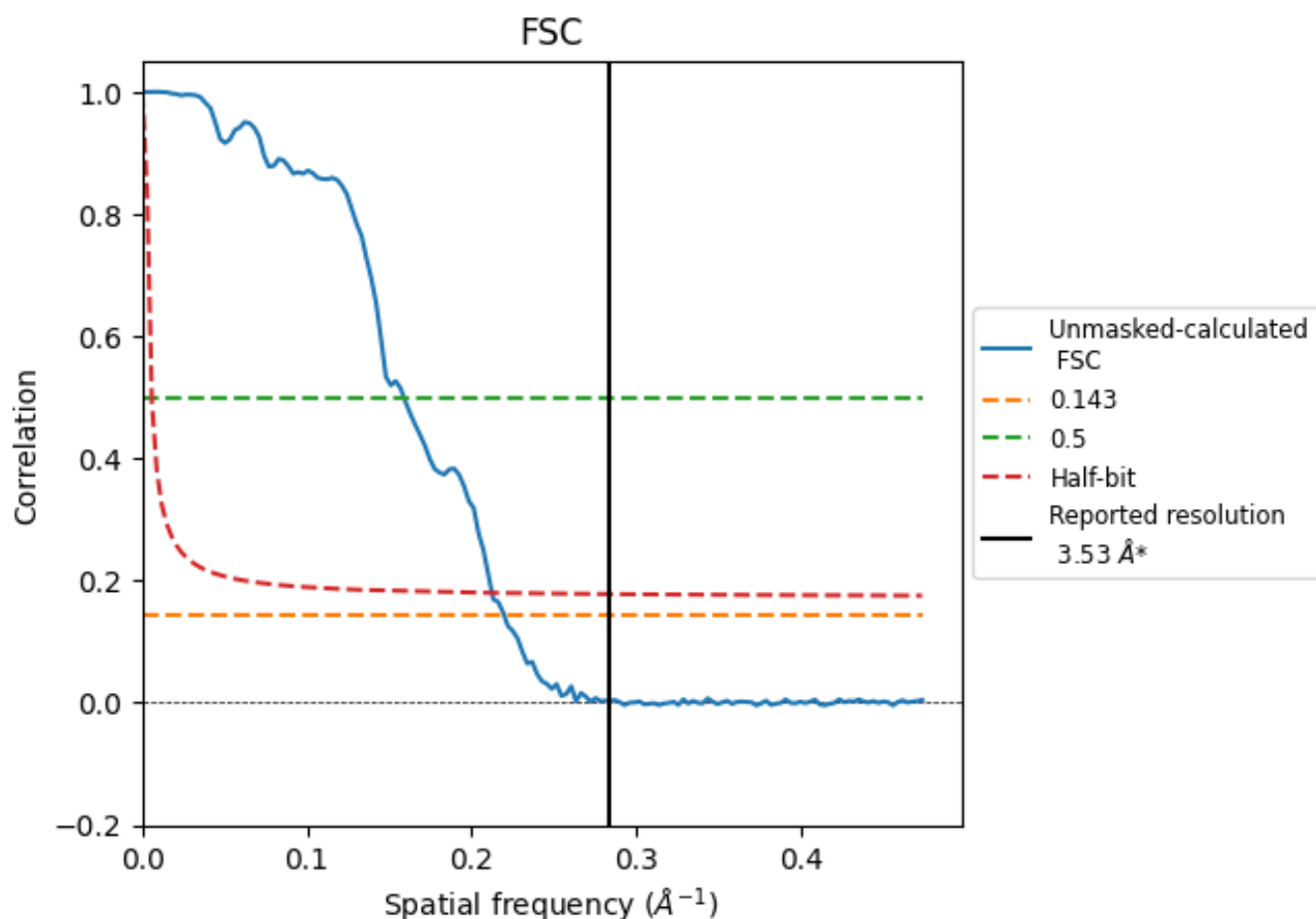


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

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 0.283 Å⁻¹

8.2 Resolution estimates [i](#)

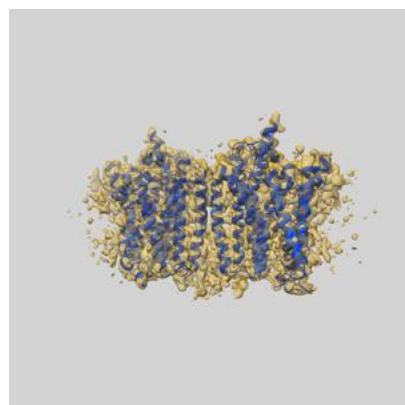
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	6.29	4.71

*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 4.55 differs from the reported value 3.53 by more than 10 %

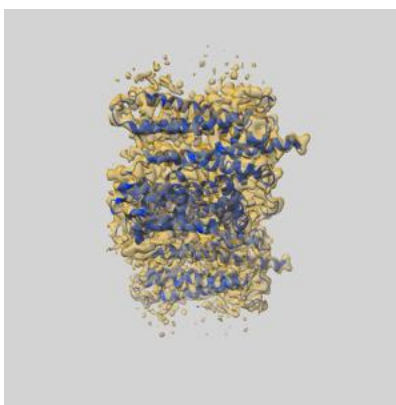
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61877 and PDB model 9JXR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

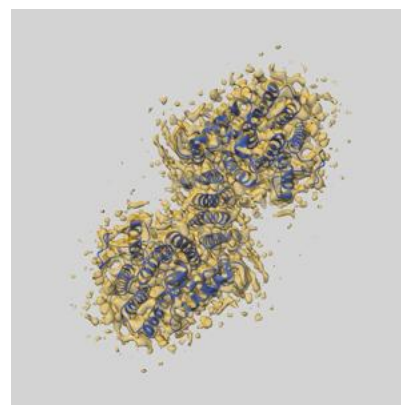
9.1 Map-model overlay [i](#)



X



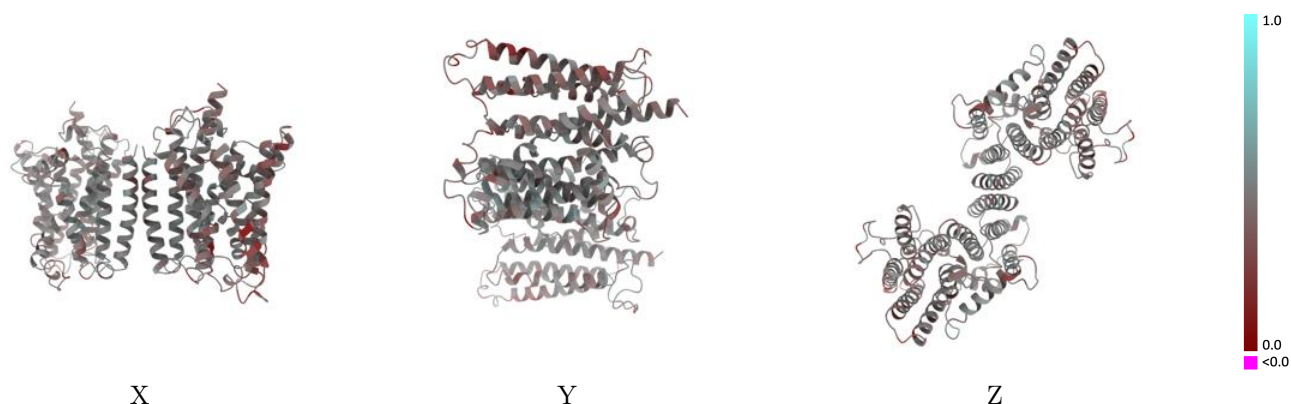
Y



Z

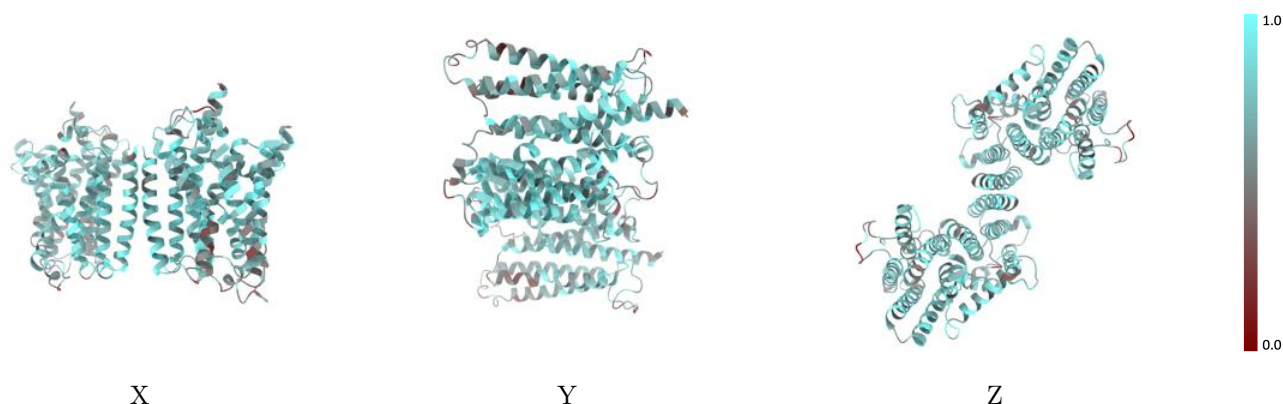
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



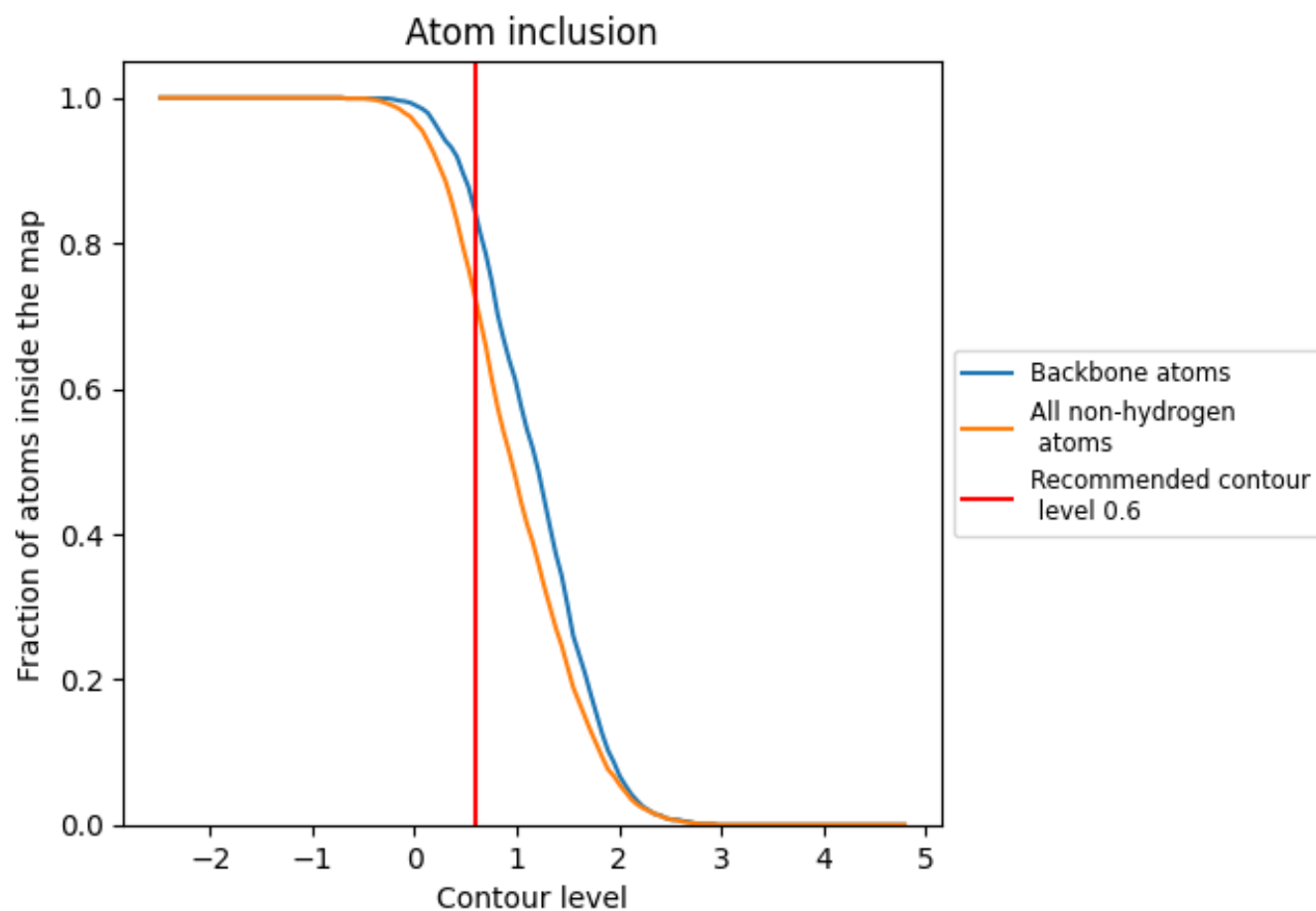
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 72% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.4290
A	0.7210	0.4300
B	0.7230	0.4280

