



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:40 PM UTC

PDB ID : 9JY1 / pdb_00009jy1
EMDB ID : EMD-61884
Title : delta epsilon/delta epsilon Fab-TCR tetramer
Authors : Wang, L.; Li, J.; Li, Z.
Deposited on : 2024-10-12
Resolution : 3.08 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

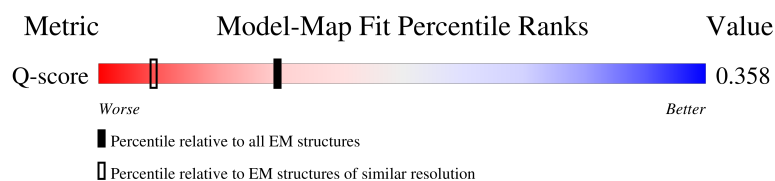
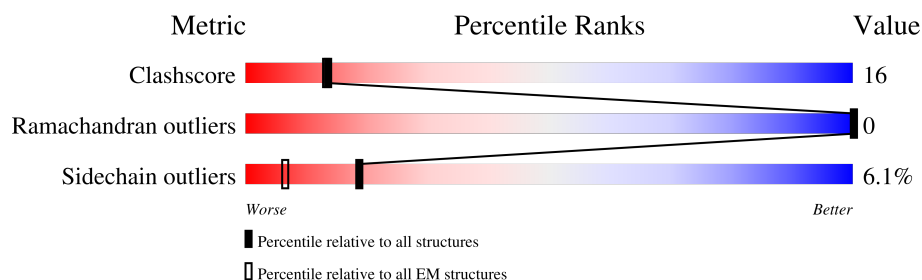
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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	14000 (2.58 - 3.58)

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	P	222	
1	R	222	
2	O	212	
2	Q	212	

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Mol	Chain	Length	Quality of chain
3	A	166	
3	B	166	
3	a	166	
3	b	166	
4	D	171	
4	d	171	
5	E	207	
5	F	207	
5	e	207	
5	f	207	
6	G	182	
6	g	182	
7	M	292	
7	m	292	
8	N	315	
8	n	315	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15642 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	196	Total	C	N	O	S	0	0
			1511	972	237	293	9		
1	R	196	Total	C	N	O	S	0	0
			1511	972	237	293	9		

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	209	Total	C	N	O	S	0	0
			1583	988	268	321	6		
2	Q	209	Total	C	N	O	S	0	0
			1583	988	268	321	6		

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
3	b	29	Total	C	N	O	S	0	0
			237	166	34	36	1		
3	A	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
3	B	29	Total	C	N	O	S	0	0
			237	166	34	36	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	165	SER	-	expression tag	UNP P20963
a	166	ALA	-	expression tag	UNP P20963
b	165	SER	-	expression tag	UNP P20963
b	166	ALA	-	expression tag	UNP P20963
A	165	SER	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	-	expression tag	UNP P20963
B	165	SER	-	expression tag	UNP P20963
B	166	ALA	-	expression tag	UNP P20963

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	105	Total	C	N	O	S	0	0
			817	521	135	155	6		
4	D	105	Total	C	N	O	S	0	0
			817	521	135	155	6		

- Molecule 5 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
5	f	118	Total	C	N	O	S	0	0
			933	594	148	183	8		
5	E	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
5	F	118	Total	C	N	O	S	0	0
			933	594	148	183	8		

- Molecule 6 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	115	Total	C	N	O	S	0	0
			907	582	150	168	7		
6	G	115	Total	C	N	O	S	0	0
			907	582	150	168	7		

- Molecule 7 is a protein called T cell receptor delta variable 2,T cell receptor delta constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	36	Total	C	N	O	S	0	0
			285	191	46	45	3		
7	M	36	Total	C	N	O	S	0	0
			285	191	46	45	3		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	114	LEU	-	linker	UNP A0JD36
m	115	GLY	-	linker	UNP A0JD36
m	116	MET	-	linker	UNP A0JD36
m	117	GLY	-	linker	UNP A0JD36
m	118	GLY	-	linker	UNP A0JD36
m	119	GLU	-	linker	UNP A0JD36
m	120	TYR	-	linker	UNP A0JD36
m	121	THR	-	linker	UNP A0JD36
m	122	ASP	-	linker	UNP A0JD36
m	123	LYS	-	linker	UNP A0JD36
m	124	LEU	-	linker	UNP A0JD36
m	125	ILE	-	linker	UNP A0JD36
m	126	PHE	-	linker	UNP A0JD36
m	127	GLY	-	linker	UNP A0JD36
m	128	LYS	-	linker	UNP A0JD36
m	129	GLY	-	linker	UNP A0JD36
m	130	THR	-	linker	UNP A0JD36
m	131	ARG	-	linker	UNP A0JD36
m	132	VAL	-	linker	UNP A0JD36
m	133	THR	-	linker	UNP A0JD36
m	134	VAL	-	linker	UNP A0JD36
m	135	GLU	-	linker	UNP A0JD36
m	136	PRO	-	linker	UNP A0JD36
m	137	ARG	-	linker	UNP A0JD36
M	114	LEU	-	linker	UNP A0JD36
M	115	GLY	-	linker	UNP A0JD36
M	116	MET	-	linker	UNP A0JD36
M	117	GLY	-	linker	UNP A0JD36
M	118	GLY	-	linker	UNP A0JD36
M	119	GLU	-	linker	UNP A0JD36
M	120	TYR	-	linker	UNP A0JD36
M	121	THR	-	linker	UNP A0JD36
M	122	ASP	-	linker	UNP A0JD36
M	123	LYS	-	linker	UNP A0JD36
M	124	LEU	-	linker	UNP A0JD36
M	125	ILE	-	linker	UNP A0JD36
M	126	PHE	-	linker	UNP A0JD36
M	127	GLY	-	linker	UNP A0JD36
M	128	LYS	-	linker	UNP A0JD36
M	129	GLY	-	linker	UNP A0JD36
M	130	THR	-	linker	UNP A0JD36
M	131	ARG	-	linker	UNP A0JD36
M	132	VAL	-	linker	UNP A0JD36

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Chain	Residue	Modelled	Actual	Comment	Reference
M	133	THR	-	linker	UNP A0JD36
M	134	VAL	-	linker	UNP A0JD36
M	135	GLU	-	linker	UNP A0JD36
M	136	PRO	-	linker	UNP A0JD36
M	137	ARG	-	linker	UNP A0JD36

- Molecule 8 is a protein called T cell receptor gamma variable 9,T cell receptor gamma constant 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	n	38	Total	C	N	O	S	0	0
			310	207	47	53	3		
8	N	38	Total	C	N	O	S	0	0
			310	207	47	53	3		

There are 44 discrepancies between the modelled and reference sequences:

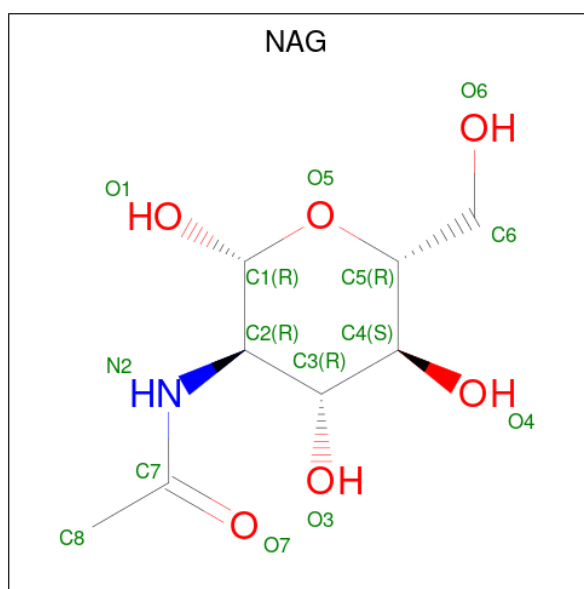
Chain	Residue	Modelled	Actual	Comment	Reference
n	104	ALA	-	linker	UNP Q99603
n	105	GLN	-	linker	UNP Q99603
n	106	GLN	-	linker	UNP Q99603
n	107	GLU	-	linker	UNP Q99603
n	108	LEU	-	linker	UNP Q99603
n	109	GLY	-	linker	UNP Q99603
n	110	LYS	-	linker	UNP Q99603
n	111	LYS	-	linker	UNP Q99603
n	112	ILE	-	linker	UNP Q99603
n	113	LYS	-	linker	UNP Q99603
n	114	VAL	-	linker	UNP Q99603
n	115	PHE	-	linker	UNP Q99603
n	116	GLY	-	linker	UNP Q99603
n	117	PRO	-	linker	UNP Q99603
n	118	GLY	-	linker	UNP Q99603
n	119	THR	-	linker	UNP Q99603
n	120	LYS	-	linker	UNP Q99603
n	121	LEU	-	linker	UNP Q99603
n	122	ILE	-	linker	UNP Q99603
n	123	ILE	-	linker	UNP Q99603
n	124	THR	-	linker	UNP Q99603
n	171	GLU	GLN	conflict	UNP P0CF51
N	104	ALA	-	linker	UNP Q99603
N	105	GLN	-	linker	UNP Q99603

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Chain	Residue	Modelled	Actual	Comment	Reference
N	106	GLN	-	linker	UNP Q99603
N	107	GLU	-	linker	UNP Q99603
N	108	LEU	-	linker	UNP Q99603
N	109	GLY	-	linker	UNP Q99603
N	110	LYS	-	linker	UNP Q99603
N	111	LYS	-	linker	UNP Q99603
N	112	ILE	-	linker	UNP Q99603
N	113	LYS	-	linker	UNP Q99603
N	114	VAL	-	linker	UNP Q99603
N	115	PHE	-	linker	UNP Q99603
N	116	GLY	-	linker	UNP Q99603
N	117	PRO	-	linker	UNP Q99603
N	118	GLY	-	linker	UNP Q99603
N	119	THR	-	linker	UNP Q99603
N	120	LYS	-	linker	UNP Q99603
N	121	LEU	-	linker	UNP Q99603
N	122	ILE	-	linker	UNP Q99603
N	123	ILE	-	linker	UNP Q99603
N	124	THR	-	linker	UNP Q99603
N	171	GLU	GLN	conflict	UNP P0CF51

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	d	1	Total	C	N	O	0
			14	8	1	5	

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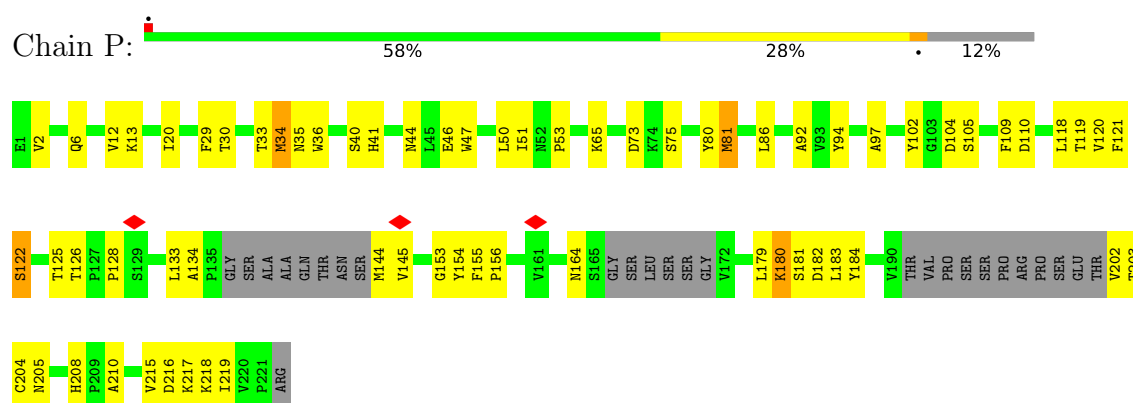
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Mol	Chain	Residues	Atoms				AltConf
9	d	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	

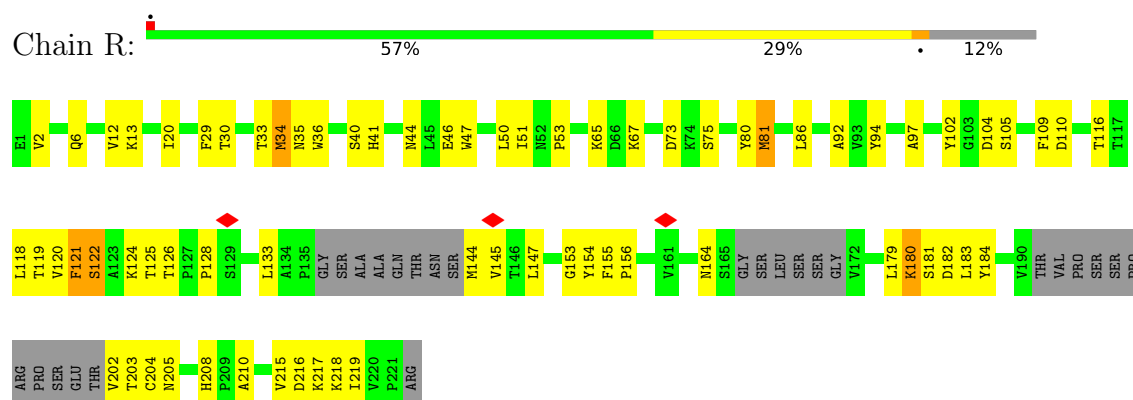
3 Residue-property plots

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

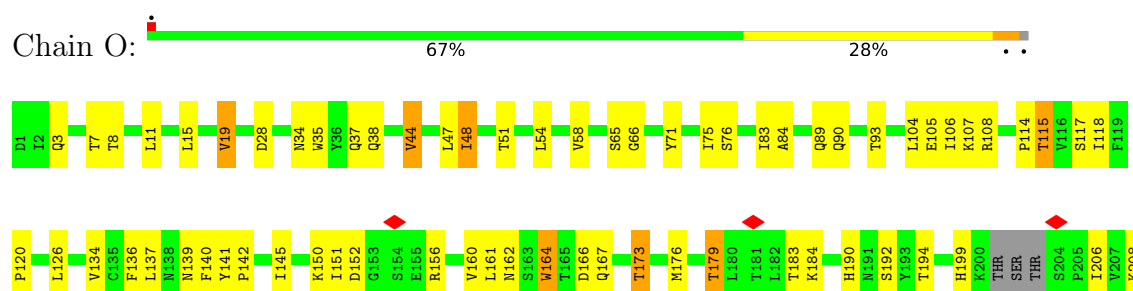
• Molecule 1: Fab heavy chain



• Molecule 1: Fab heavy chain



• Molecule 2: Fab light chain



SER
GLN
GLY
ILE
GLY
MET
LYS
LYS
GLY
GLU
ARG
ARG
ARG
GLY
LYS
GLY
HIS
ASP
GLY
LEU
TYR
GLN
GLY
LEU
SER
THR
GLY
ALA
THR
LYS
ASP
ASP
THR
TYR
ASP
ALA
LEU
LEU
PRO
PRO
ARG
SER
ALA

- Molecule 3: T-cell surface glycoprotein CD3 zeta chain

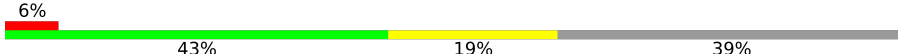
Chain B:  10% 7% 83%

MET
LYS
TRP
LYS
ALA
PHE
THR
ALA
ILE
GLN
ALA
LEU
PRO
ILE
GLY
GLU
ALA
GLN
SER
PHE
GLY
LEU
L27
K30
L31
C32
Y33
L34
L35
L39
F40
I41
Y42
G43
V44
I45
L46
T47
A48
L49
V53
K54
F55
SER
ARG
LYS
SER
MET
ALA
ASP
ALA
PRO
TYR
GLN

GLN
GLY
GLN
ASN
GLN
LEU
TYR
ASN
GLY
ARG
GLY
ARG
GLY
TYR
GLN
VAL
SER
LEU
THR
ALA
ASP
LYS
PRO
GLY
MET
HIS
GLN
LEU
PRO
PRO
ARG
SER
SER
ALA

ILE
GLY
MET
LYS
GLY
GLY
ARG
ARG
ARG
GLY
LYS
GLY
HIS
ASP
GLY
LEU
TYR
GLN
VAL
SER
LEU
THR
ALA
ASP
LYS
PRO
GLY
MET
HIS
GLN
LEU
PRO
PRO
ARG
SER
SER
ALA

- Molecule 4: T-cell surface glycoprotein CD3 delta chain

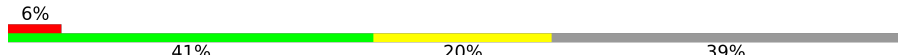
Chain d:  6% 43% 19% 39%

MET
GLU
HIS
SER
THR
PHE
LEU
SER
GLY
LEU
VAL
LEU
ALA
THR
LEU
LEU
GLN
VAL
SER
PRO
F22
K23
I24
V33
F34
N38
T39
E45
G46
T47
I55
T56
D59
L60
R63
P67
I70
Y71
C72
R73
N74
G75
T76
D77
Y79
V86
Q87
Y90

R93
M92
S95
C96
V97
D100
P101
A102
T103
V104
A105
V109
I113
A114
T115
L116
A119
L120
G121
V122
F123
C124
F125
A126
GLY
HIS
GLU
THR
ASN
ARG
LEU
SER
GLY
ALA
ALA
ASP
THR
GLN
ALA
Y71
LEU
LEU
ARG
ASN
ASP
GLN
VAL
TYR
GLN
PRO
LEU
ARG
ASP
ASP
ASP

ALA
GLN
TYR
SER
HIS
LEU
GLY
ASN
TRP
ALA
ALA
ASN
LYS

- Molecule 4: T-cell surface glycoprotein CD3 delta chain

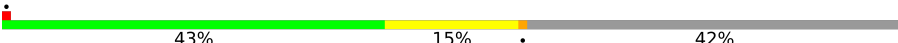
Chain D:  6% 41% 20% 39%

MET
GLU
HIS
SER
THR
PHE
LEU
SER
GLY
LEU
VAL
LEU
ALA
THR
LEU
LEU
GLN
VAL
SER
PRO
F22
K23
I24
L29
V33
F34
T39
S40
I41
E45
G46
T47
I55
T56
D59
L60
R63
P67
I70
Y71
R72
C73
N74
G75
T76
D77
K80
D81

V86
Q87
Y90
M92
S95
C96
V97
D100
P101
A102
T103
V104
A105
V109
I113
A114
T115
L116
A119
L120
G121
V122
F123
C124
F125
A126
GLY
HIS
GLU
THR
GLY
ARG
LEU
SER
GLY
ALA
ALA
ASP
THR
GLN
ALA
LEU
LEU
ARG
ASN
ASP
GLN
VAL
TYR
GLN
PRO
LEU
ARG

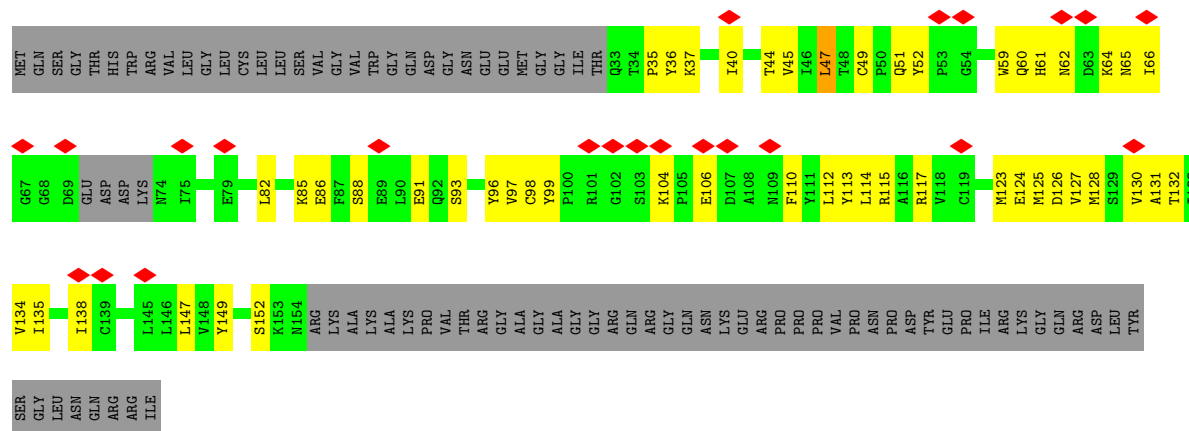
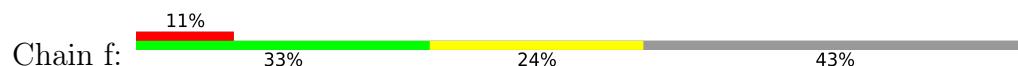
ASP
ARG
ASP
ASP
ALA
GLN
TYR
SER
HIS
LEU
GLY
GLY
ASN
TRP
ALA
ALA
ASN
LYS

- Molecule 5: T-cell surface glycoprotein CD3 epsilon chain

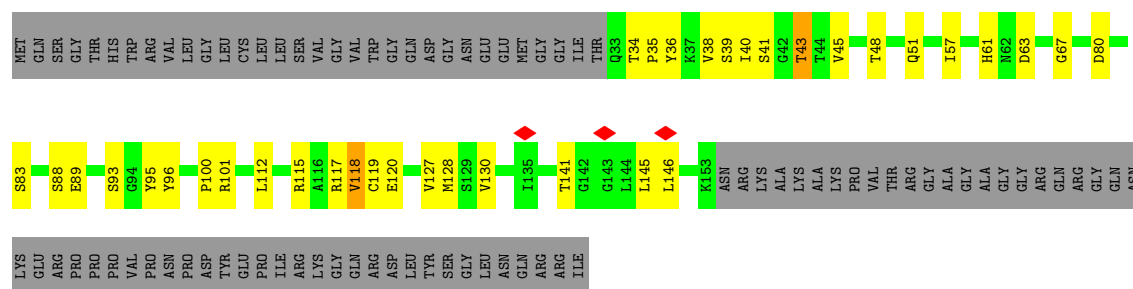
Chain e:  43% 15% 42%

MET
GLN
SER
GLY
THR
HIS
TRP
ARG
VAL
GLY
GLY
CYS
LEU
LEU
SER
VAL
GLY
VAL
TRP
GLY
GLN
ASP
GLY
ASN
GLU
MET
GLY
GLY
ILE
THR
Q33
T34
P35
V38
S39
I40
S41
G42
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V45
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C49
P50
Q51
E56
I57
D63
G67
S68
E69

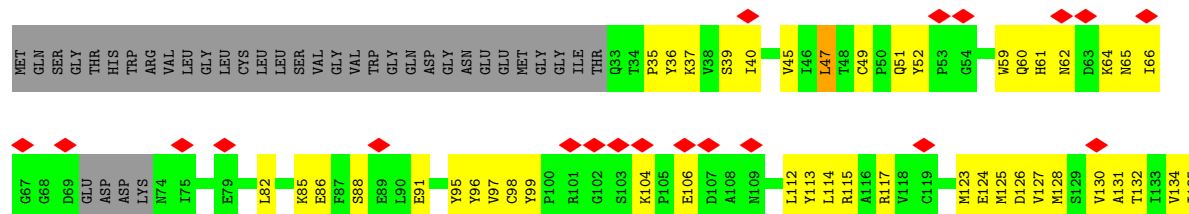
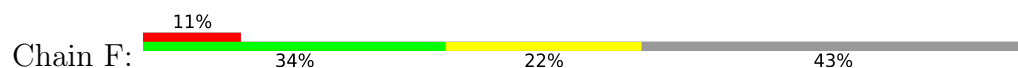
- Molecule 5: T-cell surface glycoprotein CD3 epsilon chain

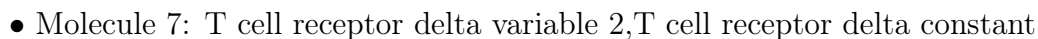


- Molecule 5: T-cell surface glycoprotein CD3 epsilon chain



- Molecule 5: T-cell surface glycoprotein CD3 epsilon chain





- [illegible]

VAL	ASP	GLN	GLU	ILE	ILE	PHE	PRO	PRO	PRO	ILE	LYS	THR	ASP	VAL	ILE	THR	MET	ASP	PRO	LYS	ASP	ASN	ALA	ASN	D251	T252	L253	L254	L255	T258	N259	Y266	L267	L268	L269	L270	L271	V274	V275	Y276	L280	T288	ALA	PHE	CYS	CYS	ASN	GLY	GLU	LYS	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66511	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.658	Depositor
Minimum map value	-1.027	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0699	Depositor
Map size (Å)	421.888, 421.888, 421.888	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	P	0.19	0/1551	0.40	0/2113
1	R	0.19	0/1551	0.40	0/2113
2	O	0.21	0/1616	0.50	2/2197 (0.1%)
2	Q	0.20	0/1616	0.43	0/2197
3	A	0.21	0/256	0.64	0/346
3	B	0.19	0/242	0.47	0/327
3	a	0.21	0/256	0.63	0/346
3	b	0.19	0/242	0.47	0/327
4	D	0.18	0/829	0.46	0/1127
4	d	0.15	0/829	0.41	0/1127
5	E	0.15	0/980	0.32	0/1331
5	F	0.13	0/953	0.33	0/1294
5	e	0.15	0/980	0.32	0/1331
5	f	0.13	0/953	0.33	0/1294
6	G	0.13	0/925	0.39	0/1244
6	g	0.13	0/925	0.41	0/1244
7	M	0.17	0/289	0.44	0/388
7	m	0.16	0/289	0.42	0/388
8	N	0.17	0/314	0.45	0/427
8	n	0.18	0/314	0.44	0/427
All	All	0.17	0/15910	0.42	2/21588 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	108	ARG	CA-C-N	6.40	133.22	121.70
2	O	108	ARG	C-N-CA	6.40	133.22	121.70

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	P	1511	0	1478	46	0
1	R	1511	0	1478	50	0
2	O	1583	0	1497	44	0
2	Q	1583	0	1497	44	0
3	A	251	0	276	20	0
3	B	237	0	260	11	0
3	a	251	0	276	19	0
3	b	237	0	260	13	0
4	D	817	0	826	26	0
4	d	817	0	826	23	0
5	E	959	0	921	23	0
5	F	933	0	897	44	0
5	e	959	0	921	21	0
5	f	933	0	897	49	0
6	G	907	0	897	39	0
6	g	907	0	897	45	0
7	M	285	0	312	17	0
7	m	285	0	312	15	0
8	N	310	0	336	10	0
8	n	310	0	336	14	0
9	D	28	0	26	0	0
9	d	28	0	26	1	0
All	All	15642	0	15452	496	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 16.

All (496) 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)
7:m:283:LEU:HD11	8:n:280:ILE:HD12	1.48	0.95
6:G:86:GLN:HG3	6:G:96:PRO:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:86:GLN:HG3	6:g:96:PRO:HB3	1.62	0.79
5:e:89:GLU:O	5:e:93:SER:OG	2.00	0.79
5:E:89:GLU:O	5:E:93:SER:OG	2.01	0.78
7:m:256:THR:OG1	7:m:260:ASN:ND2	2.18	0.76
3:A:31:LEU:HD11	5:E:130:VAL:HG21	1.67	0.76
7:M:256:THR:OG1	7:M:260:ASN:ND2	2.18	0.75
4:D:76:THR:HG22	4:D:77:ASP:H	1.54	0.73
4:d:73:CYS:SG	4:d:74:ASN:N	2.61	0.73
3:a:31:LEU:HD11	5:e:130:VAL:HG21	1.71	0.72
1:P:41:HIS:ND1	2:Q:3:GLN:OE1	2.25	0.69
7:M:256:THR:O	7:M:260:ASN:ND2	2.26	0.68
3:a:27:LEU:HB3	3:a:31:LEU:HG	1.75	0.68
2:Q:151:ILE:HD12	2:Q:151:ILE:O	1.94	0.68
2:Q:162:ASN:HB3	2:Q:164:TRP:HE1	1.59	0.68
5:f:117:ARG:HH12	6:g:103:MET:HA	1.59	0.68
2:O:151:ILE:HD12	2:O:151:ILE:O	1.94	0.67
1:R:35:ASN:HD22	1:R:47:TRP:HE1	1.43	0.67
1:P:97:ALA:HB1	1:P:109:PHE:HB3	1.76	0.67
5:F:117:ARG:NH2	6:G:104:CYS:O	2.28	0.66
7:m:256:THR:O	7:m:260:ASN:ND2	2.28	0.66
5:F:113:TYR:OH	5:F:115:ARG:NH1	2.29	0.66
1:P:35:ASN:HD22	1:P:47:TRP:HE1	1.43	0.66
1:R:205:ASN:ND2	1:R:216:ASP:OD2	2.28	0.66
1:R:97:ALA:HB1	1:R:109:PHE:HB3	1.76	0.66
5:F:130:VAL:O	5:F:134:VAL:HG23	1.96	0.66
2:O:162:ASN:HB3	2:O:164:TRP:HE1	1.59	0.66
5:f:117:ARG:NH2	6:g:104:CYS:O	2.28	0.66
1:P:205:ASN:ND2	1:P:216:ASP:OD2	2.28	0.66
4:D:73:CYS:SG	4:D:74:ASN:N	2.68	0.65
5:f:130:VAL:O	5:f:134:VAL:HG23	1.96	0.65
5:F:117:ARG:HH12	6:G:103:MET:HA	1.61	0.65
5:f:96:TYR:HB2	5:f:112:LEU:HB3	1.79	0.64
2:Q:137:LEU:HB2	2:Q:176:MET:HB3	1.79	0.64
6:g:122:GLU:O	6:g:126:ILE:HG13	1.98	0.64
1:P:203:THR:HB	1:P:218:LYS:HE3	1.81	0.63
2:O:137:LEU:HB2	2:O:176:MET:HB3	1.79	0.63
5:f:128:MET:O	5:f:132:THR:HG23	1.98	0.63
1:P:20:ILE:HD11	1:P:118:LEU:HD11	1.80	0.63
5:F:128:MET:O	5:F:132:THR:HG23	1.98	0.63
4:d:55:ILE:HD12	4:d:56:THR:H	1.63	0.62
5:f:126:ASP:OD2	5:f:127:VAL:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:20:ILE:HD11	1:R:118:LEU:HD11	1.80	0.62
3:A:27:LEU:HB3	3:A:31:LEU:HG	1.79	0.61
5:F:126:ASP:OD2	5:F:127:VAL:N	2.32	0.61
1:R:203:THR:HB	1:R:218:LYS:HE3	1.80	0.61
3:B:30:LYS:O	3:B:34:LEU:HG	2.00	0.61
3:A:47:THR:HB	3:B:46:LEU:HD11	1.81	0.61
4:D:80:LYS:HE3	4:D:80:LYS:HA	1.81	0.61
5:F:96:TYR:HB2	5:F:112:LEU:HB3	1.80	0.61
6:G:122:GLU:O	6:G:126:ILE:HG13	2.00	0.61
3:a:47:THR:HB	3:b:46:LEU:HD11	1.82	0.61
5:f:134:VAL:HG13	8:n:271:LEU:HD13	1.83	0.61
7:m:255:HIS:O	7:m:255:HIS:ND1	2.34	0.60
3:b:30:LYS:O	3:b:34:LEU:HG	2.01	0.60
5:F:134:VAL:HG13	8:N:271:LEU:HD13	1.83	0.60
6:g:56:PHE:HB2	6:g:86:GLN:HB2	1.83	0.60
2:O:48:ILE:HG22	2:O:54:LEU:HD13	1.83	0.59
3:a:38:ILE:O	3:a:41:ILE:HG13	2.02	0.59
5:f:131:ALA:O	5:f:135:ILE:HG12	2.02	0.59
5:F:60:GLN:HB2	5:F:97:VAL:HB	1.84	0.59
2:Q:48:ILE:HG22	2:Q:54:LEU:HD13	1.83	0.59
5:F:125:MET:HE3	6:G:108:ILE:HG12	1.84	0.59
6:g:44:LEU:HD11	6:g:74:LEU:HD23	1.83	0.59
3:A:38:ILE:O	3:A:41:ILE:HG13	2.02	0.59
4:D:97:VAL:HG12	7:M:260:ASN:HB3	1.84	0.59
4:d:97:VAL:HG12	7:m:260:ASN:HB3	1.82	0.59
5:F:131:ALA:O	5:F:135:ILE:HG12	2.02	0.59
8:n:254:LEU:O	8:n:258:THR:HG23	2.03	0.59
6:G:56:PHE:HB2	6:G:86:GLN:HB2	1.83	0.59
5:f:49:CYS:HB2	5:f:51:GLN:HE21	1.68	0.58
8:N:254:LEU:O	8:N:258:THR:HG23	2.03	0.58
3:a:44:VAL:HA	3:a:47:THR:HG22	1.85	0.58
3:b:40:PHE:O	3:b:44:VAL:HG22	2.04	0.58
5:F:49:CYS:HB2	5:F:51:GLN:HE21	1.68	0.58
7:M:255:HIS:O	7:M:255:HIS:ND1	2.35	0.58
6:G:44:LEU:HD11	6:G:74:LEU:HD23	1.83	0.58
3:A:44:VAL:HA	3:A:47:THR:HG22	1.85	0.58
5:f:60:GLN:HB2	5:f:97:VAL:HB	1.84	0.57
5:E:119:CYS:SG	5:E:120:GLU:N	2.77	0.57
5:e:119:CYS:SG	5:e:120:GLU:N	2.77	0.57
5:F:115:ARG:HB3	6:G:103:MET:HE1	1.86	0.57
1:R:180:LYS:HB3	2:Q:161:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:TYR:OH	5:e:67:GLY:O	2.16	0.57
4:d:115:THR:HG23	5:e:141:THR:HG23	1.87	0.57
5:f:125:MET:HE3	6:g:108:ILE:HG12	1.86	0.57
2:O:3:GLN:OE1	1:R:41:HIS:ND1	2.37	0.57
8:n:267:LEU:O	8:n:271:LEU:HG	2.05	0.57
4:D:47:THR:O	4:D:71:TYR:OH	2.15	0.57
2:O:114:PRO:HB3	2:O:140:PHE:HB3	1.87	0.56
3:a:30:LYS:HA	3:a:33:TYR:HD2	1.69	0.56
3:A:30:LYS:HA	3:A:33:TYR:HD2	1.68	0.56
4:d:76:THR:HG22	4:d:77:ASP:H	1.70	0.56
1:P:180:LYS:HB3	2:O:161:LEU:HD21	1.86	0.56
1:R:86:LEU:HD13	1:R:120:VAL:HG22	1.88	0.56
1:R:204:CYS:HB3	1:R:217:LYS:HE3	1.87	0.56
7:m:261:MET:O	7:m:265:THR:HG23	2.06	0.56
1:R:154:TYR:HB2	1:R:208:HIS:NE2	2.21	0.56
2:Q:106:ILE:O	2:Q:141:TYR:OH	2.19	0.56
4:D:39:THR:HG21	4:D:74:ASN:HB3	1.88	0.56
1:P:204:CYS:HB3	1:P:217:LYS:HE3	1.88	0.55
1:R:33:THR:OG1	5:E:101:ARG:NH2	2.39	0.55
6:G:56:PHE:HA	6:G:61:MET:HA	1.88	0.55
1:P:154:TYR:HB2	1:P:208:HIS:NE2	2.21	0.55
2:O:15:LEU:HD12	2:O:15:LEU:H	1.72	0.55
6:g:56:PHE:HA	6:g:61:MET:HA	1.88	0.55
5:E:40:ILE:HG23	5:E:45:VAL:HG22	1.88	0.55
7:M:270:ARG:HA	7:M:270:ARG:CZ	2.36	0.55
1:P:33:THR:OG1	5:e:101:ARG:NH2	2.39	0.55
5:e:89:GLU:HG2	6:g:38:GLU:HG3	1.88	0.55
6:g:119:LEU:HA	6:g:122:GLU:OE2	2.07	0.55
1:R:102:TYR:OH	5:E:67:GLY:O	2.16	0.55
4:D:115:THR:HG23	5:E:141:THR:HG23	1.88	0.55
6:g:53:ILE:HA	6:g:89:GLY:HA2	1.88	0.55
6:g:88:LYS:HE2	6:g:93:LYS:HB3	1.89	0.55
1:P:86:LEU:HD13	1:P:120:VAL:HG22	1.88	0.55
3:b:35:LEU:O	3:b:39:LEU:HG	2.07	0.55
6:g:119:LEU:HD12	6:g:120:PHE:HD1	1.72	0.55
8:N:267:LEU:O	8:N:271:LEU:HG	2.07	0.55
2:O:83:ILE:HD11	2:O:106:ILE:HG23	1.89	0.54
2:Q:15:LEU:HD12	2:Q:15:LEU:H	1.71	0.54
4:d:47:THR:O	4:d:71:TYR:OH	2.14	0.54
4:d:125:PHE:HA	7:m:286:LYS:HD3	1.90	0.54
5:f:104:LYS:HG3	5:f:106:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ASP:OD1	2:O:166:ASP:N	2.40	0.54
5:e:117:ARG:HH11	6:g:39:ASP:HA	1.72	0.54
4:d:39:THR:HG21	4:d:74:ASN:HB3	1.89	0.54
5:E:117:ARG:HH11	6:G:39:ASP:HA	1.73	0.54
4:D:63:ARG:HD3	4:D:92:MET:SD	2.48	0.54
3:B:35:LEU:O	3:B:39:LEU:HG	2.08	0.54
6:G:53:ILE:HA	6:G:89:GLY:HA2	1.88	0.54
6:G:103:MET:HE2	6:G:103:MET:N	2.23	0.54
5:e:40:ILE:HG23	5:e:45:VAL:HG22	1.88	0.54
1:P:125:THR:O	1:P:125:THR:OG1	2.25	0.53
5:F:106:GLU:HB2	6:G:27:GLY:HA3	1.90	0.53
6:G:69:LYS:HE3	6:G:71:LYS:O	2.08	0.53
5:F:104:LYS:HG3	5:F:106:GLU:HG3	1.89	0.53
2:Q:7:THR:HG22	2:Q:8:THR:HG23	1.91	0.53
5:F:85:LYS:O	5:F:86:GLU:HG3	2.09	0.53
6:G:88:LYS:HE2	6:G:93:LYS:HB3	1.89	0.53
6:G:119:LEU:HA	6:G:122:GLU:HG2	1.90	0.53
1:P:144:MET:HE2	1:P:145:VAL:O	2.08	0.53
6:g:103:MET:HE2	6:g:103:MET:N	2.24	0.53
2:Q:166:ASP:OD1	2:Q:166:ASP:N	2.40	0.53
5:E:89:GLU:HG2	6:G:38:GLU:HG3	1.91	0.53
4:d:63:ARG:HD3	4:d:92:MET:SD	2.48	0.53
3:a:50:PHE:HZ	3:b:53:VAL:HG21	1.74	0.53
6:g:69:LYS:HE3	6:g:71:LYS:O	2.08	0.53
1:R:144:MET:HE2	1:R:145:VAL:O	2.09	0.53
2:Q:126:LEU:HB3	2:Q:184:LYS:HE2	1.91	0.53
2:Q:134:VAL:HG22	2:Q:179:THR:HG22	1.91	0.53
3:B:54:LYS:HD2	3:B:54:LYS:C	2.34	0.53
2:O:114:PRO:HG2	2:O:206:ILE:HD13	1.91	0.53
3:A:27:LEU:O	3:A:31:LEU:HD23	2.08	0.53
4:d:34:PHE:CE1	4:d:59:ASP:HB3	2.44	0.52
4:d:33:VAL:HG23	4:d:60:LEU:HB2	1.90	0.52
2:Q:115:THR:O	2:Q:115:THR:OG1	2.25	0.52
2:O:7:THR:HG22	2:O:8:THR:HG23	1.90	0.52
4:d:33:VAL:HG21	4:d:67:PRO:HG2	1.90	0.52
3:a:27:LEU:O	3:a:31:LEU:HD23	2.09	0.52
6:g:126:ILE:HA	6:g:129:LEU:HG	1.90	0.52
7:M:270:ARG:HA	7:M:270:ARG:NE	2.25	0.52
4:D:33:VAL:HG23	4:D:60:LEU:HB2	1.90	0.52
4:D:34:PHE:CE1	4:D:59:ASP:HB3	2.44	0.52
5:F:112:LEU:HD12	6:G:98:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:39:LEU:HD12	3:b:40:PHE:N	2.25	0.52
1:R:40:SER:HB3	1:R:92:ALA:HB2	1.91	0.52
6:g:101:TYR:CD2	6:g:103:MET:HE3	2.45	0.52
5:f:106:GLU:HB2	6:g:27:GLY:HA3	1.90	0.52
2:O:126:LEU:HB3	2:O:184:LYS:HE2	1.92	0.52
2:Q:65:SER:OG	2:Q:66:GLY:N	2.42	0.52
4:D:33:VAL:HG21	4:D:67:PRO:HG2	1.90	0.52
5:f:85:LYS:O	5:f:86:GLU:HG3	2.09	0.52
1:P:40:SER:HB3	1:P:92:ALA:HB2	1.91	0.51
4:d:23:LYS:NZ	5:e:63:ASP:OD1	2.37	0.51
6:g:87:CYS:O	6:g:94:SER:N	2.39	0.51
4:D:70:ILE:HD11	5:E:35:PRO:HB3	1.93	0.51
6:G:126:ILE:HA	6:G:129:LEU:HG	1.91	0.51
4:D:100:ASP:O	4:D:104:VAL:HG23	2.10	0.51
4:d:100:ASP:O	4:d:104:VAL:HG23	2.10	0.51
3:A:37:GLY:HA2	3:A:40:PHE:CD2	2.46	0.51
1:R:208:HIS:NE2	1:R:210:ALA:HB3	2.25	0.51
4:D:23:LYS:NZ	5:E:63:ASP:OD1	2.37	0.51
2:O:134:VAL:HG22	2:O:179:THR:HG22	1.91	0.51
5:f:60:GLN:HG3	5:f:99:TYR:HE1	1.76	0.51
1:R:125:THR:O	1:R:125:THR:OG1	2.25	0.51
6:g:54:THR:HG22	6:g:64:PHE:HA	1.93	0.51
1:P:208:HIS:NE2	1:P:210:ALA:HB3	2.25	0.50
8:n:262:ALA:HA	8:n:265:MET:HE3	1.93	0.50
1:R:73:ASP:OD1	1:R:75:SER:OG	2.28	0.50
2:Q:152:ASP:OD1	2:Q:190:HIS:HB3	2.12	0.50
1:R:180:LYS:HD2	2:Q:161:LEU:HD11	1.92	0.50
3:B:39:LEU:HD12	3:B:40:PHE:N	2.26	0.50
4:d:70:ILE:HD11	5:e:35:PRO:HB3	1.93	0.50
5:e:141:THR:O	5:e:145:LEU:HG	2.11	0.50
2:O:115:THR:O	2:O:115:THR:OG1	2.27	0.50
1:R:13:LYS:NZ	1:R:122:SER:OG	2.45	0.50
5:E:141:THR:O	5:E:145:LEU:HG	2.12	0.50
3:a:37:GLY:HA2	3:a:40:PHE:CD2	2.47	0.50
5:F:61:HIS:O	5:F:64:LYS:HG2	2.12	0.50
5:F:112:LEU:HG	5:F:114:LEU:HD21	1.94	0.50
1:P:73:ASP:OD1	1:P:75:SER:OG	2.28	0.50
5:f:47:LEU:HD12	5:f:82:LEU:HD23	1.94	0.50
5:f:59:TRP:CG	5:f:82:LEU:HD22	2.47	0.50
2:Q:90:GLN:NE2	2:Q:93:THR:O	2.45	0.50
2:Q:114:PRO:HG2	2:Q:206:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:263:SER:N	8:N:259:ASN:HD21	2.10	0.50
1:P:13:LYS:NZ	1:P:122:SER:OG	2.45	0.50
1:P:180:LYS:HD2	2:O:161:LEU:HD11	1.92	0.50
2:O:90:GLN:NE2	2:O:93:THR:O	2.45	0.50
7:m:283:LEU:CD1	8:n:280:ILE:HD12	2.32	0.50
1:P:36:TRP:CE3	1:P:81:MET:HE2	2.47	0.49
2:O:152:ASP:OD1	2:O:190:HIS:HB3	2.11	0.49
5:f:61:HIS:O	5:f:64:LYS:HG2	2.12	0.49
5:f:112:LEU:HD12	6:g:98:GLN:HB3	1.94	0.49
5:f:112:LEU:HG	5:f:114:LEU:HD21	1.93	0.49
7:M:263:SER:O	7:M:267:LEU:HG	2.12	0.49
1:P:133:LEU:HD21	2:O:134:VAL:HG21	1.94	0.49
3:b:30:LYS:HA	3:b:33:TYR:CD1	2.47	0.49
3:B:44:VAL:HG13	7:M:281:PHE:HE2	1.77	0.49
2:Q:150:LYS:N	2:Q:194:THR:O	2.38	0.49
2:O:65:SER:OG	2:O:66:GLY:N	2.42	0.49
5:e:49:CYS:SG	5:e:51:GLN:NE2	2.85	0.49
6:g:41:SER:HA	6:g:76:SER:HA	1.95	0.49
1:R:36:TRP:CE3	1:R:81:MET:HE2	2.47	0.49
5:F:59:TRP:CG	5:F:82:LEU:HD22	2.47	0.49
2:Q:117:SER:HB2	2:Q:136:PHE:HB2	1.95	0.49
3:A:50:PHE:HZ	3:B:53:VAL:HG21	1.76	0.49
5:F:35:PRO:O	5:F:37:LYS:NZ	2.46	0.49
5:F:47:LEU:HD12	5:F:82:LEU:HD23	1.94	0.49
4:D:125:PHE:HA	7:M:286:LYS:HD3	1.95	0.49
3:a:38:ILE:HG13	3:a:39:LEU:N	2.28	0.49
6:G:54:THR:N	6:G:88:LYS:O	2.44	0.49
5:F:60:GLN:HG3	5:F:99:TYR:HE1	1.76	0.49
6:G:54:THR:HG22	6:G:64:PHE:HA	1.93	0.49
5:F:60:GLN:HG2	5:F:65:ASN:HA	1.95	0.48
5:F:61:HIS:HB3	5:F:66:ILE:HG13	1.95	0.48
6:G:101:TYR:CD2	6:G:103:MET:HE3	2.48	0.48
5:f:35:PRO:O	5:f:37:LYS:NZ	2.45	0.48
6:G:87:CYS:O	6:G:94:SER:N	2.39	0.48
1:P:20:ILE:O	1:P:80:TYR:HA	2.14	0.48
8:n:276:TYR:CE1	8:n:280:ILE:HD13	2.49	0.48
1:P:44:ASN:ND2	2:Q:3:GLN:HE22	2.12	0.48
7:m:263:SER:N	8:n:259:ASN:HD21	2.11	0.48
5:F:59:TRP:CE2	5:F:82:LEU:HB2	2.49	0.48
6:G:115:ILE:HD12	6:G:118:PHE:HD2	1.77	0.48
1:P:128:PRO:HD3	1:P:208:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:164:TRP:N	2:O:164:TRP:CD1	2.82	0.48
5:f:61:HIS:HB3	5:f:66:ILE:HG13	1.95	0.48
5:f:59:TRP:CE2	5:f:82:LEU:HB2	2.49	0.48
5:f:115:ARG:HE	6:g:36:TYR:HE2	1.61	0.48
1:R:128:PRO:HD3	1:R:208:HIS:ND1	2.29	0.48
2:Q:164:TRP:N	2:Q:164:TRP:CD1	2.82	0.48
1:R:180:LYS:NZ	1:R:181:SER:H	2.12	0.48
3:A:38:ILE:HG13	3:A:39:LEU:N	2.27	0.48
1:P:12:VAL:HG11	1:P:86:LEU:HD21	1.95	0.47
2:Q:11:LEU:HD11	2:Q:19:VAL:HG21	1.96	0.47
2:O:117:SER:HB2	2:O:136:PHE:HB2	1.94	0.47
6:G:41:SER:HA	6:G:76:SER:HA	1.95	0.47
2:O:139:ASN:HA	2:O:173:THR:HB	1.95	0.47
1:R:133:LEU:HD21	2:Q:134:VAL:HG21	1.94	0.47
5:f:60:GLN:HG2	5:f:65:ASN:HA	1.95	0.47
1:P:180:LYS:NZ	1:P:181:SER:H	2.12	0.47
7:m:266:VAL:O	7:m:270:ARG:HG2	2.15	0.47
1:R:20:ILE:O	1:R:80:TYR:HA	2.14	0.47
2:O:89:GLN:HG2	2:O:90:GLN:N	2.29	0.47
2:Q:89:GLN:HG2	2:Q:90:GLN:N	2.29	0.47
2:Q:114:PRO:HB3	2:Q:140:PHE:HB3	1.97	0.47
4:D:95:SER:O	4:D:95:SER:OG	2.32	0.47
5:f:113:TYR:OH	5:f:115:ARG:NH1	2.48	0.47
1:P:202:VAL:O	1:P:219:ILE:HG12	2.15	0.47
5:f:61:HIS:HB2	5:f:96:TYR:CE1	2.50	0.47
7:M:266:VAL:O	7:M:270:ARG:HG2	2.15	0.47
1:P:86:LEU:HD12	1:P:86:LEU:O	2.15	0.47
2:Q:19:VAL:HG13	2:Q:75:ILE:HB	1.97	0.47
5:F:36:TYR:HE2	5:F:98:CYS:HB3	1.79	0.47
2:O:19:VAL:HG13	2:O:75:ILE:HB	1.98	0.46
1:R:202:VAL:O	1:R:219:ILE:HG12	2.15	0.46
5:f:36:TYR:HE2	5:f:98:CYS:HB3	1.79	0.46
5:F:60:GLN:NE2	5:F:99:TYR:OH	2.47	0.46
5:F:61:HIS:HB2	5:F:96:TYR:CE1	2.51	0.46
2:Q:83:ILE:HG23	2:Q:104:LEU:O	2.16	0.46
1:P:144:MET:HG3	1:P:145:VAL:N	2.31	0.46
2:O:11:LEU:HD11	2:O:19:VAL:HG21	1.96	0.46
2:O:150:LYS:N	2:O:194:THR:O	2.37	0.46
1:R:12:VAL:HG11	1:R:86:LEU:HD21	1.95	0.46
3:A:34:LEU:O	3:A:38:ILE:HG23	2.16	0.46
4:d:38:ASN:HD22	4:d:76:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:113:TYR:CE2	6:g:33:VAL:HG11	2.50	0.46
1:R:144:MET:HG3	1:R:145:VAL:H	1.79	0.46
5:f:60:GLN:NE2	5:f:99:TYR:OH	2.47	0.46
5:f:88:SER:HB2	5:f:91:GLU:HB2	1.98	0.46
1:R:144:MET:HG3	1:R:145:VAL:N	2.31	0.46
5:f:115:ARG:HB3	6:g:103:MET:HE1	1.97	0.46
3:A:41:ILE:HA	3:A:44:VAL:HG22	1.98	0.46
7:m:283:LEU:C	7:m:283:LEU:HD12	2.41	0.46
1:P:144:MET:HG3	1:P:145:VAL:H	1.79	0.46
1:P:179:LEU:HD12	1:P:184:TYR:CE2	2.51	0.46
2:Q:83:ILE:HD11	2:Q:106:ILE:HG23	1.98	0.46
3:A:30:LYS:HD2	3:A:33:TYR:HB2	1.98	0.46
5:F:88:SER:HB2	5:F:91:GLU:HB2	1.98	0.46
2:Q:47:LEU:HA	2:Q:58:VAL:HG21	1.97	0.46
5:F:62:ASN:HB2	5:F:64:LYS:HZ2	1.80	0.46
7:M:270:ARG:CZ	8:N:266:TYR:CD1	2.98	0.46
1:P:182:ASP:O	1:P:183:LEU:HD22	2.16	0.45
1:P:94:TYR:CD2	1:P:118:LEU:HD13	2.52	0.45
2:O:83:ILE:HG23	2:O:104:LEU:O	2.17	0.45
5:e:89:GLU:OE1	5:e:115:ARG:NH1	2.48	0.45
1:R:86:LEU:HD12	1:R:86:LEU:O	2.15	0.45
1:R:182:ASP:O	1:R:183:LEU:HD22	2.16	0.45
5:F:65:ASN:O	5:F:66:ILE:HD13	2.17	0.45
5:f:62:ASN:HB2	5:f:64:LYS:HZ2	1.82	0.45
5:f:65:ASN:O	5:f:66:ILE:HD13	2.17	0.45
6:g:35:ASP:HA	6:g:37:GLN:NE2	2.32	0.45
2:O:47:LEU:HA	2:O:58:VAL:HG21	1.97	0.45
3:a:41:ILE:HA	3:a:44:VAL:HG22	1.98	0.45
5:f:37:LYS:HD3	5:f:37:LYS:HA	1.60	0.45
6:g:134:TYR:HD1	6:g:135:PHE:HD2	1.65	0.45
6:G:35:ASP:HA	6:G:37:GLN:HE21	1.80	0.45
1:R:94:TYR:CD2	1:R:118:LEU:HD13	2.52	0.45
1:P:110:ASP:OD1	1:P:110:ASP:N	2.45	0.45
2:O:141:TYR:CD1	2:O:142:PRO:HA	2.51	0.45
6:g:115:ILE:HD12	6:g:118:PHE:HD1	1.81	0.45
1:R:121:PHE:HD1	1:R:121:PHE:HA	1.71	0.45
5:F:117:ARG:NH1	6:G:103:MET:HA	2.30	0.45
3:a:30:LYS:HD2	3:a:33:TYR:HB2	1.98	0.45
3:A:40:PHE:O	3:A:44:VAL:HG13	2.17	0.45
4:d:79:TYR:HE2	9:d:202:NAG:H81	1.82	0.45
6:g:119:LEU:HA	6:g:122:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:179:LEU:HD12	1:R:184:TYR:CE2	2.52	0.45
5:E:89:GLU:OE1	5:E:115:ARG:NH1	2.48	0.44
5:F:37:LYS:HA	5:F:37:LYS:HD3	1.60	0.44
3:b:44:VAL:HG12	7:m:281:PHE:CE1	2.52	0.44
4:D:55:ILE:O	4:D:56:THR:OG1	2.25	0.44
5:E:80:ASP:OD2	5:E:80:ASP:N	2.40	0.44
4:d:24:ILE:O	5:e:95:TYR:OH	2.33	0.44
4:D:40:SER:N	4:D:56:THR:HG22	2.33	0.44
6:G:35:ASP:HA	6:G:37:GLN:NE2	2.32	0.44
8:n:251:ASP:HB3	8:n:252:THR:H	1.57	0.44
3:A:30:LYS:HA	3:A:33:TYR:CD2	2.50	0.44
6:g:130:ALA:HA	6:g:133:VAL:HG12	1.99	0.44
2:Q:161:LEU:HB2	2:Q:179:THR:OG1	2.18	0.44
5:E:34:THR:O	5:E:51:GLN:NE2	2.51	0.44
6:G:130:ALA:HA	6:G:133:VAL:HG12	1.99	0.44
8:N:271:LEU:HA	8:N:274:VAL:HG22	2.00	0.44
1:P:203:THR:HA	1:P:218:LYS:HA	2.00	0.44
5:f:59:TRP:CZ3	5:f:98:CYS:HB2	2.53	0.44
2:O:152:ASP:HA	2:O:192:SER:HB3	2.00	0.43
3:b:32:CYS:O	3:b:35:LEU:HG	2.18	0.43
8:n:277:PHE:HA	8:n:280:ILE:HG12	1.99	0.43
1:P:13:LYS:HE3	1:P:13:LYS:HB3	1.72	0.43
1:R:86:LEU:HD13	1:R:120:VAL:CG2	2.48	0.43
3:A:36:ASP:HB3	3:B:35:LEU:HD11	1.99	0.43
3:b:30:LYS:HA	3:b:30:LYS:HD3	1.82	0.43
6:g:32:LYS:HZ1	6:g:47:ASP:HB2	1.84	0.43
1:R:34:MET:HE3	1:R:34:MET:HB2	1.72	0.43
1:R:203:THR:HA	1:R:218:LYS:HA	2.00	0.43
5:F:59:TRP:CZ3	5:F:98:CYS:HB2	2.53	0.43
8:N:276:TYR:O	8:N:280:ILE:HG23	2.19	0.43
3:a:52:ARG:HD3	3:a:52:ARG:HA	1.66	0.43
2:Q:152:ASP:HA	2:Q:192:SER:HB3	1.99	0.43
3:a:40:PHE:O	3:a:44:VAL:HG13	2.17	0.43
5:f:123:MET:HG2	5:f:124:GLU:N	2.34	0.43
7:m:263:SER:O	7:m:267:LEU:HG	2.19	0.43
8:n:255:LEU:O	8:n:259:ASN:HB2	2.19	0.43
1:R:110:ASP:OD1	1:R:110:ASP:N	2.45	0.43
1:R:124:LYS:HE3	1:R:124:LYS:HB3	1.84	0.43
3:A:52:ARG:HA	3:A:52:ARG:HD3	1.66	0.43
6:G:28:ASN:O	6:G:95:LYS:N	2.42	0.43
7:M:271:MET:HE1	7:M:272:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:40:ILE:HB	5:f:45:VAL:HG13	1.99	0.43
6:g:88:LYS:HG3	6:g:93:LYS:HA	2.01	0.43
3:B:32:CYS:O	3:B:35:LEU:HG	2.18	0.43
5:F:123:MET:HG2	5:F:124:GLU:N	2.33	0.43
6:G:119:LEU:HA	6:G:122:GLU:OE2	2.18	0.43
1:R:67:LYS:HD3	1:R:67:LYS:HA	1.74	0.43
4:D:24:ILE:HD12	4:D:86:VAL:HG12	2.00	0.43
5:F:147:LEU:HD23	5:F:147:LEU:HA	1.90	0.43
2:O:118:ILE:HG12	2:O:208:LYS:HG2	2.01	0.43
2:O:161:LEU:HB2	2:O:179:THR:OG1	2.18	0.43
4:D:24:ILE:O	5:E:95:TYR:OH	2.33	0.43
1:P:86:LEU:HD13	1:P:120:VAL:CG2	2.48	0.43
5:f:147:LEU:HD23	5:f:147:LEU:HA	1.90	0.43
4:D:33:VAL:HG11	4:D:90:TYR:CZ	2.54	0.43
4:D:87:GLN:O	5:E:112:LEU:HD12	2.19	0.43
3:a:34:LEU:O	3:a:38:ILE:HG23	2.19	0.42
2:O:28:ASP:OD1	2:O:28:ASP:C	2.62	0.42
3:b:51:LEU:O	3:b:54:LYS:HG3	2.19	0.42
7:m:280:ASN:O	7:m:284:THR:OG1	2.33	0.42
6:G:88:LYS:HG3	6:G:93:LYS:HA	2.01	0.42
2:O:105:GLU:HB3	2:O:167:GLN:CD	2.44	0.42
4:d:38:ASN:HD22	4:d:76:THR:CG2	2.32	0.42
8:n:276:TYR:O	8:n:280:ILE:HG23	2.19	0.42
1:R:154:TYR:HB2	1:R:208:HIS:HE2	1.83	0.42
5:F:40:ILE:HB	5:F:45:VAL:HG13	1.99	0.42
2:O:140:PHE:CE2	2:O:145:ILE:HG21	2.55	0.42
4:d:24:ILE:HD12	4:d:86:VAL:HG12	2.00	0.42
1:R:29:PHE:CE2	1:R:53:PRO:HB3	2.54	0.42
4:D:87:GLN:OE1	5:E:36:TYR:N	2.50	0.42
5:F:106:GLU:O	6:G:95:LYS:NZ	2.53	0.42
1:P:47:TRP:HZ2	1:P:50:LEU:HD23	1.85	0.42
8:n:271:LEU:HA	8:n:274:VAL:HG22	2.02	0.42
7:M:261:MET:HE3	7:M:265:THR:HG23	2.01	0.42
1:P:29:PHE:CE2	1:P:53:PRO:HB3	2.54	0.42
5:e:57:ILE:HA	5:e:100:PRO:HA	2.02	0.42
7:m:268:GLY:O	7:m:272:LEU:HD23	2.19	0.42
5:F:114:LEU:HD22	6:G:100:TYR:HB3	2.00	0.42
3:a:36:ASP:HB3	3:b:35:LEU:HD11	2.02	0.42
5:f:106:GLU:O	6:g:95:LYS:NZ	2.53	0.42
4:D:41:ILE:HD13	4:D:73:CYS:HB2	2.02	0.42
7:M:269:LEU:HB3	7:M:270:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:33:VAL:HG11	4:d:90:TYR:CZ	2.54	0.42
4:d:95:SER:O	4:d:95:SER:OG	2.32	0.42
5:f:117:ARG:NH1	6:g:103:MET:HA	2.30	0.42
2:Q:35:TRP:HD1	2:Q:48:ILE:HD11	1.85	0.42
5:E:57:ILE:HA	5:E:100:PRO:HA	2.02	0.42
1:P:153:GLY:HA2	1:P:183:LEU:HG	2.02	0.42
5:f:135:ILE:HA	5:f:138:ILE:HG22	2.02	0.42
6:g:50:ALA:H	6:g:53:ILE:HD11	1.85	0.42
2:Q:4:MET:HE3	2:Q:4:MET:HB3	1.79	0.42
3:A:31:LEU:HD21	5:E:127:VAL:HG12	2.01	0.42
1:P:104:ASP:OD1	1:P:105:SER:N	2.53	0.41
3:b:49:LEU:O	3:b:53:VAL:HG23	2.20	0.41
6:g:28:ASN:O	6:g:95:LYS:N	2.42	0.41
6:g:35:ASP:HA	6:g:37:GLN:HE21	1.84	0.41
5:E:43:THR:HA	5:E:118:VAL:CG1	2.50	0.41
8:N:251:ASP:HB3	8:N:252:THR:H	1.57	0.41
2:O:38:GLN:O	2:O:84:ALA:HB1	2.19	0.41
6:g:120:PHE:O	6:g:124:VAL:HG13	2.21	0.41
5:F:123:MET:O	5:F:125:MET:HE2	2.20	0.41
1:P:34:MET:HE3	1:P:34:MET:HB2	1.72	0.41
2:O:136:PHE:HD1	2:O:136:PHE:HA	1.73	0.41
8:n:270:LEU:HD23	8:n:270:LEU:HA	1.82	0.41
2:Q:38:GLN:O	2:Q:84:ALA:HB1	2.20	0.41
3:A:37:GLY:O	3:A:41:ILE:HG23	2.21	0.41
6:G:50:ALA:H	6:G:53:ILE:HD11	1.85	0.41
7:M:268:GLY:O	7:M:272:LEU:HD23	2.20	0.41
3:a:30:LYS:HA	3:a:33:TYR:CD2	2.52	0.41
4:d:87:GLN:O	5:e:112:LEU:HD12	2.19	0.41
5:f:149:TYR:CD1	6:g:137:ALA:HB2	2.56	0.41
6:g:54:THR:N	6:g:88:LYS:O	2.44	0.41
1:R:104:ASP:OD1	1:R:105:SER:N	2.53	0.41
2:Q:150:LYS:HD2	2:Q:150:LYS:HA	1.97	0.41
4:D:77:ASP:HA	4:D:80:LYS:NZ	2.35	0.41
2:O:51:THR:HG23	2:O:71:TYR:HD1	1.86	0.41
2:O:107:LYS:HA	2:O:141:TYR:OH	2.20	0.41
3:a:47:THR:O	3:a:51:LEU:HG	2.21	0.41
2:Q:136:PHE:HD1	2:Q:136:PHE:HA	1.73	0.41
5:F:113:TYR:CE2	6:G:33:VAL:HG11	2.56	0.41
2:O:151:ILE:HG12	2:O:156:ARG:NH2	2.36	0.41
1:R:164:ASN:HA	1:R:203:THR:HG22	2.02	0.41
2:Q:28:ASP:OD1	2:Q:28:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:27:LEU:HD22	3:A:31:LEU:HG	2.02	0.41
2:Q:151:ILE:HG12	2:Q:156:ARG:NH2	2.36	0.41
5:E:61:HIS:HB2	5:E:96:TYR:CE2	2.56	0.41
1:P:155:PHE:HB3	1:P:156:PRO:HD3	2.02	0.41
1:P:164:ASN:HA	1:P:203:THR:HG22	2.02	0.41
2:O:35:TRP:HD1	2:O:48:ILE:HD11	1.85	0.41
5:e:43:THR:HA	5:e:118:VAL:CG1	2.50	0.41
5:f:123:MET:O	5:f:125:MET:HE2	2.21	0.41
1:R:47:TRP:HZ2	1:R:50:LEU:HD23	1.85	0.41
1:R:147:LEU:HD13	1:R:219:ILE:HB	2.03	0.41
1:R:155:PHE:HB3	1:R:156:PRO:HD3	2.02	0.41
2:Q:51:THR:HG23	2:Q:71:TYR:HD1	1.86	0.41
2:Q:105:GLU:HB3	2:Q:167:GLN:CD	2.46	0.41
3:B:49:LEU:O	3:B:53:VAL:HG23	2.21	0.41
4:D:24:ILE:HD13	4:D:73:CYS:HB3	2.03	0.41
5:E:83:SER:O	5:E:83:SER:OG	2.36	0.41
8:N:270:LEU:HD23	8:N:270:LEU:HA	1.83	0.41
2:O:37:GLN:O	2:O:44:VAL:HA	2.21	0.41
5:e:56:GLU:O	5:e:101:ARG:N	2.53	0.41
1:R:20:ILE:HD12	1:R:116:THR:OG1	2.21	0.41
1:R:125:THR:HA	1:R:156:PRO:HD3	2.03	0.41
1:R:153:GLY:HA2	1:R:183:LEU:HG	2.02	0.41
2:Q:140:PHE:CE2	2:Q:145:ILE:HG21	2.56	0.41
7:M:275:LYS:HE3	7:M:275:LYS:HB2	1.90	0.41
5:f:152:SER:OG	6:g:137:ALA:HB3	2.21	0.40
1:R:51:ILE:O	1:R:53:PRO:HD3	2.21	0.40
5:F:149:TYR:CD1	6:G:137:ALA:HB2	2.56	0.40
6:G:120:PHE:O	6:G:124:VAL:HG13	2.20	0.40
8:N:255:LEU:O	8:N:259:ASN:HB2	2.21	0.40
5:e:117:ARG:NH1	6:g:39:ASP:HA	2.35	0.40
5:f:114:LEU:HD22	6:g:100:TYR:HB3	2.03	0.40
1:P:51:ILE:O	1:P:53:PRO:HD3	2.21	0.40
1:P:134:ALA:O	2:O:120:PRO:HD2	2.21	0.40
5:f:110:PHE:CD1	6:g:96:PRO:HG2	2.57	0.40
2:Q:37:GLN:O	2:Q:44:VAL:HA	2.22	0.40
3:B:30:LYS:HA	3:B:33:TYR:CD1	2.56	0.40
5:F:95:TYR:CD1	5:F:113:TYR:HB2	2.56	0.40
3:a:37:GLY:O	3:a:41:ILE:HG23	2.21	0.40
5:e:57:ILE:HD12	5:e:98:CYS:HB2	2.03	0.40
5:f:44:THR:HB	5:f:85:LYS:NZ	2.37	0.40
5:f:93:SER:HB3	5:f:115:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:118:ILE:HG12	2:Q:208:LYS:HG2	2.01	0.40
6:G:53:ILE:HB	6:G:65:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	188/222 (85%)	179 (95%)	9 (5%)	0	100	100
1	R	188/222 (85%)	179 (95%)	9 (5%)	0	100	100
2	O	205/212 (97%)	195 (95%)	10 (5%)	0	100	100
2	Q	205/212 (97%)	193 (94%)	12 (6%)	0	100	100
3	A	29/166 (18%)	27 (93%)	2 (7%)	0	100	100
3	B	27/166 (16%)	27 (100%)	0	0	100	100
3	a	29/166 (18%)	27 (93%)	2 (7%)	0	100	100
3	b	27/166 (16%)	27 (100%)	0	0	100	100
4	D	103/171 (60%)	102 (99%)	1 (1%)	0	100	100
4	d	103/171 (60%)	102 (99%)	1 (1%)	0	100	100
5	E	119/207 (58%)	118 (99%)	1 (1%)	0	100	100
5	F	114/207 (55%)	111 (97%)	3 (3%)	0	100	100
5	e	119/207 (58%)	118 (99%)	1 (1%)	0	100	100
5	f	114/207 (55%)	110 (96%)	4 (4%)	0	100	100
6	G	113/182 (62%)	106 (94%)	7 (6%)	0	100	100
6	g	113/182 (62%)	106 (94%)	7 (6%)	0	100	100
7	M	34/292 (12%)	34 (100%)	0	0	100	100
7	m	34/292 (12%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	N	36/315 (11%)	36 (100%)	0	0	100	100
8	n	36/315 (11%)	36 (100%)	0	0	100	100
All	All	1936/4280 (45%)	1867 (96%)	69 (4%)	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	P	172/193 (89%)	159 (92%)	13 (8%)	12	37
1	R	172/193 (89%)	158 (92%)	14 (8%)	11	34
2	O	175/189 (93%)	163 (93%)	12 (7%)	14	40
2	Q	175/189 (93%)	165 (94%)	10 (6%)	18	46
3	A	28/136 (21%)	26 (93%)	2 (7%)	13	39
3	B	26/136 (19%)	25 (96%)	1 (4%)	29	57
3	a	28/136 (21%)	26 (93%)	2 (7%)	13	39
3	b	26/136 (19%)	25 (96%)	1 (4%)	29	57
4	D	93/147 (63%)	89 (96%)	4 (4%)	26	55
4	d	93/147 (63%)	91 (98%)	2 (2%)	45	68
5	E	109/177 (62%)	100 (92%)	9 (8%)	10	33
5	F	106/177 (60%)	103 (97%)	3 (3%)	38	63
5	e	109/177 (62%)	99 (91%)	10 (9%)	8	29
5	f	106/177 (60%)	104 (98%)	2 (2%)	50	70
6	G	97/155 (63%)	91 (94%)	6 (6%)	16	43
6	g	97/155 (63%)	91 (94%)	6 (6%)	16	43
7	M	32/259 (12%)	30 (94%)	2 (6%)	16	43
7	m	32/259 (12%)	28 (88%)	4 (12%)	4	17
8	N	36/284 (13%)	34 (94%)	2 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	n	36/284 (13%)	35 (97%)	1 (3%)	38 63
All	All	1748/3706 (47%)	1642 (94%)	106 (6%)	19 44

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	2	VAL
1	P	6	GLN
1	P	30	THR
1	P	34	MET
1	P	46	GLU
1	P	65	LYS
1	P	81	MET
1	P	119	THR
1	P	121	PHE
1	P	122	SER
1	P	126	THR
1	P	180	LYS
1	P	215	VAL
2	O	19	VAL
2	O	34	ASN
2	O	44	VAL
2	O	48	ILE
2	O	76	SER
2	O	115	THR
2	O	160	VAL
2	O	164	TRP
2	O	173	THR
2	O	179	THR
2	O	183	THR
2	O	199	HIS
3	a	28	ASP
3	a	38	ILE
3	b	46	LEU
4	d	45	GLU
4	d	120	LEU
5	e	34	THR
5	e	38	VAL
5	e	39	SER
5	e	41	SER
5	e	43	THR
5	e	48	THR

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Mol	Chain	Res	Type
5	e	88	SER
5	e	118	VAL
5	e	128	MET
5	e	146	LEU
5	f	47	LEU
5	f	52	TYR
6	g	41	SER
6	g	43	LEU
6	g	44	LEU
6	g	61	MET
6	g	64	PHE
6	g	76	SER
7	m	264	LEU
7	m	266	VAL
7	m	280	ASN
7	m	281	PHE
8	n	254	LEU
1	R	2	VAL
1	R	6	GLN
1	R	30	THR
1	R	34	MET
1	R	44	ASN
1	R	46	GLU
1	R	65	LYS
1	R	81	MET
1	R	119	THR
1	R	121	PHE
1	R	122	SER
1	R	126	THR
1	R	180	LYS
1	R	215	VAL
2	Q	19	VAL
2	Q	34	ASN
2	Q	48	ILE
2	Q	76	SER
2	Q	115	THR
2	Q	160	VAL
2	Q	164	TRP
2	Q	173	THR
2	Q	179	THR
2	Q	199	HIS
3	A	28	ASP

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Mol	Chain	Res	Type
3	A	38	ILE
3	B	46	LEU
4	D	29	LEU
4	D	45	GLU
4	D	81	ASP
4	D	120	LEU
5	E	38	VAL
5	E	39	SER
5	E	41	SER
5	E	43	THR
5	E	48	THR
5	E	88	SER
5	E	118	VAL
5	E	128	MET
5	E	146	LEU
5	F	39	SER
5	F	47	LEU
5	F	52	TYR
6	G	41	SER
6	G	43	LEU
6	G	44	LEU
6	G	61	MET
6	G	64	PHE
6	G	76	SER
7	M	280	ASN
7	M	288	PHE
8	N	254	LEU
8	N	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	35	ASN
1	P	44	ASN
5	e	51	GLN
5	f	60	GLN
5	f	92	GLN
5	f	121	ASN
6	g	92	ASN
8	n	259	ASN
1	R	35	ASN
1	R	173	HIS

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Mol	Chain	Res	Type
2	Q	139	ASN
5	F	60	GLN
5	F	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	NAG	d	201	4	14,14,15	0.66	0	17,19,21	1.44	1 (5%)
9	NAG	D	202	4	14,14,15	0.80	0	17,19,21	1.84	3 (17%)
9	NAG	D	201	4	14,14,15	0.69	0	17,19,21	1.53	3 (17%)
9	NAG	d	202	4	14,14,15	0.75	0	17,19,21	1.05	1 (5%)

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
9	NAG	d	201	4	-	1/6/23/26	0/1/1/1
9	NAG	D	202	4	-	2/6/23/26	0/1/1/1
9	NAG	D	201	4	-	1/6/23/26	0/1/1/1
9	NAG	d	202	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	202	NAG	C1-O5-C5	5.94	120.15	112.19
9	d	201	NAG	C1-O5-C5	-4.64	105.96	112.19
9	D	201	NAG	C1-O5-C5	-4.40	106.29	112.19
9	d	202	NAG	C1-O5-C5	2.65	115.73	112.19
9	D	201	NAG	C3-C4-C5	2.56	114.87	110.23
9	D	201	NAG	O4-C4-C3	-2.16	105.28	110.38
9	D	202	NAG	C3-C4-C5	-2.10	106.42	110.23
9	D	202	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	201	NAG	O5-C5-C6-O6
9	d	201	NAG	O5-C5-C6-O6
9	D	202	NAG	C4-C5-C6-O6
9	D	202	NAG	O5-C5-C6-O6

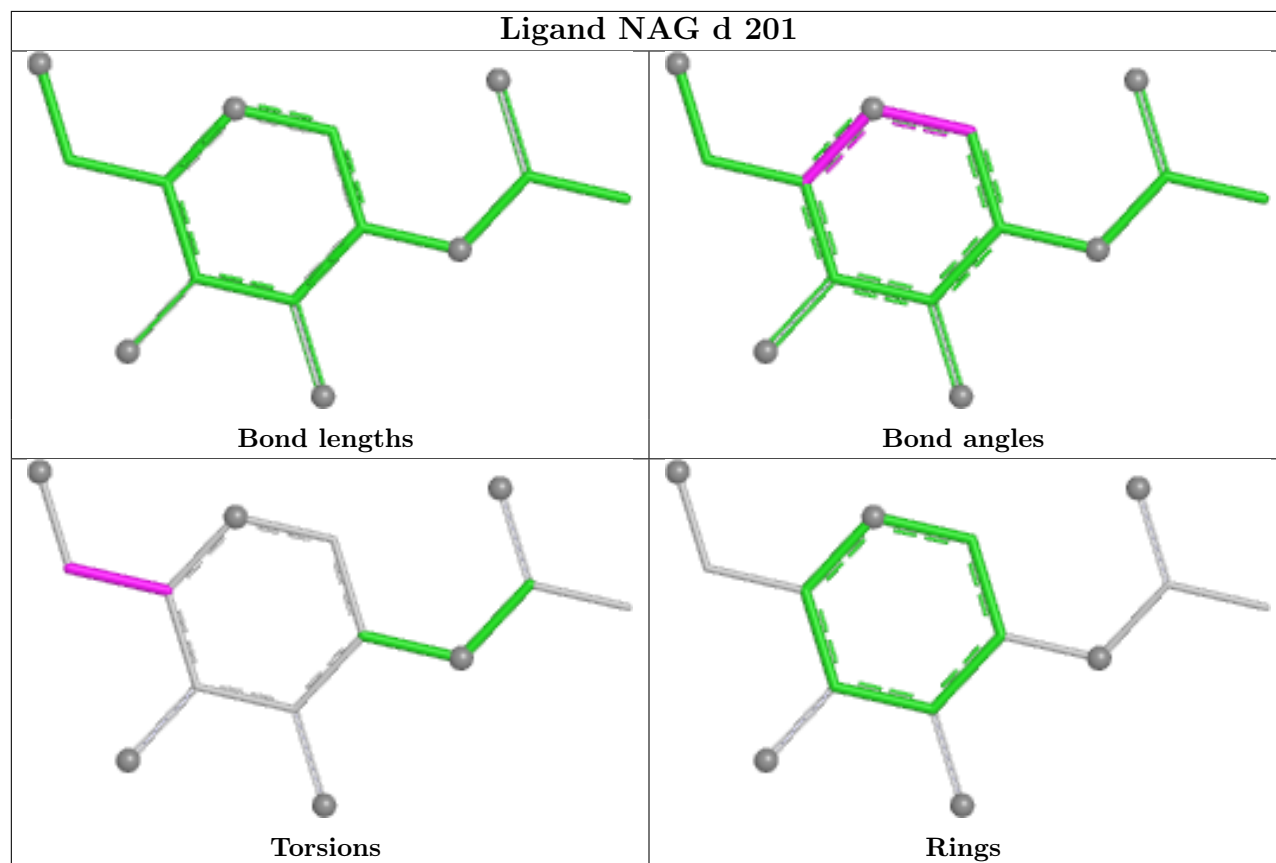
There are no ring outliers.

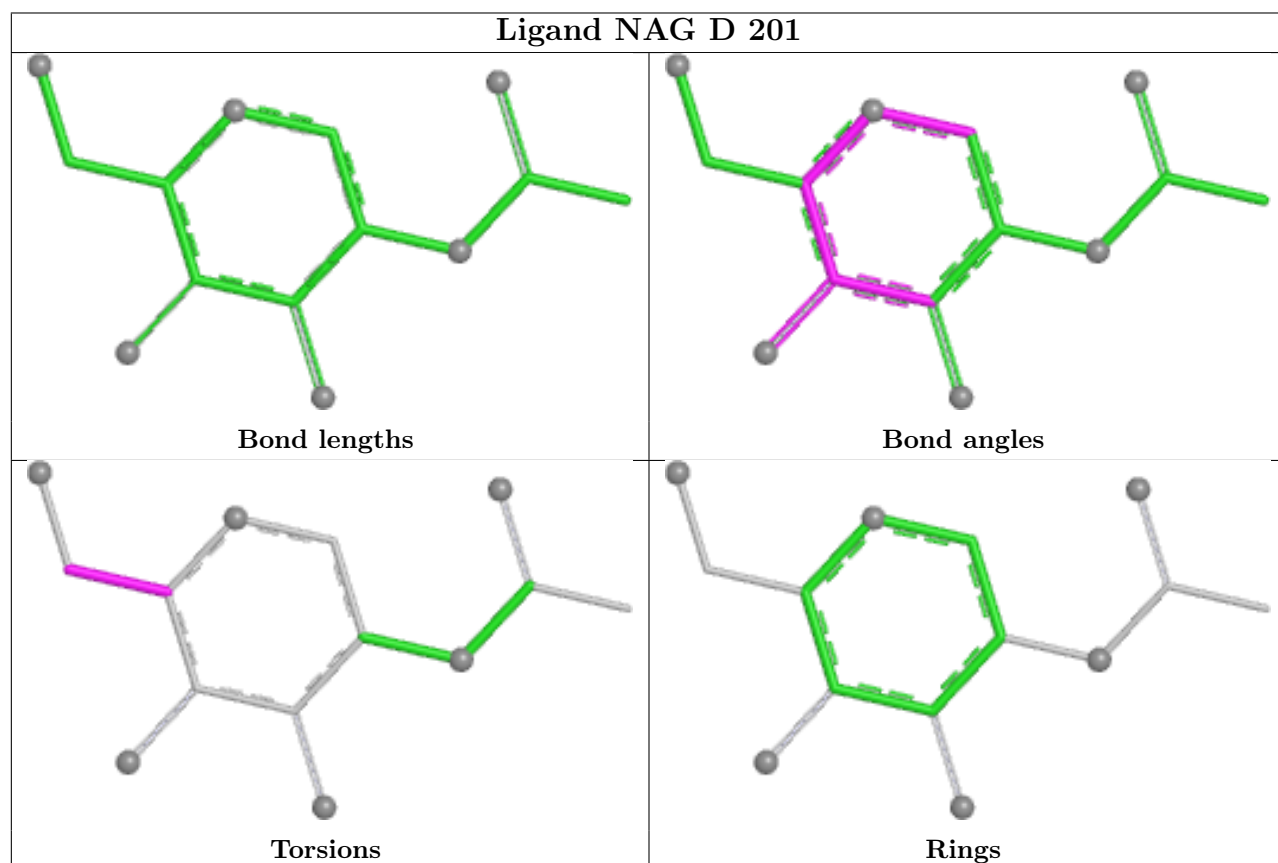
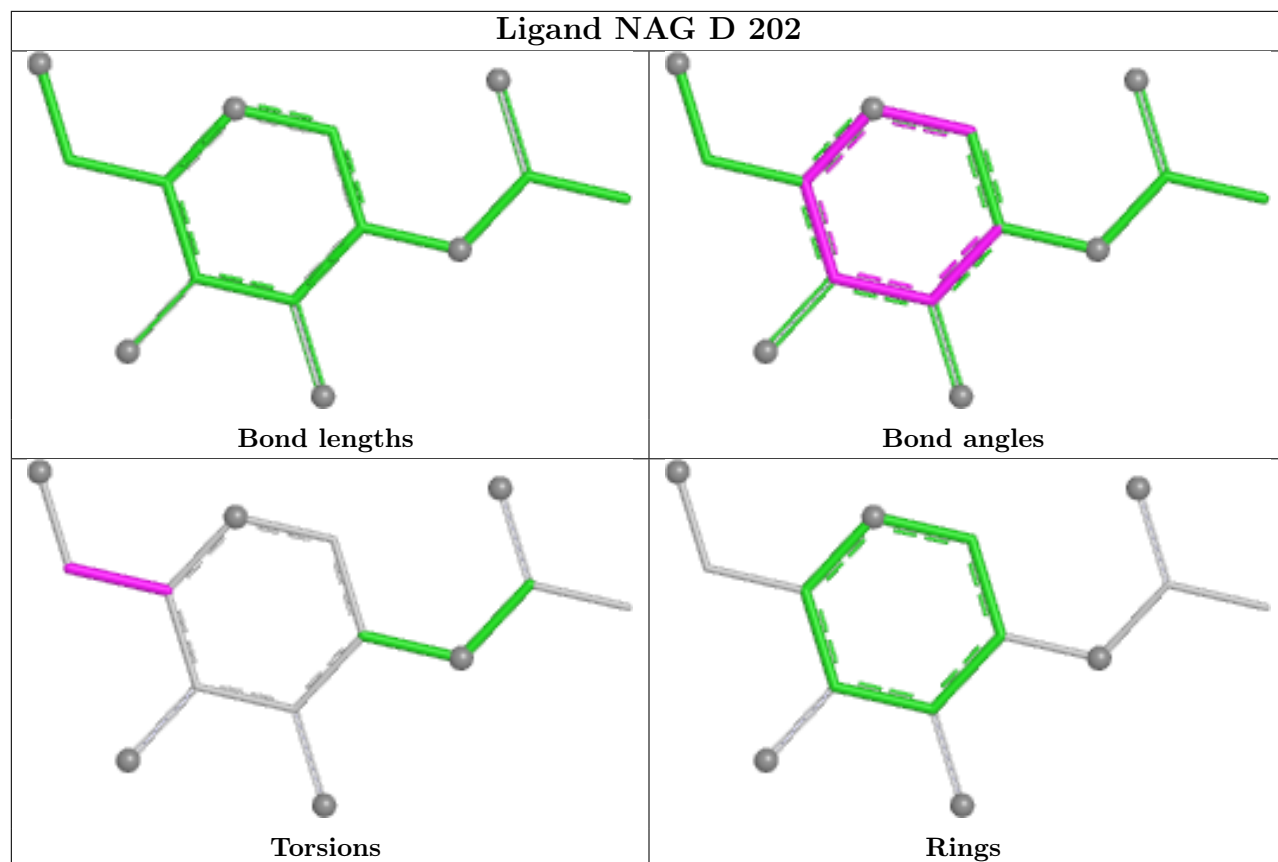
1 monomer is involved in 1 short contact:

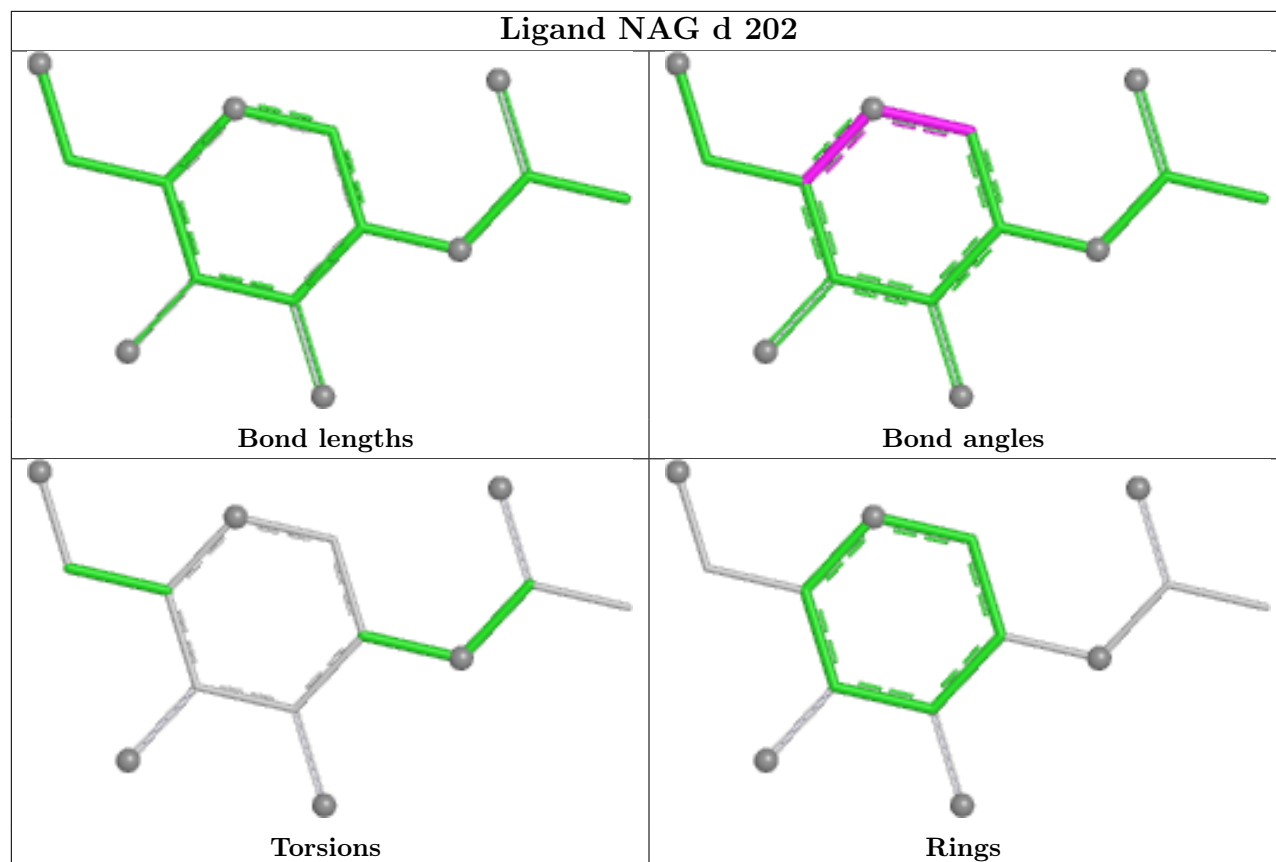
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	d	202	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

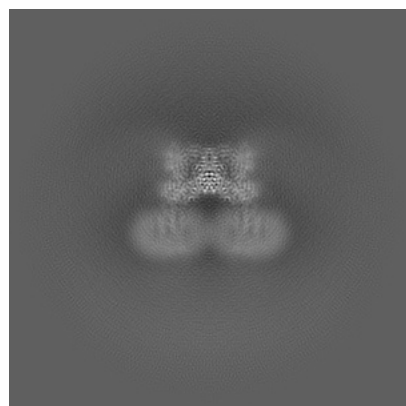
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61884. These allow visual inspection of the internal detail of the map and identification of artifacts.

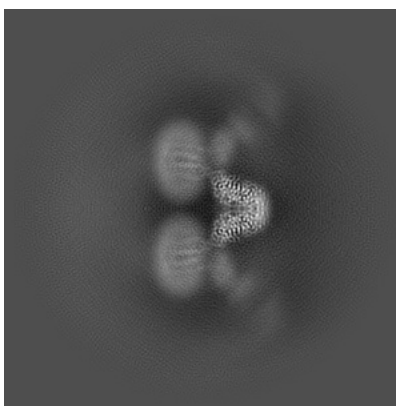
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

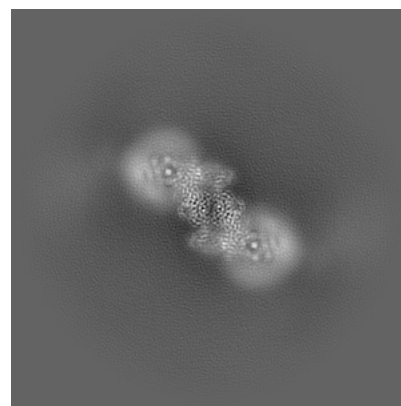
6.1.1 Primary map



X

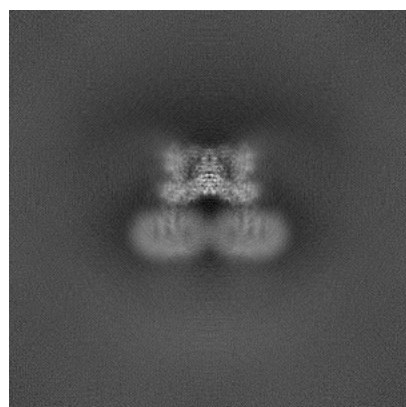


Y

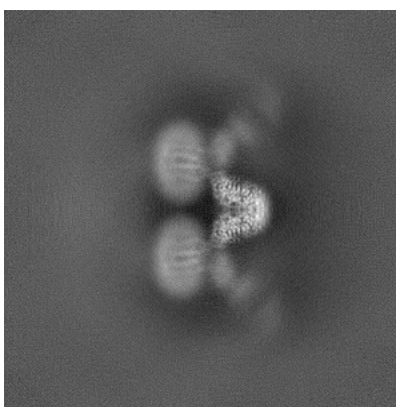


Z

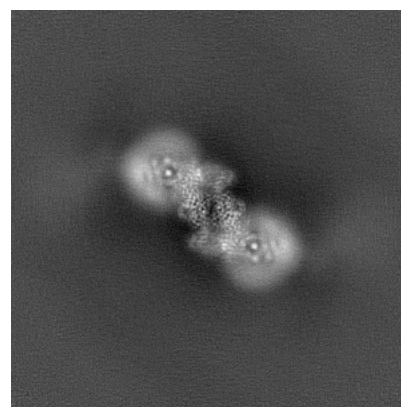
6.1.2 Raw map



X



Y

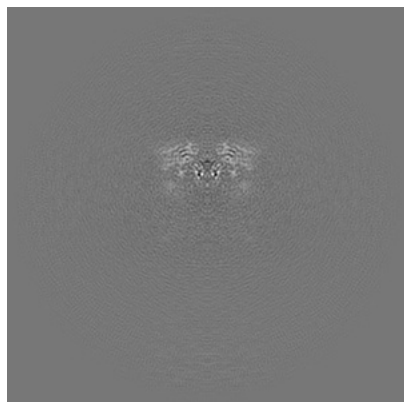


Z

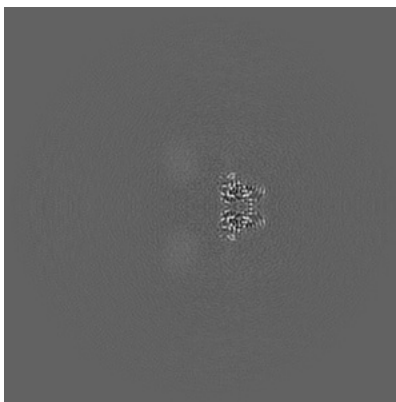
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

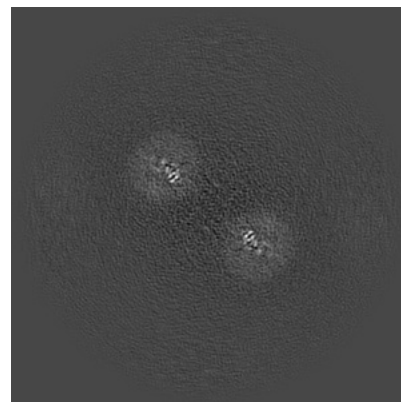
6.2.1 Primary map



X Index: 256



Y Index: 256

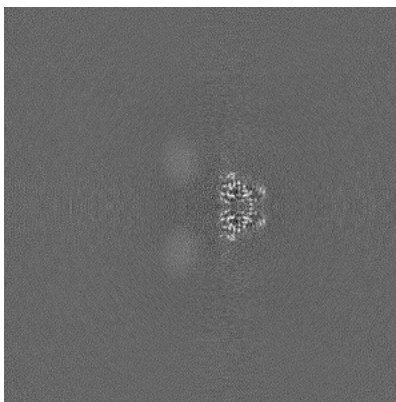


Z Index: 256

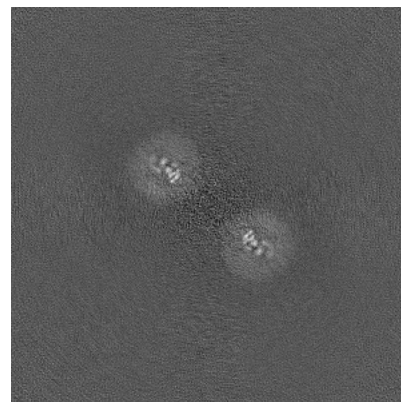
6.2.2 Raw map



X Index: 256



Y Index: 256

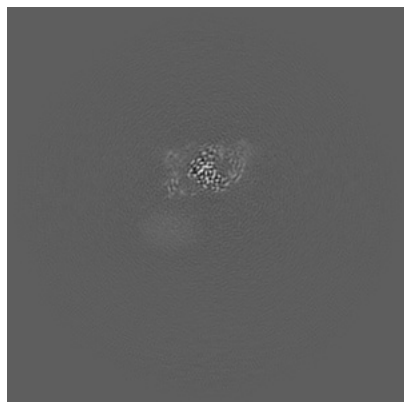


Z Index: 256

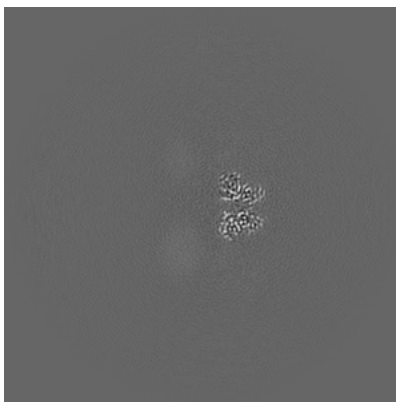
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

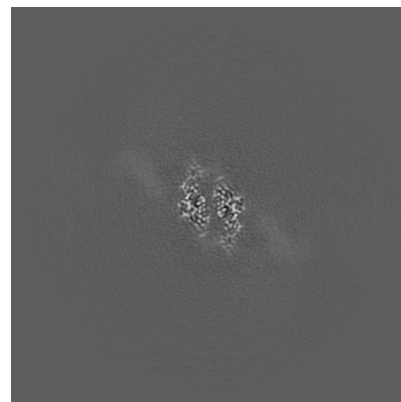
6.3.1 Primary map



X Index: 270



Y Index: 259

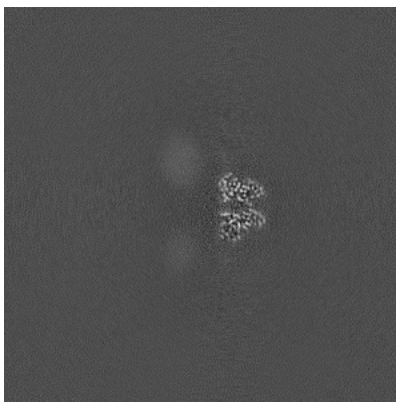


Z Index: 289

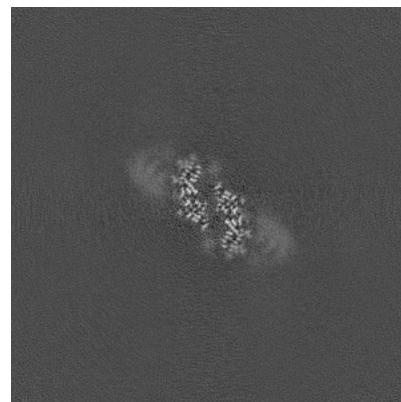
6.3.2 Raw map



X Index: 271



Y Index: 253

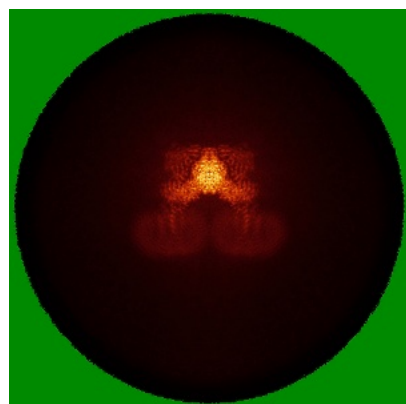


Z Index: 281

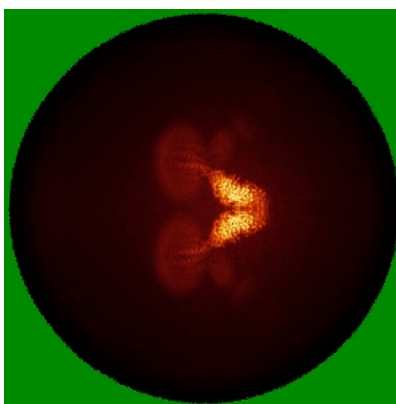
The images above show the largest variance slices of the map in three orthogonal directions.

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

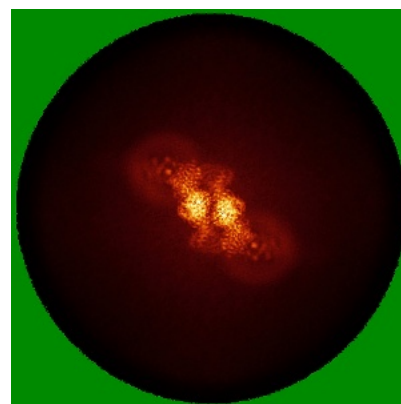
6.4.1 Primary map



X



Y

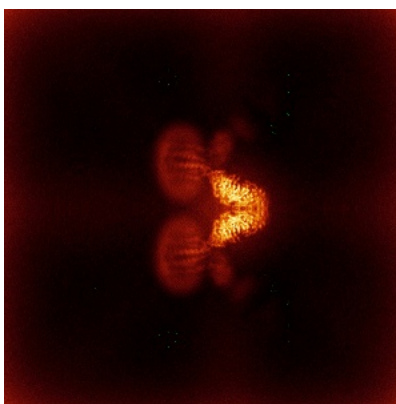


Z

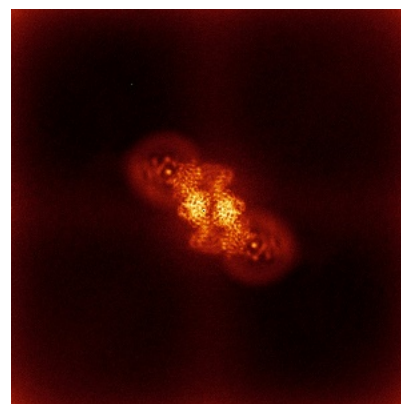
6.4.2 Raw map



X



Y

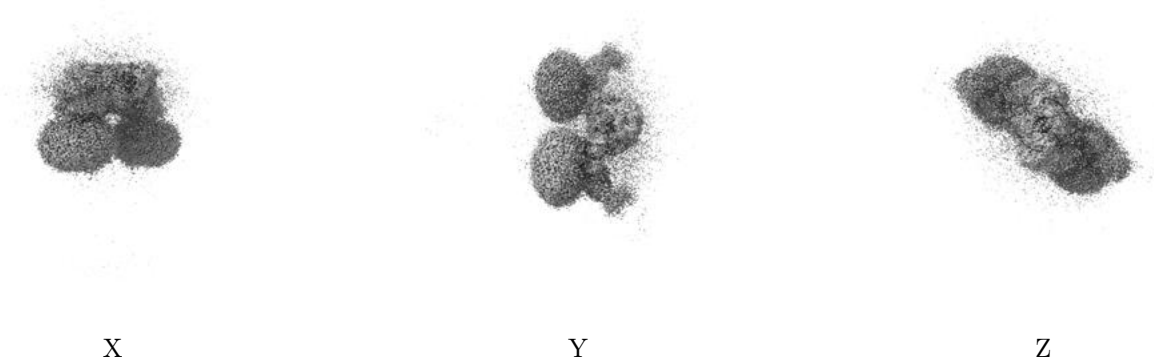


Z

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 0.0699. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

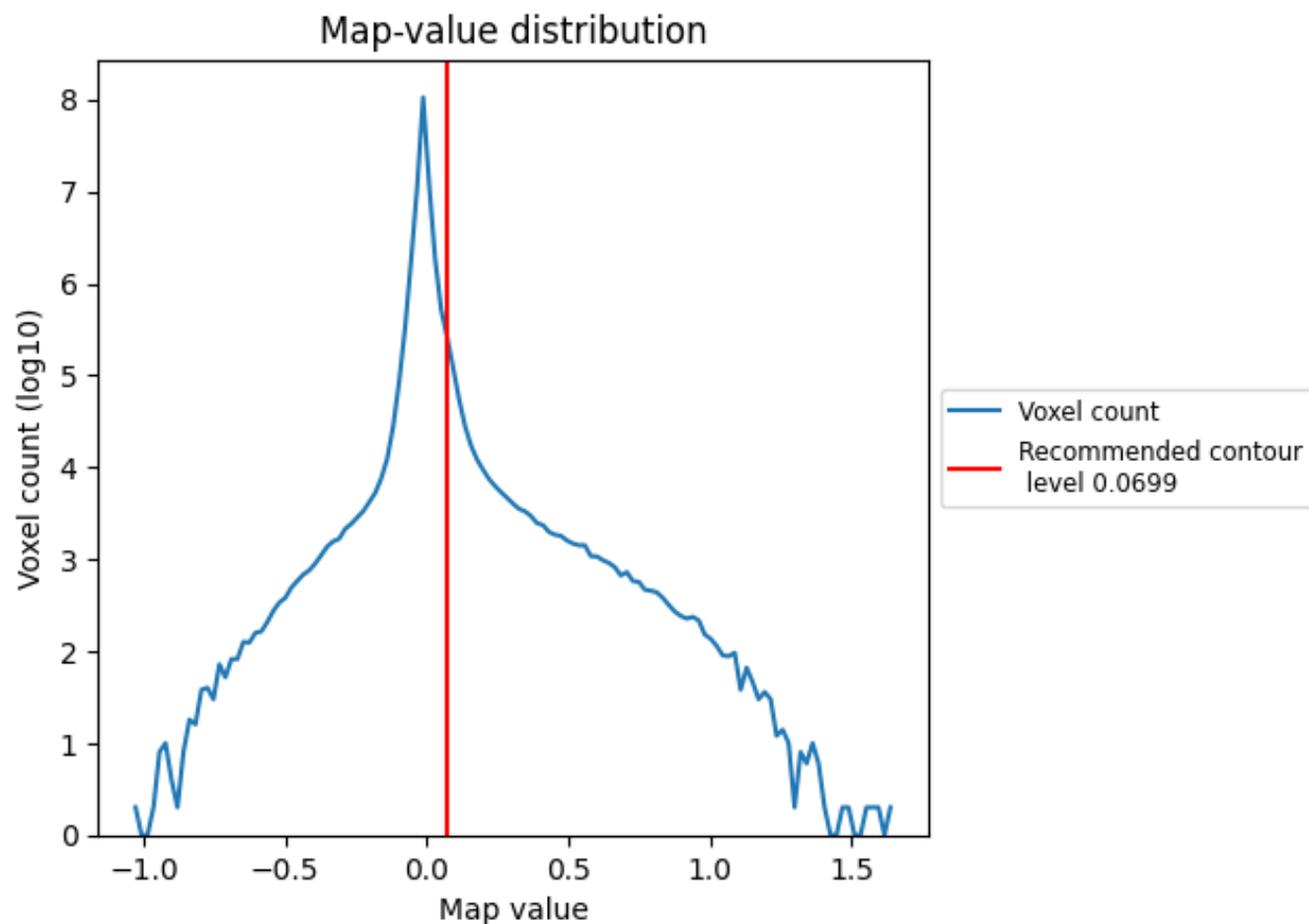
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

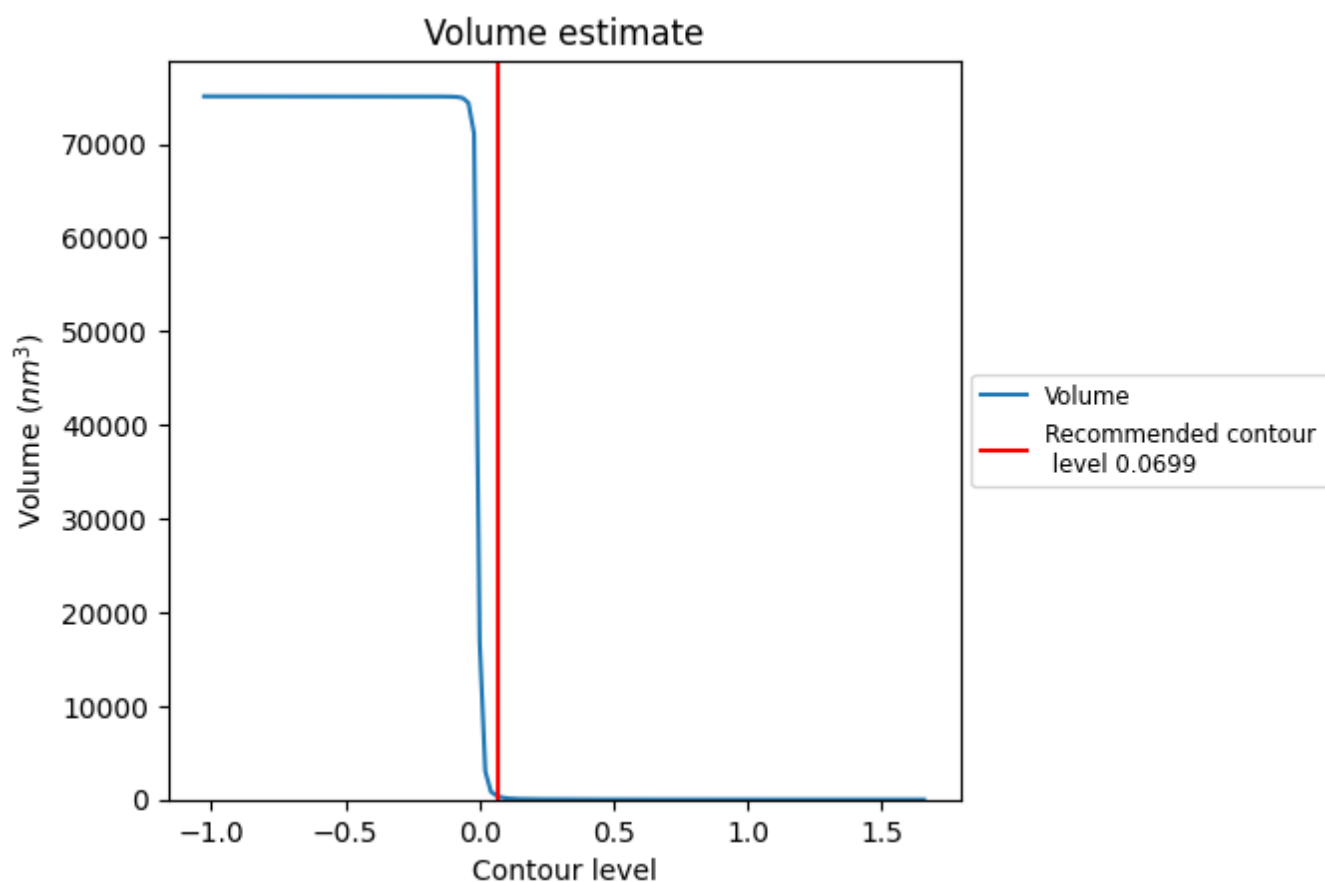
This section contains the results of statistical analysis of the map.

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.

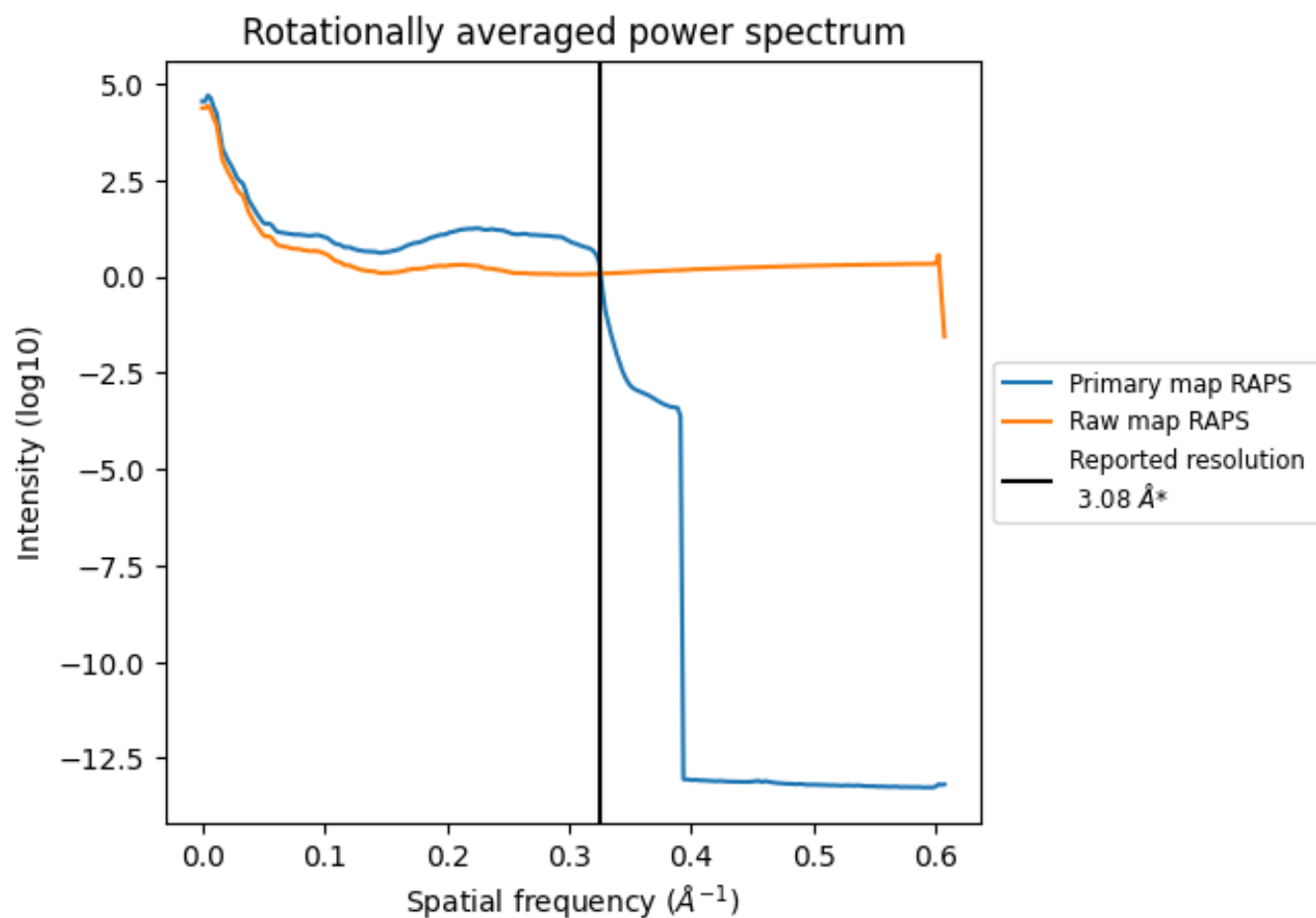
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 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 ⓘ

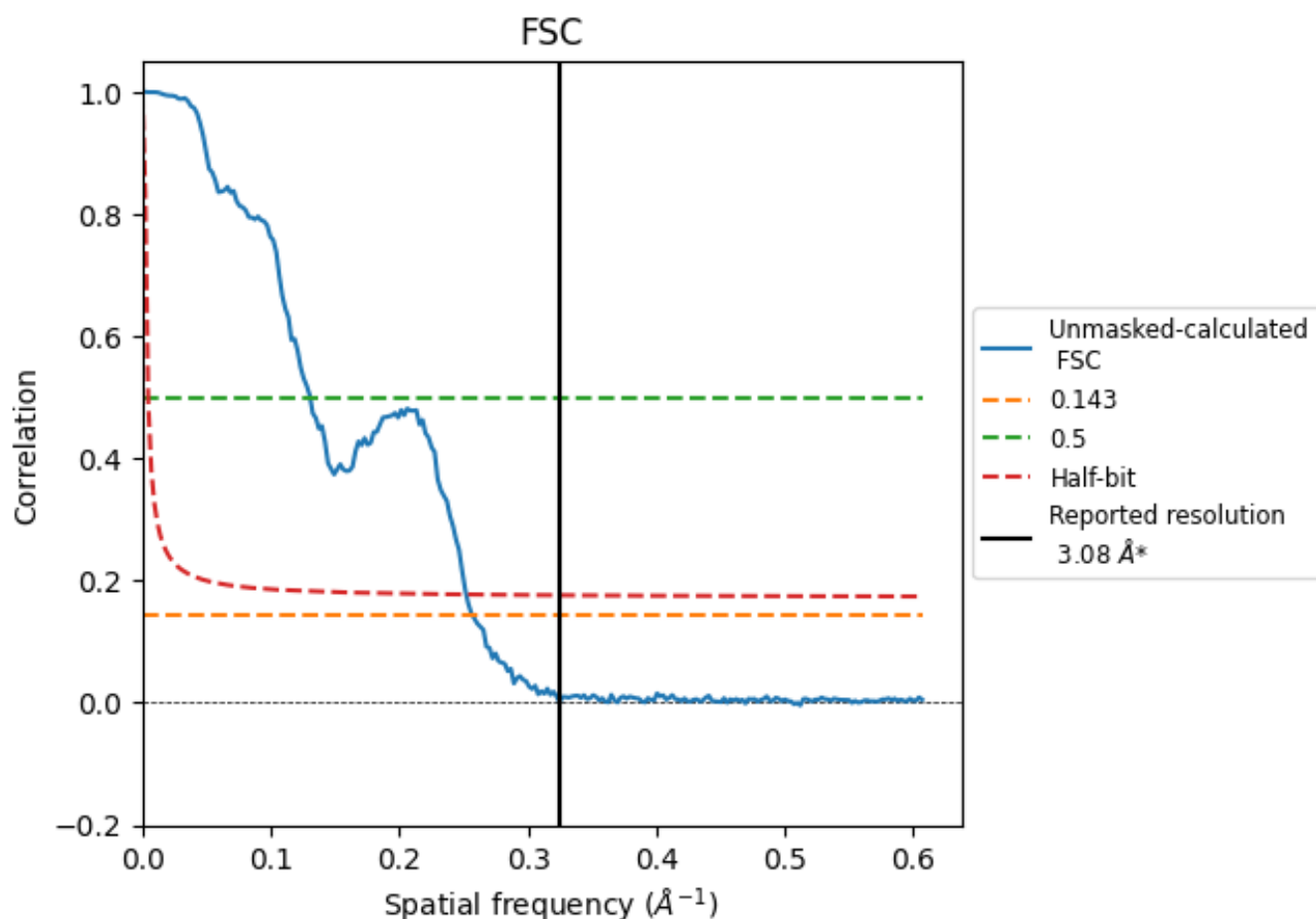


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

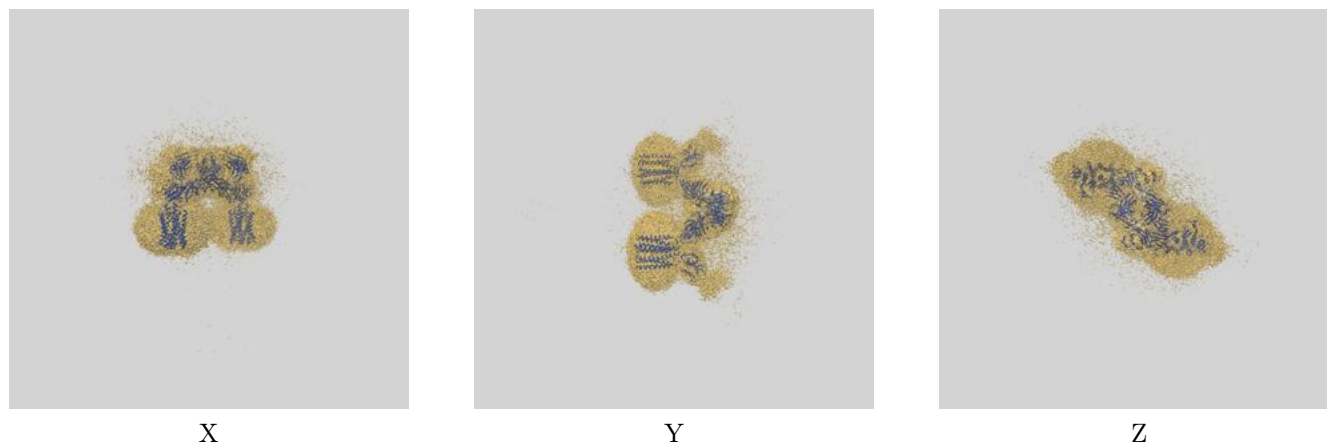
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	7.66	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

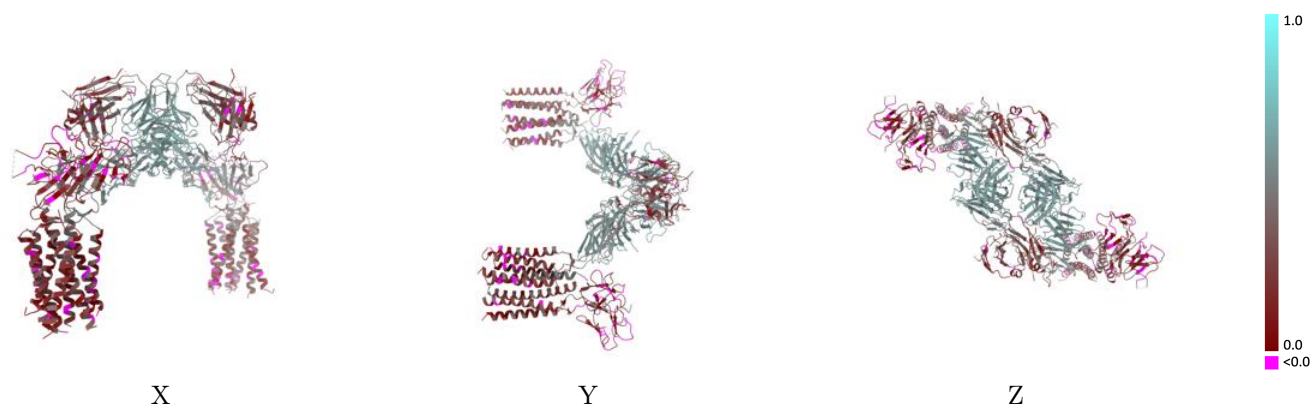
This section contains information regarding the fit between EMDB map EMD-61884 and PDB model 9JY1. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



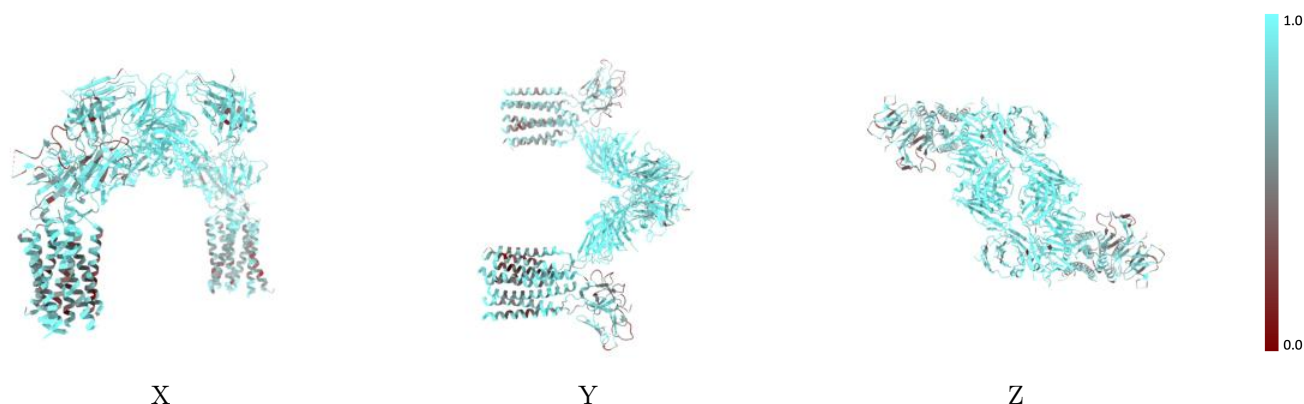
The images above show the 3D surface view of the map at the recommended contour level 0.0699 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



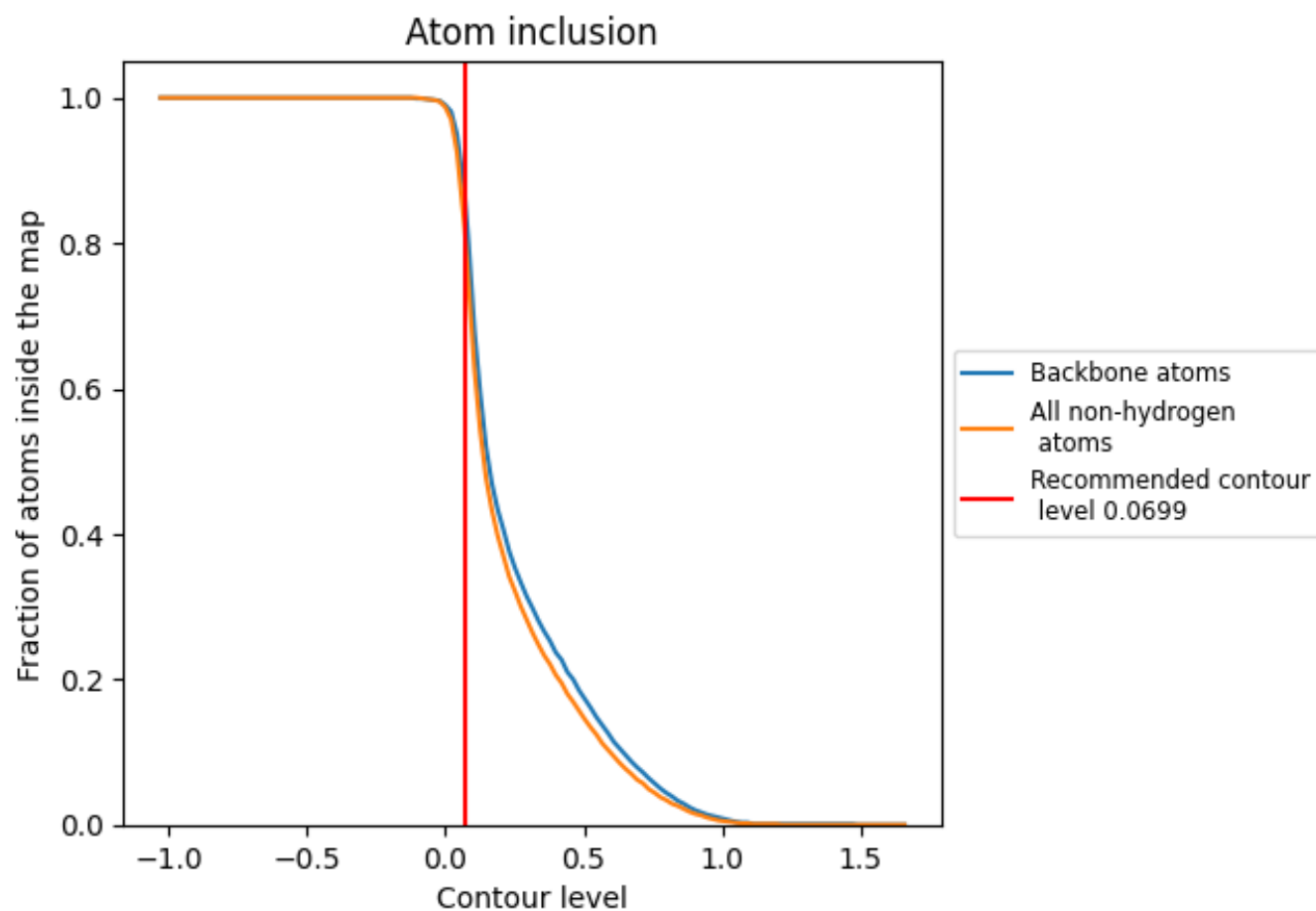
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0699).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.0699) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.3580
A	 0.6360	 0.1960
B	 0.6950	 0.2060
D	 0.8580	 0.3990
E	 0.9020	 0.4770
F	 0.6630	 0.1480
G	 0.6390	 0.1760
M	 0.7700	 0.3000
N	 0.7780	 0.2770
O	 0.9160	 0.4550
P	 0.9270	 0.4740
Q	 0.9130	 0.4550
R	 0.9270	 0.4750
a	 0.6360	 0.2020
b	 0.7120	 0.2110
d	 0.8590	 0.4050
e	 0.9020	 0.4770
f	 0.6630	 0.1470
g	 0.6360	 0.1730
m	 0.7740	 0.3080
n	 0.7810	 0.2860

