



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 09:34 AM UTC

PDB ID : 7B05 / pdb_00007b05
EMDB ID : EMD-11957
Title : TRPC4 in complex with inhibitor GFB-8749
Authors : Vinayagam, D.; Quentin, D.; Sistel, O.; Merino, F.; Stabrin, M.; Hofnagel, O.;
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Deposited on : 2020-11-18
Resolution : 3.80 Å(reported)
Based on initial model : 6GIK

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

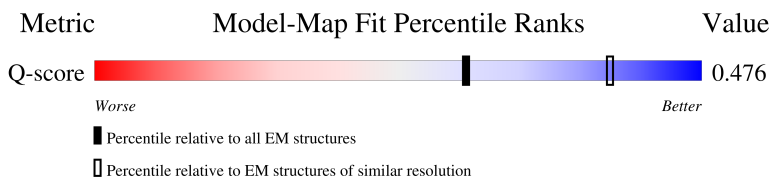
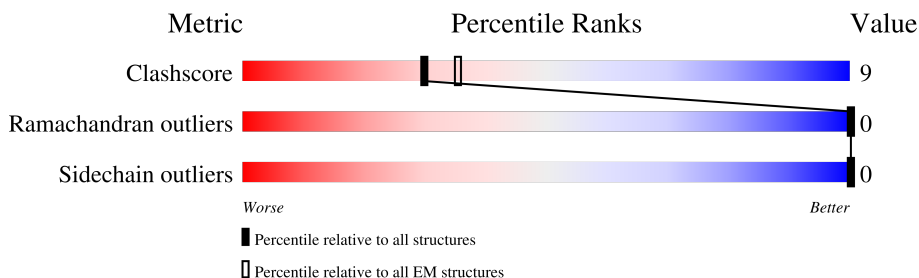
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	915	 55% 16% 30%
1	B	915	 55% 16% 30%
1	C	915	 55% 16% 30%
1	D	915	 55% 16% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21056 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.

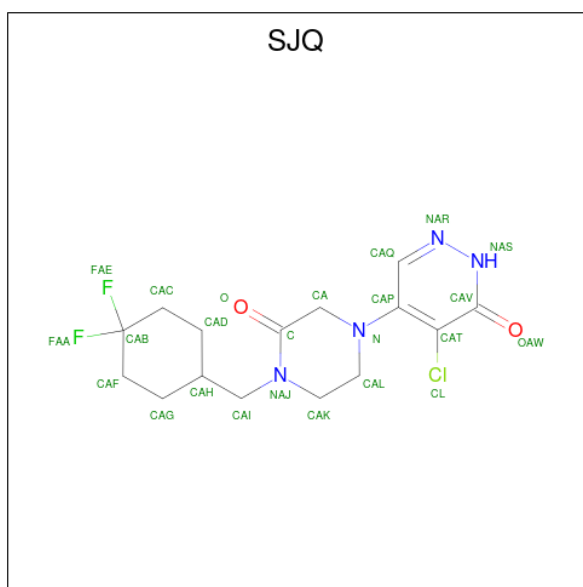
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily c member 4a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			5215	3410	859	919	27		
1	B	645	Total	C	N	O	S	0	0
			5215	3410	859	919	27		
1	C	645	Total	C	N	O	S	0	0
			5215	3410	859	919	27		
1	D	645	Total	C	N	O	S	0	0
			5215	3410	859	919	27		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP U3N7D8
B	1	GLY	-	expression tag	UNP U3N7D8
C	1	GLY	-	expression tag	UNP U3N7D8
D	1	GLY	-	expression tag	UNP U3N7D8

- Molecule 2 is 4-[4-[[4,4-bis(fluoranyl)cyclohexyl]methyl]-3-oxidanylidene-piperazin-1-yl]-5-chloranyl-1 {H}-pyridazin-6-one (CCD ID: SJQ) (formula: C₁₅H₁₉ClF₂N₄O₂) (labeled as "Ligand of Interest" by depositor).

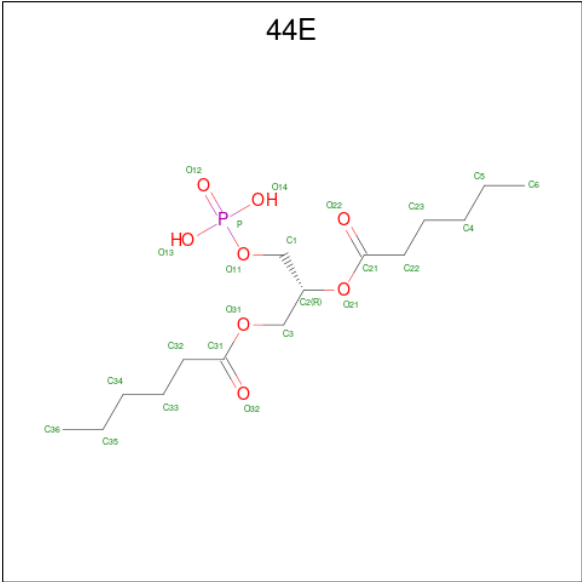


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Cl	F	N	O
			24	15	1	2	4	2
2	B	1	Total	C	Cl	F	N	O
			24	15	1	2	4	2
2	C	1	Total	C	Cl	F	N	O
			24	15	1	2	4	2
2	D	1	Total	C	Cl	F	N	O
			24	15	1	2	4	2

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

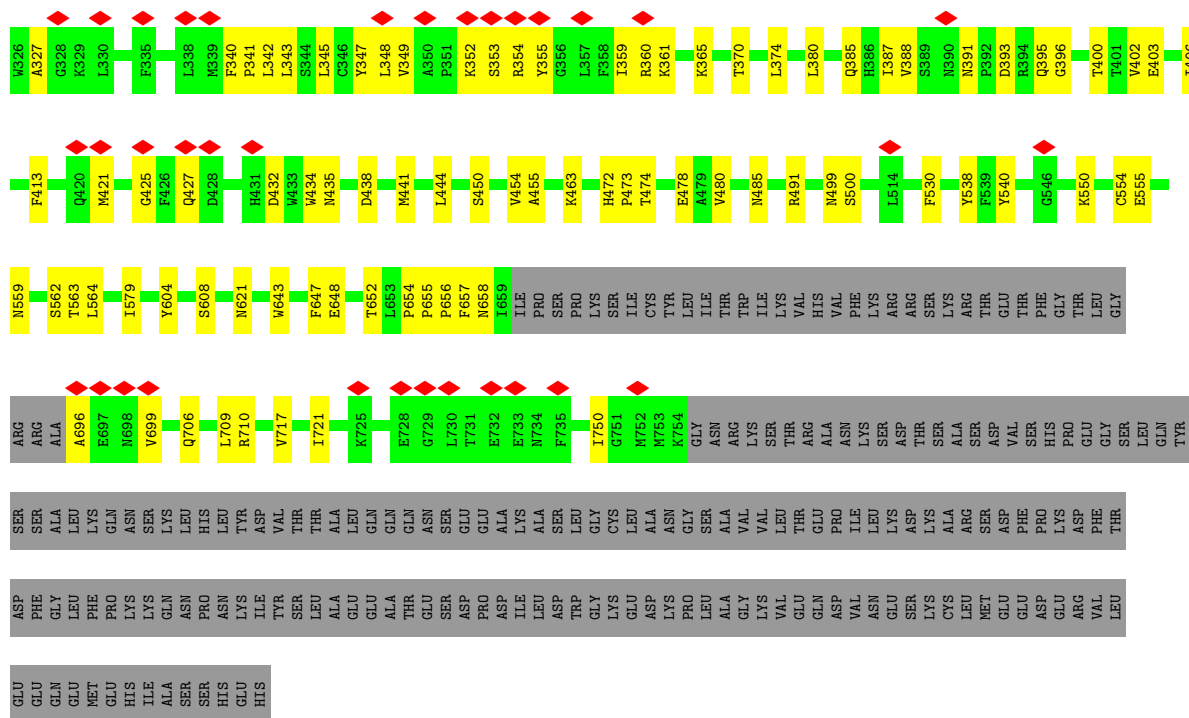
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is (2R)-3-(phosphonooxy)propane-1,2-diyl dihexanoate (CCD ID: 44E) (formula: C₁₅H₂₉O₈P).



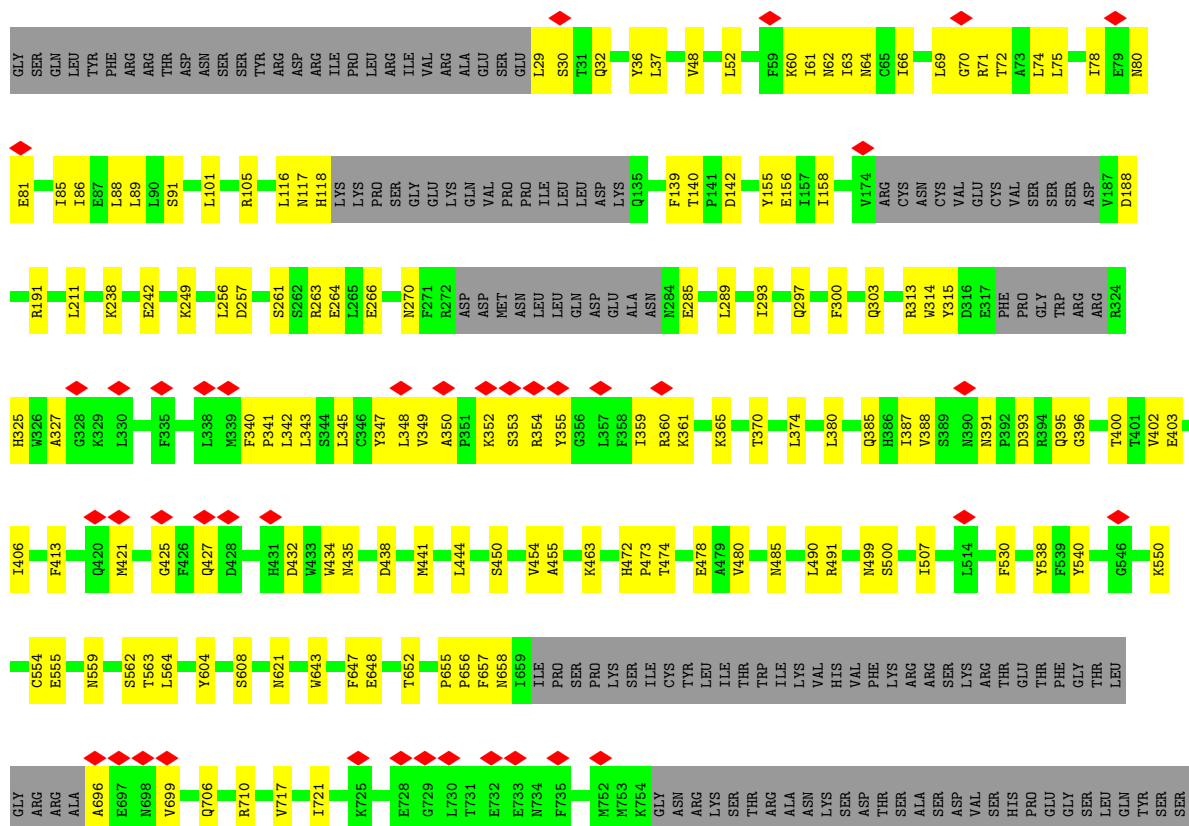
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			24	15	8	1	
4	B	1	Total	C	O	P	0
			24	15	8	1	
4	C	1	Total	C	O	P	0
			24	15	8	1	
4	D	1	Total	C	O	P	0
			24	15	8	1	





• Molecule 1: Transient receptor potential cation channel subfamily c member 4a

Chain D: 55% 16% 30%



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

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

GLN
GLU
MET
GLU
HIS
ILE
ALA
SER
SER
HIS
GLU
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	44989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	860	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	54945	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0093	Depositor
Map size ($\text{\AA}$)	262.08002, 262.08002, 262.08002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9100001, 0.9100001, 0.9100001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 44E, CA, SJQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/5341	0.45	0/7241
1	B	0.35	0/5341	0.45	0/7241
1	C	0.35	0/5341	0.45	0/7241
1	D	0.35	0/5341	0.45	0/7241
All	All	0.35	0/21364	0.45	0/28964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5215	0	5222	99	0
1	B	5215	0	5222	99	0
1	C	5215	0	5222	97	0
1	D	5215	0	5222	98	0
2	A	24	0	0	1	0
2	B	24	0	0	1	0
2	C	24	0	0	1	0
2	D	24	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	29	0	0
4	B	24	0	29	0	0
4	C	24	0	29	0	0
4	D	24	0	29	0	0
All	All	21056	0	21004	383	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 9.

All (383) 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:C:717:VAL:HG23	1:C:721:ILE:HD11	1.56	0.87
1:D:717:VAL:HG23	1:D:721:ILE:HD11	1.56	0.86
1:A:717:VAL:HG23	1:A:721:ILE:HD11	1.56	0.86
1:B:717:VAL:HG23	1:B:721:ILE:HD11	1.56	0.85
1:A:395:GLN:HE22	1:A:463:LYS:HB3	1.49	0.78
1:B:395:GLN:HE22	1:B:463:LYS:HB3	1.49	0.77
1:D:395:GLN:HE22	1:D:463:LYS:HB3	1.49	0.77
1:C:395:GLN:HE22	1:C:463:LYS:HB3	1.49	0.76
1:A:387:ILE:HG13	1:A:388:VAL:HG13	1.69	0.74
1:D:387:ILE:HG13	1:D:388:VAL:HG13	1.69	0.73
1:A:441:MET:HE3	2:A:1001:SJQ:CAV	2.19	0.73
1:B:441:MET:HE3	2:B:1001:SJQ:CAV	2.19	0.73
1:C:387:ILE:HG13	1:C:388:VAL:HG13	1.69	0.72
1:B:387:ILE:HG13	1:B:388:VAL:HG13	1.69	0.72
1:D:441:MET:HE3	2:D:1001:SJQ:CAV	2.19	0.72
1:C:441:MET:HE3	2:C:1001:SJQ:CAV	2.19	0.72
1:C:29:LEU:HG	1:C:30:SER:H	1.60	0.67
1:C:117:ASN:O	1:C:118:HIS:ND1	2.28	0.66
1:A:188:ASP:OD2	1:A:191:ARG:NH2	2.29	0.66
1:A:29:LEU:HG	1:A:30:SER:H	1.60	0.66
1:D:117:ASN:O	1:D:118:HIS:ND1	2.28	0.66
1:B:29:LEU:HG	1:B:30:SER:H	1.60	0.66
1:B:117:ASN:O	1:B:118:HIS:ND1	2.28	0.66
1:B:499:ASN:OD1	1:B:500:SER:N	2.29	0.66
1:D:29:LEU:HG	1:D:30:SER:H	1.60	0.66
1:D:499:ASN:OD1	1:D:500:SER:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:OD2	1:B:191:ARG:NH2	2.29	0.65
1:D:188:ASP:OD2	1:D:191:ARG:NH2	2.29	0.65
1:C:499:ASN:OD1	1:C:500:SER:N	2.29	0.65
1:A:257:ASP:OD1	1:A:303:GLN:NE2	2.30	0.65
1:A:117:ASN:O	1:A:118:HIS:ND1	2.28	0.65
1:C:188:ASP:OD2	1:C:191:ARG:NH2	2.29	0.65
1:D:257:ASP:OD1	1:D:303:GLN:NE2	2.30	0.65
1:A:499:ASN:OD1	1:A:500:SER:N	2.29	0.64
1:C:257:ASP:OD1	1:C:303:GLN:NE2	2.30	0.64
1:D:270:ASN:ND2	1:D:285:GLU:OE1	2.31	0.64
1:A:270:ASN:ND2	1:A:285:GLU:OE1	2.31	0.64
1:B:257:ASP:OD1	1:B:303:GLN:NE2	2.30	0.64
1:C:621:ASN:ND2	1:D:621:ASN:HD21	1.96	0.64
1:A:621:ASN:ND2	1:B:621:ASN:HD21	1.96	0.63
1:B:621:ASN:ND2	1:C:621:ASN:HD21	1.96	0.63
1:C:249:LYS:HA	1:C:297:GLN:HE22	1.64	0.63
1:C:270:ASN:ND2	1:C:285:GLU:OE1	2.31	0.63
1:A:621:ASN:HD21	1:D:621:ASN:ND2	1.96	0.62
1:D:249:LYS:HA	1:D:297:GLN:HE22	1.64	0.62
1:B:270:ASN:ND2	1:B:285:GLU:OE1	2.31	0.62
1:B:249:LYS:HA	1:B:297:GLN:HE22	1.64	0.62
1:D:105:ARG:HE	1:D:139:PHE:HZ	1.48	0.62
1:A:249:LYS:HA	1:A:297:GLN:HE22	1.64	0.61
1:A:105:ARG:HE	1:A:139:PHE:HZ	1.48	0.61
1:C:105:ARG:HE	1:C:139:PHE:HZ	1.48	0.60
1:B:105:ARG:HE	1:B:139:PHE:HZ	1.48	0.59
1:C:438:ASP:HA	1:C:441:MET:HE2	1.86	0.58
1:D:72:THR:HG22	1:D:74:LEU:H	1.70	0.57
1:D:438:ASP:HA	1:D:441:MET:HE2	1.86	0.57
1:A:444:LEU:HD22	1:A:480:VAL:HG13	1.86	0.57
1:B:444:LEU:HD22	1:B:480:VAL:HG13	1.86	0.57
1:B:438:ASP:HA	1:B:441:MET:HE2	1.86	0.57
1:C:261:SER:HB3	1:C:264:GLU:HB2	1.87	0.57
1:C:156:GLU:OE2	1:C:156:GLU:N	2.30	0.57
1:D:554:CYS:SG	1:D:555:GLU:N	2.78	0.57
1:B:554:CYS:SG	1:B:555:GLU:N	2.78	0.57
1:C:72:THR:HG22	1:C:74:LEU:H	1.70	0.57
1:B:72:THR:HG22	1:B:74:LEU:H	1.70	0.57
1:A:438:ASP:HA	1:A:441:MET:HE2	1.86	0.57
1:B:261:SER:HB3	1:B:264:GLU:HB2	1.87	0.57
1:A:60:LYS:HE2	1:A:61:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HG13	1:A:66:ILE:O	2.05	0.56
1:B:365:LYS:HE2	1:B:652:THR:HA	1.87	0.56
1:D:66:ILE:O	1:D:66:ILE:HG13	2.05	0.56
1:D:365:LYS:HE2	1:D:652:THR:HA	1.87	0.56
1:A:261:SER:HB3	1:A:264:GLU:HB2	1.87	0.56
1:A:554:CYS:SG	1:A:555:GLU:N	2.78	0.56
1:B:60:LYS:HE2	1:B:61:ILE:HG23	1.87	0.56
1:D:60:LYS:HE2	1:D:61:ILE:HG23	1.87	0.56
1:D:261:SER:HB3	1:D:264:GLU:HB2	1.87	0.56
1:A:72:THR:HG22	1:A:74:LEU:H	1.70	0.56
1:B:66:ILE:HG13	1:B:66:ILE:O	2.05	0.56
1:C:444:LEU:HD22	1:C:480:VAL:HG13	1.86	0.56
1:C:66:ILE:HG13	1:C:66:ILE:O	2.05	0.56
1:C:554:CYS:SG	1:C:555:GLU:N	2.78	0.56
1:D:444:LEU:HD22	1:D:480:VAL:HG13	1.86	0.56
1:A:365:LYS:HE2	1:A:652:THR:HA	1.87	0.56
1:B:66:ILE:HD12	1:B:70:GLY:HA2	1.88	0.56
1:C:66:ILE:HD12	1:C:70:GLY:HA2	1.88	0.56
1:C:365:LYS:HE2	1:C:652:THR:HA	1.87	0.55
1:A:66:ILE:HD12	1:A:70:GLY:HA2	1.88	0.55
1:C:60:LYS:HE2	1:C:61:ILE:HG23	1.87	0.55
1:D:66:ILE:HD12	1:D:70:GLY:HA2	1.88	0.55
1:B:345:LEU:HD23	1:B:348:LEU:HD21	1.88	0.55
1:A:101:LEU:HB3	1:A:139:PHE:CE1	2.42	0.55
1:D:345:LEU:HD23	1:D:348:LEU:HD21	1.88	0.55
1:D:101:LEU:HB3	1:D:139:PHE:CE1	2.42	0.54
1:A:345:LEU:HD23	1:A:348:LEU:HD21	1.88	0.54
1:A:156:GLU:OE2	1:A:156:GLU:N	2.30	0.54
1:B:101:LEU:HB3	1:B:139:PHE:CE1	2.42	0.54
1:A:402:VAL:O	1:A:406:ILE:HG12	2.08	0.54
1:C:402:VAL:O	1:C:406:ILE:HG12	2.08	0.54
1:B:402:VAL:O	1:B:406:ILE:HG12	2.08	0.53
1:C:101:LEU:HB3	1:C:139:PHE:CE1	2.42	0.53
1:C:345:LEU:HD23	1:C:348:LEU:HD21	1.88	0.53
1:B:530:PHE:CD2	1:B:604:TYR:HB2	2.44	0.53
1:D:402:VAL:O	1:D:406:ILE:HG12	2.08	0.53
1:A:530:PHE:CD2	1:A:604:TYR:HB2	2.44	0.53
1:D:530:PHE:CD2	1:D:604:TYR:HB2	2.44	0.52
1:D:455:ALA:HB2	1:D:473:PRO:HB2	1.92	0.52
1:B:455:ALA:HB2	1:B:473:PRO:HB2	1.92	0.52
1:C:88:LEU:O	1:C:91:SER:OG	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:PRO:N	1:D:656:PRO:HD2	2.26	0.51
1:A:455:ALA:HB2	1:A:473:PRO:HB2	1.92	0.51
1:A:655:PRO:N	1:A:656:PRO:HD2	2.26	0.51
1:C:530:PHE:CD2	1:C:604:TYR:HB2	2.44	0.51
1:D:340:PHE:CD1	1:D:341:PRO:HD3	2.46	0.51
1:A:340:PHE:CD1	1:A:341:PRO:HD3	2.46	0.51
1:B:340:PHE:CD1	1:B:341:PRO:HD3	2.46	0.51
1:C:455:ALA:HB2	1:C:473:PRO:HB2	1.92	0.51
1:C:340:PHE:CD1	1:C:341:PRO:HD3	2.46	0.51
1:B:88:LEU:O	1:B:91:SER:OG	2.27	0.51
1:C:648:GLU:OE1	1:C:648:GLU:N	2.43	0.51
1:D:648:GLU:OE1	1:D:648:GLU:N	2.43	0.51
1:B:156:GLU:OE2	1:B:156:GLU:N	2.30	0.50
1:C:30:SER:O	1:C:32:GLN:HG3	2.11	0.50
1:B:30:SER:O	1:B:32:GLN:HG3	2.11	0.50
1:B:550:LYS:HE3	1:B:559:ASN:ND2	2.26	0.50
1:C:352:LYS:HG2	1:C:353:SER:H	1.77	0.50
1:A:88:LEU:O	1:A:91:SER:OG	2.27	0.50
1:C:655:PRO:N	1:C:656:PRO:HD2	2.26	0.50
1:D:550:LYS:HE3	1:D:559:ASN:ND2	2.26	0.50
1:A:550:LYS:HE3	1:A:559:ASN:ND2	2.26	0.50
1:B:36:TYR:HD2	1:B:37:LEU:HD22	1.76	0.50
1:B:655:PRO:N	1:B:656:PRO:HD2	2.26	0.50
1:C:550:LYS:HE3	1:C:559:ASN:ND2	2.26	0.50
1:B:140:THR:HG22	1:B:142:ASP:H	1.77	0.50
1:B:352:LYS:HG2	1:B:353:SER:H	1.77	0.50
1:D:30:SER:O	1:D:32:GLN:HG3	2.11	0.50
1:D:352:LYS:HG2	1:D:353:SER:H	1.77	0.50
1:A:30:SER:O	1:A:32:GLN:HG3	2.11	0.50
1:C:140:THR:HG22	1:C:142:ASP:H	1.77	0.50
1:A:434:TRP:HB3	1:A:491:ARG:NH1	2.27	0.50
1:B:434:TRP:HB3	1:B:491:ARG:NH1	2.27	0.50
1:A:36:TYR:HD2	1:A:37:LEU:HD22	1.76	0.49
1:A:352:LYS:HG2	1:A:353:SER:H	1.77	0.49
1:C:36:TYR:HD2	1:C:37:LEU:HD22	1.76	0.49
1:C:434:TRP:HB3	1:C:491:ARG:NH1	2.27	0.49
1:A:238:LYS:O	1:A:242:GLU:HG2	2.13	0.49
1:A:140:THR:HG22	1:A:142:ASP:H	1.77	0.49
1:B:238:LYS:O	1:B:242:GLU:HG2	2.13	0.49
1:D:140:THR:HG22	1:D:142:ASP:H	1.77	0.49
1:D:238:LYS:O	1:D:242:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:TRP:HB3	1:D:491:ARG:NH1	2.27	0.49
1:C:655:PRO:HA	1:C:658:ASN:HB2	1.95	0.48
1:C:48:VAL:O	1:C:52:LEU:HD23	2.13	0.48
1:A:48:VAL:O	1:A:52:LEU:HD23	2.13	0.48
1:C:69:LEU:HB2	1:C:71:ARG:HD2	1.96	0.48
1:C:238:LYS:O	1:C:242:GLU:HG2	2.13	0.48
1:D:36:TYR:HD2	1:D:37:LEU:HD22	1.76	0.48
1:D:69:LEU:HB2	1:D:71:ARG:HD2	1.96	0.48
1:D:63:ILE:H	1:D:63:ILE:HD12	1.79	0.48
1:B:648:GLU:OE1	1:B:648:GLU:N	2.43	0.48
1:A:655:PRO:HA	1:A:658:ASN:HB2	1.95	0.48
1:B:655:PRO:HA	1:B:658:ASN:HB2	1.95	0.48
1:A:648:GLU:N	1:A:648:GLU:OE1	2.43	0.48
1:C:63:ILE:HD12	1:C:63:ILE:H	1.79	0.48
1:A:696:ALA:N	1:A:699:VAL:HB	2.29	0.48
1:B:48:VAL:O	1:B:52:LEU:HD23	2.13	0.48
1:D:156:GLU:OE2	1:D:156:GLU:N	2.30	0.48
1:A:63:ILE:HD12	1:A:63:ILE:H	1.79	0.48
1:B:696:ALA:N	1:B:699:VAL:HB	2.29	0.48
1:D:263:ARG:O	1:D:266:GLU:HG3	2.14	0.48
1:B:354:ARG:HG3	1:B:355:TYR:CD2	2.49	0.47
1:D:354:ARG:HG3	1:D:355:TYR:CD2	2.49	0.47
1:D:655:PRO:HA	1:D:658:ASN:HB2	1.95	0.47
1:A:62:ASN:ND2	1:A:64:ASN:OD1	2.48	0.47
1:A:354:ARG:HG3	1:A:355:TYR:CD2	2.49	0.47
1:C:354:ARG:HG3	1:C:355:TYR:CD2	2.49	0.47
1:D:696:ALA:N	1:D:699:VAL:HB	2.29	0.47
1:B:263:ARG:O	1:B:266:GLU:HG3	2.14	0.47
1:D:48:VAL:O	1:D:52:LEU:HD23	2.13	0.47
1:D:380:LEU:HD21	1:D:485:ASN:CG	2.39	0.47
1:A:263:ARG:O	1:A:266:GLU:HG3	2.14	0.47
1:B:63:ILE:HD12	1:B:63:ILE:H	1.79	0.47
1:B:314:TRP:HD1	1:B:315:TYR:CD1	2.32	0.47
1:B:380:LEU:HD21	1:B:485:ASN:CG	2.39	0.47
1:A:60:LYS:HB2	1:A:60:LYS:HE3	1.73	0.47
1:B:69:LEU:HB2	1:B:71:ARG:HD2	1.96	0.47
1:C:263:ARG:O	1:C:266:GLU:HG3	2.14	0.47
1:C:621:ASN:ND2	1:D:621:ASN:ND2	2.63	0.47
1:A:69:LEU:HB2	1:A:71:ARG:HD2	1.96	0.47
1:A:314:TRP:HD1	1:A:315:TYR:CD1	2.32	0.47
1:C:60:LYS:HG3	1:C:61:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:TRP:HD1	1:D:315:TYR:CD1	2.32	0.47
1:A:354:ARG:HG3	1:A:355:TYR:CE2	2.50	0.47
1:D:62:ASN:ND2	1:D:64:ASN:OD1	2.48	0.47
1:A:413:PHE:HE2	1:A:655:PRO:HG2	1.80	0.46
1:C:696:ALA:N	1:C:699:VAL:HB	2.29	0.46
1:D:60:LYS:HG3	1:D:61:ILE:N	2.30	0.46
1:D:345:LEU:HA	1:D:348:LEU:HG	1.98	0.46
1:D:354:ARG:HG3	1:D:355:TYR:CE2	2.50	0.46
1:A:60:LYS:HG3	1:A:61:ILE:N	2.30	0.46
1:B:62:ASN:ND2	1:B:64:ASN:OD1	2.48	0.46
1:A:345:LEU:HA	1:A:348:LEU:HG	1.98	0.46
1:C:325:HIS:NE2	1:C:327:ALA:HB3	2.31	0.46
1:C:413:PHE:HE2	1:C:655:PRO:HG2	1.80	0.46
1:D:88:LEU:O	1:D:91:SER:OG	2.27	0.46
1:B:354:ARG:HG3	1:B:355:TYR:CE2	2.50	0.46
1:A:380:LEU:HD21	1:A:485:ASN:CG	2.39	0.46
1:B:325:HIS:NE2	1:B:327:ALA:HB3	2.31	0.46
1:C:314:TRP:HD1	1:C:315:TYR:CD1	2.32	0.46
1:C:345:LEU:HA	1:C:348:LEU:HG	1.98	0.46
1:D:472:HIS:ND1	1:D:473:PRO:HD2	2.31	0.46
1:C:62:ASN:ND2	1:C:64:ASN:OD1	2.48	0.46
1:C:380:LEU:HD21	1:C:485:ASN:CG	2.39	0.46
1:A:354:ARG:HA	1:A:354:ARG:HD2	1.75	0.46
1:D:325:HIS:NE2	1:D:327:ALA:HB3	2.31	0.46
1:B:345:LEU:HA	1:B:348:LEU:HG	1.98	0.46
1:D:256:LEU:HD22	1:D:300:PHE:CE1	2.51	0.46
1:A:256:LEU:HD22	1:A:300:PHE:CE1	2.51	0.46
1:B:60:LYS:HG3	1:B:61:ILE:N	2.30	0.46
1:B:472:HIS:ND1	1:B:473:PRO:HD2	2.31	0.46
1:B:621:ASN:ND2	1:C:621:ASN:ND2	2.63	0.46
1:D:413:PHE:HE2	1:D:655:PRO:HG2	1.80	0.46
1:A:621:ASN:ND2	1:B:621:ASN:ND2	2.63	0.45
1:B:256:LEU:HD22	1:B:300:PHE:CE1	2.51	0.45
1:A:325:HIS:NE2	1:A:327:ALA:HB3	2.31	0.45
1:B:413:PHE:HE2	1:B:655:PRO:HG2	1.80	0.45
1:C:472:HIS:ND1	1:C:473:PRO:HD2	2.31	0.45
1:C:709:LEU:HD23	1:C:709:LEU:HA	1.83	0.45
1:A:472:HIS:ND1	1:A:473:PRO:HD2	2.31	0.45
1:A:621:ASN:ND2	1:D:621:ASN:ND2	2.63	0.45
1:C:354:ARG:HG3	1:C:355:TYR:CE2	2.50	0.45
1:C:360:ARG:HA	1:C:360:ARG:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLY:C	1:A:427:GLN:H	2.25	0.45
1:A:421:MET:O	1:A:425:GLY:N	2.50	0.45
1:C:256:LEU:HD22	1:C:300:PHE:CE1	2.51	0.45
1:D:538:TYR:O	1:D:540:TYR:N	2.50	0.45
1:C:538:TYR:O	1:C:540:TYR:N	2.50	0.44
1:D:474:THR:O	1:D:478:GLU:HG3	2.17	0.44
1:D:425:GLY:C	1:D:427:GLN:H	2.25	0.44
1:B:421:MET:O	1:B:425:GLY:N	2.50	0.44
1:A:391:ASN:OD1	1:A:393:ASP:N	2.51	0.44
1:B:289:LEU:O	1:B:293:ILE:HG12	2.18	0.44
1:B:474:THR:O	1:B:478:GLU:HG3	2.17	0.44
1:C:361:LYS:HD3	1:C:361:LYS:HA	1.84	0.44
1:A:158:ILE:H	1:A:158:ILE:HD12	1.82	0.44
1:B:158:ILE:HD12	1:B:158:ILE:H	1.82	0.44
1:C:343:LEU:CD2	1:C:359:ILE:HB	2.48	0.44
1:B:391:ASN:OD1	1:B:393:ASP:N	2.51	0.44
1:B:425:GLY:C	1:B:427:GLN:H	2.25	0.44
1:D:343:LEU:CD2	1:D:359:ILE:HB	2.48	0.44
1:A:343:LEU:CD2	1:A:359:ILE:HB	2.48	0.44
1:B:342:LEU:HA	1:B:345:LEU:HD12	2.00	0.44
1:D:158:ILE:HD12	1:D:158:ILE:H	1.82	0.44
1:D:391:ASN:OD1	1:D:393:ASP:N	2.51	0.44
1:C:72:THR:HB	1:C:75:LEU:HD13	2.00	0.44
1:C:158:ILE:HD12	1:C:158:ILE:H	1.82	0.44
1:C:474:THR:O	1:C:478:GLU:HG3	2.17	0.44
1:D:72:THR:HB	1:D:75:LEU:HD13	2.00	0.44
1:A:289:LEU:O	1:A:293:ILE:HG12	2.18	0.44
1:A:538:TYR:O	1:A:540:TYR:N	2.50	0.44
1:C:313:ARG:HD3	1:C:647:PHE:CE1	2.53	0.44
1:C:345:LEU:O	1:C:349:VAL:HG12	2.18	0.44
1:C:643:TRP:HB3	1:C:647:PHE:HE2	1.82	0.44
1:A:608:SER:O	1:A:608:SER:OG	2.34	0.43
1:B:72:THR:HB	1:B:75:LEU:HD13	2.00	0.43
1:B:643:TRP:HB3	1:B:647:PHE:HE2	1.82	0.43
1:D:345:LEU:O	1:D:349:VAL:HG12	2.18	0.43
1:A:313:ARG:HD3	1:A:647:PHE:CE1	2.53	0.43
1:B:343:LEU:CD2	1:B:359:ILE:HB	2.48	0.43
1:C:391:ASN:OD1	1:C:393:ASP:N	2.51	0.43
1:D:289:LEU:O	1:D:293:ILE:HG12	2.18	0.43
1:D:342:LEU:HA	1:D:345:LEU:HD12	2.00	0.43
1:B:345:LEU:O	1:B:349:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:TYR:O	1:B:540:TYR:N	2.50	0.43
1:D:313:ARG:HD3	1:D:647:PHE:CE1	2.53	0.43
1:A:72:THR:HB	1:A:75:LEU:HD13	2.00	0.43
1:A:342:LEU:HA	1:A:345:LEU:HD12	2.00	0.43
1:A:474:THR:O	1:A:478:GLU:HG3	2.17	0.43
1:C:579:ILE:HD13	1:C:579:ILE:HA	1.88	0.43
1:B:80:ASN:O	1:B:81:GLU:HG3	2.19	0.43
1:C:421:MET:O	1:C:425:GLY:N	2.50	0.43
1:C:425:GLY:C	1:C:427:GLN:H	2.25	0.43
1:D:341:PRO:HA	1:D:657:PHE:HE2	1.83	0.43
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.81	0.43
1:C:450:SER:O	1:C:454:VAL:HG23	2.19	0.43
1:D:421:MET:O	1:D:425:GLY:N	2.50	0.43
1:D:450:SER:O	1:D:454:VAL:HG23	2.19	0.43
1:A:361:LYS:HA	1:A:361:LYS:HD3	1.84	0.43
1:B:313:ARG:HD3	1:B:647:PHE:CE1	2.53	0.43
1:B:341:PRO:HA	1:B:657:PHE:HE2	1.83	0.43
1:B:347:TYR:HB2	1:B:359:ILE:HG21	2.00	0.43
1:C:289:LEU:O	1:C:293:ILE:HG12	2.18	0.43
1:B:608:SER:O	1:B:608:SER:OG	2.34	0.43
1:C:342:LEU:HA	1:C:345:LEU:HD12	2.00	0.43
1:D:643:TRP:HB3	1:D:647:PHE:HE2	1.82	0.43
1:D:80:ASN:O	1:D:81:GLU:HG3	2.19	0.43
1:C:80:ASN:O	1:C:81:GLU:HG3	2.19	0.42
1:C:85:ILE:O	1:C:89:LEU:HD23	2.19	0.42
1:A:80:ASN:O	1:A:81:GLU:HG3	2.19	0.42
1:A:85:ILE:O	1:A:89:LEU:HD23	2.19	0.42
1:A:643:TRP:HB3	1:A:647:PHE:HE2	1.82	0.42
1:B:450:SER:O	1:B:454:VAL:HG23	2.19	0.42
1:C:341:PRO:HA	1:C:657:PHE:HE2	1.83	0.42
1:C:563:THR:HG22	1:C:564:LEU:N	2.35	0.42
1:A:385:GLN:HB3	1:A:387:ILE:HG12	2.02	0.42
1:D:432:ASP:HB3	1:D:435:ASN:ND2	2.34	0.42
1:D:608:SER:O	1:D:608:SER:OG	2.34	0.42
1:A:341:PRO:HA	1:A:657:PHE:HE2	1.83	0.42
1:A:450:SER:O	1:A:454:VAL:HG23	2.19	0.42
1:B:85:ILE:O	1:B:89:LEU:HD23	2.19	0.42
1:C:347:TYR:HB2	1:C:359:ILE:HG21	2.00	0.42
1:D:490:LEU:HA	1:D:490:LEU:HD12	1.81	0.42
1:A:347:TYR:HB2	1:A:359:ILE:HG21	2.00	0.42
1:A:400:THR:HG23	1:A:403:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASP:HB3	1:A:435:ASN:ND2	2.34	0.42
1:B:385:GLN:HB3	1:B:387:ILE:HG12	2.02	0.42
1:B:432:ASP:HB3	1:B:435:ASN:ND2	2.34	0.42
1:B:579:ILE:HD13	1:B:579:ILE:HA	1.88	0.42
1:B:750:ILE:HD13	1:B:750:ILE:HA	1.88	0.42
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.90	0.42
1:D:347:TYR:HB2	1:D:359:ILE:HG21	2.00	0.42
1:C:432:ASP:HB3	1:C:435:ASN:ND2	2.34	0.42
1:D:155:TYR:CE1	1:D:211:LEU:HD21	2.55	0.42
1:B:78:ILE:HA	1:B:86:ILE:HD11	2.02	0.42
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.90	0.42
1:B:400:THR:HG23	1:B:403:GLU:H	1.85	0.42
1:B:563:THR:HG22	1:B:564:LEU:N	2.35	0.42
1:D:563:THR:HG22	1:D:564:LEU:N	2.35	0.42
1:A:370:THR:O	1:A:374:LEU:HD23	2.20	0.42
1:C:155:TYR:CE1	1:C:211:LEU:HD21	2.55	0.42
1:D:400:THR:HG23	1:D:403:GLU:H	1.85	0.42
1:A:78:ILE:HA	1:A:86:ILE:HD11	2.02	0.42
1:B:370:THR:O	1:B:374:LEU:HD23	2.20	0.42
1:B:706:GLN:O	1:B:710:ARG:HG2	2.20	0.42
1:C:750:ILE:HD13	1:C:750:ILE:HA	1.88	0.42
1:A:155:TYR:CE1	1:A:211:LEU:HD21	2.55	0.41
1:A:345:LEU:O	1:A:349:VAL:HG12	2.18	0.41
1:B:155:TYR:CE1	1:B:211:LEU:HD21	2.55	0.41
1:C:608:SER:O	1:C:608:SER:OG	2.34	0.41
1:D:370:THR:O	1:D:374:LEU:HD23	2.20	0.41
1:D:60:LYS:HE3	1:D:60:LYS:HB2	1.73	0.41
1:D:78:ILE:HA	1:D:86:ILE:HD11	2.02	0.41
1:D:706:GLN:O	1:D:710:ARG:HG2	2.20	0.41
1:C:621:ASN:HD21	1:D:621:ASN:HD21	1.66	0.41
1:D:361:LYS:HD3	1:D:361:LYS:HA	1.84	0.41
1:B:329:LYS:HA	1:B:329:LYS:HD2	1.90	0.41
1:C:564:LEU:HD12	1:C:564:LEU:HA	1.88	0.41
1:D:385:GLN:HB3	1:D:387:ILE:HG12	2.02	0.41
1:B:621:ASN:HD21	1:C:621:ASN:HD21	1.66	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.90	0.41
1:B:60:LYS:HB2	1:B:60:LYS:HE3	1.73	0.41
1:A:341:PRO:O	1:A:345:LEU:HG	2.21	0.41
1:C:385:GLN:HB3	1:C:387:ILE:HG12	2.02	0.41
1:C:400:THR:HG23	1:C:403:GLU:H	1.85	0.41
1:C:706:GLN:O	1:C:710:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ILE:O	1:D:89:LEU:HD23	2.19	0.41
1:A:563:THR:HG22	1:A:564:LEU:N	2.35	0.41
1:C:370:THR:O	1:C:374:LEU:HD23	2.20	0.41
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.88	0.41
1:B:66:ILE:HB	1:B:70:GLY:HA2	2.03	0.41
1:B:80:ASN:C	1:B:81:GLU:HG3	2.46	0.41
1:B:396:GLY:H	1:B:474:THR:HG21	1.86	0.41
1:C:396:GLY:H	1:C:474:THR:HG21	1.86	0.41
1:C:654:PRO:HA	1:C:655:PRO:HD3	1.98	0.41
1:D:341:PRO:O	1:D:345:LEU:HG	2.21	0.41
1:D:352:LYS:HE3	1:D:352:LYS:HB2	1.76	0.41
1:A:80:ASN:C	1:A:81:GLU:HG3	2.46	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.96	0.41
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.81	0.41
1:A:706:GLN:O	1:A:710:ARG:HG2	2.20	0.41
1:B:559:ASN:OD1	1:B:562:SER:HB3	2.21	0.41
1:C:559:ASN:OD1	1:C:562:SER:HB3	2.21	0.41
1:A:66:ILE:HB	1:A:70:GLY:HA2	2.03	0.40
1:A:350:ALA:O	1:A:352:LYS:N	2.50	0.40
1:B:360:ARG:HA	1:B:360:ARG:HD2	1.83	0.40
1:D:559:ASN:OD1	1:D:562:SER:HB3	2.21	0.40
1:A:352:LYS:HE3	1:A:352:LYS:HB2	1.76	0.40
1:C:78:ILE:HA	1:C:86:ILE:HD11	2.02	0.40
1:D:350:ALA:O	1:D:352:LYS:N	2.50	0.40
1:D:396:GLY:H	1:D:474:THR:HG21	1.86	0.40
1:A:396:GLY:H	1:A:474:THR:HG21	1.86	0.40
1:B:314:TRP:CD1	1:B:315:TYR:CD1	3.10	0.40
1:D:360:ARG:HD2	1:D:360:ARG:HA	1.83	0.40
1:D:507:ILE:HD13	1:D:507:ILE:HA	1.98	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	633/915 (69%)	582 (92%)	51 (8%)	0	100	100
1	B	633/915 (69%)	582 (92%)	51 (8%)	0	100	100
1	C	633/915 (69%)	582 (92%)	51 (8%)	0	100	100
1	D	633/915 (69%)	582 (92%)	51 (8%)	0	100	100
All	All	2532/3660 (69%)	2328 (92%)	204 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/817 (69%)	563 (100%)	0	100	100
1	B	563/817 (69%)	563 (100%)	0	100	100
1	C	563/817 (69%)	563 (100%)	0	100	100
1	D	563/817 (69%)	563 (100%)	0	100	100
All	All	2252/3268 (69%)	2252 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	192	HIS
1	A	297	GLN
1	A	605	ASN
1	A	621	ASN
1	B	163	GLN
1	B	192	HIS
1	B	297	GLN
1	B	605	ASN
1	B	621	ASN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	192	HIS
1	C	297	GLN
1	C	386	HIS
1	C	605	ASN
1	C	621	ASN
1	D	163	GLN
1	D	192	HIS
1	D	297	GLN
1	D	605	ASN
1	D	621	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SJQ	A	1001	-	25,26,26	3.22	6 (24%)	31,38,38	2.68	10 (32%)
4	44E	C	1003	-	23,23,23	1.23	4 (17%)	26,28,28	1.24	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SJQ	B	1001	-	25,26,26	3.22	6 (24%)	31,38,38	2.68	10 (32%)
2	SJQ	D	1001	-	25,26,26	3.22	6 (24%)	31,38,38	2.68	10 (32%)
4	44E	B	1003	-	23,23,23	1.23	4 (17%)	26,28,28	1.24	2 (7%)
4	44E	D	1003	-	23,23,23	1.23	4 (17%)	26,28,28	1.24	2 (7%)
4	44E	A	1003	-	23,23,23	1.23	4 (17%)	26,28,28	1.24	2 (7%)
2	SJQ	C	1001	-	25,26,26	3.22	6 (24%)	31,38,38	2.68	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SJQ	A	1001	-	-	4/8/33/33	0/2/3/3
4	44E	C	1003	-	-	10/25/25/25	-
2	SJQ	B	1001	-	-	4/8/33/33	0/2/3/3
2	SJQ	D	1001	-	-	4/8/33/33	0/2/3/3
4	44E	B	1003	-	-	10/25/25/25	-
4	44E	D	1003	-	-	10/25/25/25	-
4	44E	A	1003	-	-	10/25/25/25	-
2	SJQ	C	1001	-	-	4/8/33/33	0/2/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SJQ	CAQ-NAR	9.69	1.39	1.30
2	B	1001	SJQ	CAQ-NAR	9.69	1.39	1.30
2	C	1001	SJQ	CAQ-NAR	9.69	1.39	1.30
2	D	1001	SJQ	CAQ-NAR	9.69	1.39	1.30
2	A	1001	SJQ	OAW-CAV	8.66	1.40	1.23
2	B	1001	SJQ	OAW-CAV	8.66	1.40	1.23
2	C	1001	SJQ	OAW-CAV	8.66	1.40	1.23
2	D	1001	SJQ	OAW-CAV	8.66	1.40	1.23
2	A	1001	SJQ	C-NAJ	7.51	1.44	1.34
2	B	1001	SJQ	C-NAJ	7.51	1.44	1.34
2	C	1001	SJQ	C-NAJ	7.51	1.44	1.34
2	D	1001	SJQ	C-NAJ	7.51	1.44	1.34
4	A	1003	44E	O21-C2	-2.90	1.39	1.46
4	B	1003	44E	O21-C2	-2.90	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	44E	O21-C2	-2.90	1.39	1.46
4	D	1003	44E	O21-C2	-2.90	1.39	1.46
2	A	1001	SJQ	NAS-NAR	2.82	1.42	1.36
2	B	1001	SJQ	NAS-NAR	2.82	1.42	1.36
2	C	1001	SJQ	NAS-NAR	2.82	1.42	1.36
2	D	1001	SJQ	NAS-NAR	2.82	1.42	1.36
2	A	1001	SJQ	CAT-CL	2.57	1.78	1.72
2	B	1001	SJQ	CAT-CL	2.57	1.78	1.72
2	C	1001	SJQ	CAT-CL	2.57	1.78	1.72
2	D	1001	SJQ	CAT-CL	2.57	1.78	1.72
4	A	1003	44E	O31-C31	2.33	1.40	1.33
4	B	1003	44E	O31-C31	2.33	1.40	1.33
4	C	1003	44E	O31-C31	2.33	1.40	1.33
4	D	1003	44E	O31-C31	2.33	1.40	1.33
2	A	1001	SJQ	O-C	-2.26	1.18	1.23
2	B	1001	SJQ	O-C	-2.26	1.18	1.23
2	C	1001	SJQ	O-C	-2.26	1.18	1.23
2	D	1001	SJQ	O-C	-2.26	1.18	1.23
4	A	1003	44E	O31-C3	-2.26	1.40	1.45
4	B	1003	44E	O31-C3	-2.26	1.40	1.45
4	C	1003	44E	O31-C3	-2.26	1.40	1.45
4	D	1003	44E	O31-C3	-2.26	1.40	1.45
4	A	1003	44E	O21-C21	2.02	1.40	1.34
4	B	1003	44E	O21-C21	2.02	1.40	1.34
4	C	1003	44E	O21-C21	2.02	1.40	1.34
4	D	1003	44E	O21-C21	2.02	1.40	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	SJQ	CAT-CAV-NAS	7.16	120.09	113.61
2	B	1001	SJQ	CAT-CAV-NAS	7.16	120.09	113.61
2	C	1001	SJQ	CAT-CAV-NAS	7.16	120.09	113.61
2	D	1001	SJQ	CAT-CAV-NAS	7.16	120.09	113.61
2	A	1001	SJQ	CAG-CAF-CAB	5.84	113.99	110.75
2	B	1001	SJQ	CAG-CAF-CAB	5.84	113.99	110.75
2	C	1001	SJQ	CAG-CAF-CAB	5.84	113.99	110.75
2	D	1001	SJQ	CAG-CAF-CAB	5.84	113.99	110.75
2	A	1001	SJQ	OAW-CAV-CAT	-5.81	120.05	125.43
2	B	1001	SJQ	OAW-CAV-CAT	-5.81	120.05	125.43
2	C	1001	SJQ	OAW-CAV-CAT	-5.81	120.05	125.43
2	D	1001	SJQ	OAW-CAV-CAT	-5.81	120.05	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	SJQ	CAD-CAC-CAB	5.17	113.62	110.75
2	B	1001	SJQ	CAD-CAC-CAB	5.17	113.62	110.75
2	C	1001	SJQ	CAD-CAC-CAB	5.17	113.62	110.75
2	D	1001	SJQ	CAD-CAC-CAB	5.17	113.62	110.75
4	A	1003	44E	O21-C21-C22	4.09	120.33	111.48
4	B	1003	44E	O21-C21-C22	4.09	120.33	111.48
4	C	1003	44E	O21-C21-C22	4.09	120.33	111.48
4	D	1003	44E	O21-C21-C22	4.09	120.33	111.48
2	A	1001	SJQ	CAQ-NAR-NAS	3.84	119.92	116.53
2	B	1001	SJQ	CAQ-NAR-NAS	3.84	119.92	116.53
2	C	1001	SJQ	CAQ-NAR-NAS	3.84	119.92	116.53
2	D	1001	SJQ	CAQ-NAR-NAS	3.84	119.92	116.53
2	A	1001	SJQ	O-C-NAJ	-3.84	118.84	122.77
2	B	1001	SJQ	O-C-NAJ	-3.84	118.84	122.77
2	C	1001	SJQ	O-C-NAJ	-3.84	118.84	122.77
2	D	1001	SJQ	O-C-NAJ	-3.84	118.84	122.77
2	A	1001	SJQ	CAV-NAS-NAR	-3.28	119.95	126.84
2	B	1001	SJQ	CAV-NAS-NAR	-3.28	119.95	126.84
2	C	1001	SJQ	CAV-NAS-NAR	-3.28	119.95	126.84
2	D	1001	SJQ	CAV-NAS-NAR	-3.28	119.95	126.84
2	A	1001	SJQ	CAP-CAQ-NAR	-3.19	120.02	124.54
2	B	1001	SJQ	CAP-CAQ-NAR	-3.19	120.02	124.54
2	C	1001	SJQ	CAP-CAQ-NAR	-3.19	120.02	124.54
2	D	1001	SJQ	CAP-CAQ-NAR	-3.19	120.02	124.54
4	A	1003	44E	O31-C31-C32	2.83	120.47	111.83
4	B	1003	44E	O31-C31-C32	2.83	120.47	111.83
4	C	1003	44E	O31-C31-C32	2.83	120.47	111.83
4	D	1003	44E	O31-C31-C32	2.83	120.47	111.83
2	A	1001	SJQ	C-CA-N	-2.20	111.80	115.03
2	B	1001	SJQ	C-CA-N	-2.20	111.80	115.03
2	C	1001	SJQ	C-CA-N	-2.20	111.80	115.03
2	D	1001	SJQ	C-CA-N	-2.20	111.80	115.03
2	A	1001	SJQ	CA-C-NAJ	2.16	121.36	118.20
2	B	1001	SJQ	CA-C-NAJ	2.16	121.36	118.20
2	C	1001	SJQ	CA-C-NAJ	2.16	121.36	118.20
2	D	1001	SJQ	CA-C-NAJ	2.16	121.36	118.20

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	SJQ	CAD-CAH-CAI-NAJ

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Mol	Chain	Res	Type	Atoms
2	A	1001	SJQ	CAG-CAH-CAI-NAJ
2	B	1001	SJQ	CAD-CAH-CAI-NAJ
2	B	1001	SJQ	CAG-CAH-CAI-NAJ
2	C	1001	SJQ	CAD-CAH-CAI-NAJ
2	C	1001	SJQ	CAG-CAH-CAI-NAJ
2	D	1001	SJQ	CAD-CAH-CAI-NAJ
2	D	1001	SJQ	CAG-CAH-CAI-NAJ
4	A	1003	44E	C1-O11-P-O13
4	A	1003	44E	C1-O11-P-O14
4	B	1003	44E	C1-O11-P-O13
4	B	1003	44E	C1-O11-P-O14
4	C	1003	44E	C1-O11-P-O13
4	C	1003	44E	C1-O11-P-O14
4	D	1003	44E	C1-O11-P-O13
4	D	1003	44E	C1-O11-P-O14
4	A	1003	44E	C32-C31-O31-C3
4	B	1003	44E	C32-C31-O31-C3
4	C	1003	44E	C32-C31-O31-C3
4	D	1003	44E	C32-C31-O31-C3
4	A	1003	44E	O32-C31-O31-C3
4	B	1003	44E	O32-C31-O31-C3
4	C	1003	44E	O32-C31-O31-C3
4	D	1003	44E	O32-C31-O31-C3
4	A	1003	44E	C22-C21-O21-C2
4	B	1003	44E	C22-C21-O21-C2
4	C	1003	44E	C22-C21-O21-C2
4	D	1003	44E	C22-C21-O21-C2
4	A	1003	44E	O22-C21-O21-C2
4	B	1003	44E	O22-C21-O21-C2
4	C	1003	44E	O22-C21-O21-C2
4	D	1003	44E	O22-C21-O21-C2
4	A	1003	44E	C21-C22-C23-C4
4	B	1003	44E	C21-C22-C23-C4
4	C	1003	44E	C21-C22-C23-C4
4	D	1003	44E	C21-C22-C23-C4
4	A	1003	44E	C32-C33-C34-C35
4	B	1003	44E	C32-C33-C34-C35
4	C	1003	44E	C32-C33-C34-C35
4	D	1003	44E	C32-C33-C34-C35
4	A	1003	44E	C1-O11-P-O12
4	B	1003	44E	C1-O11-P-O12
4	C	1003	44E	C1-O11-P-O12

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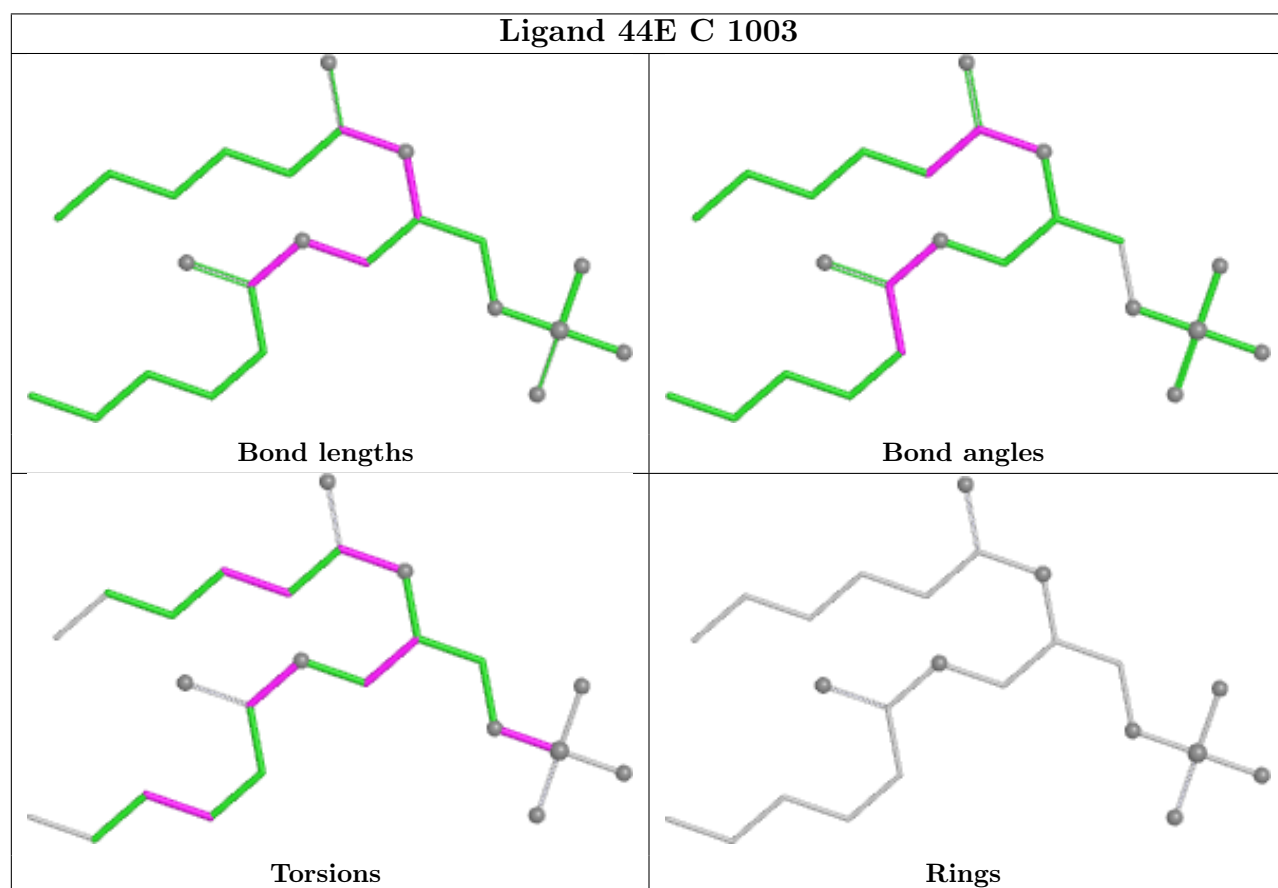
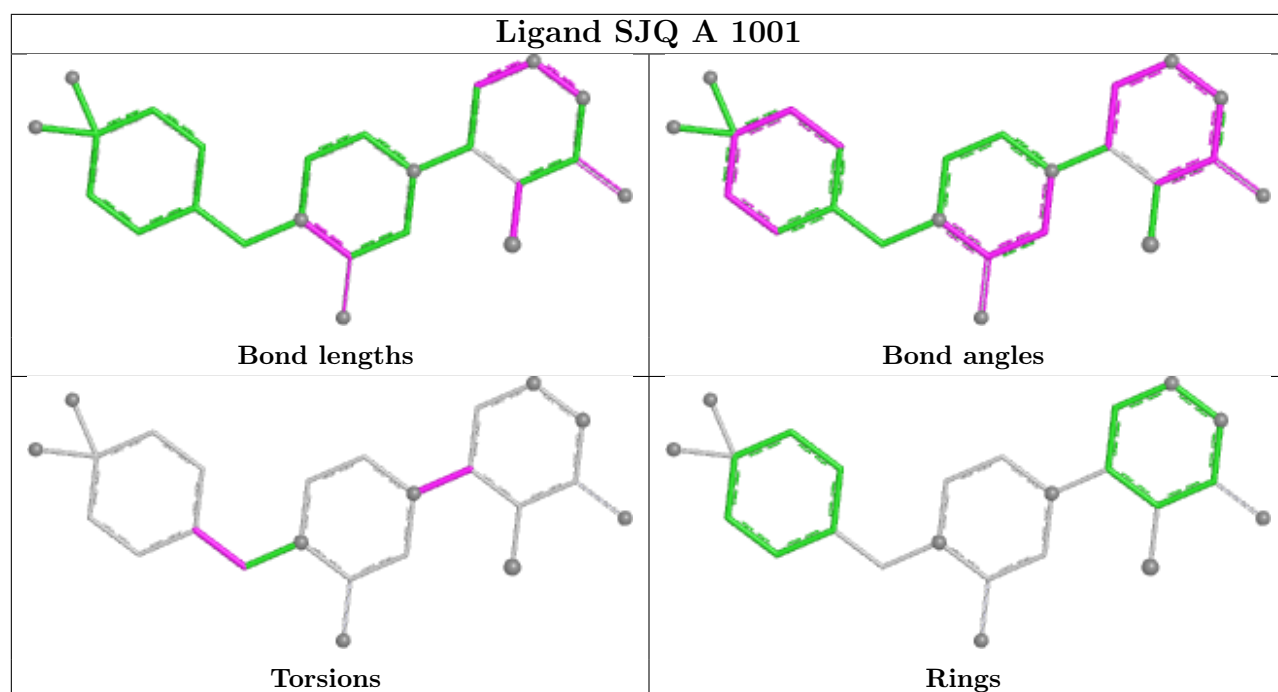
Mol	Chain	Res	Type	Atoms
4	D	1003	44E	C1-O11-P-O12
2	A	1001	SJQ	CAT-CAP-N-CAL
2	B	1001	SJQ	CAT-CAP-N-CAL
2	C	1001	SJQ	CAT-CAP-N-CAL
2	D	1001	SJQ	CAT-CAP-N-CAL
4	A	1003	44E	C1-C2-C3-O31
4	B	1003	44E	C1-C2-C3-O31
4	C	1003	44E	C1-C2-C3-O31
4	D	1003	44E	C1-C2-C3-O31
2	A	1001	SJQ	CAT-CAP-N-CA
2	B	1001	SJQ	CAT-CAP-N-CA
2	C	1001	SJQ	CAT-CAP-N-CA
2	D	1001	SJQ	CAT-CAP-N-CA

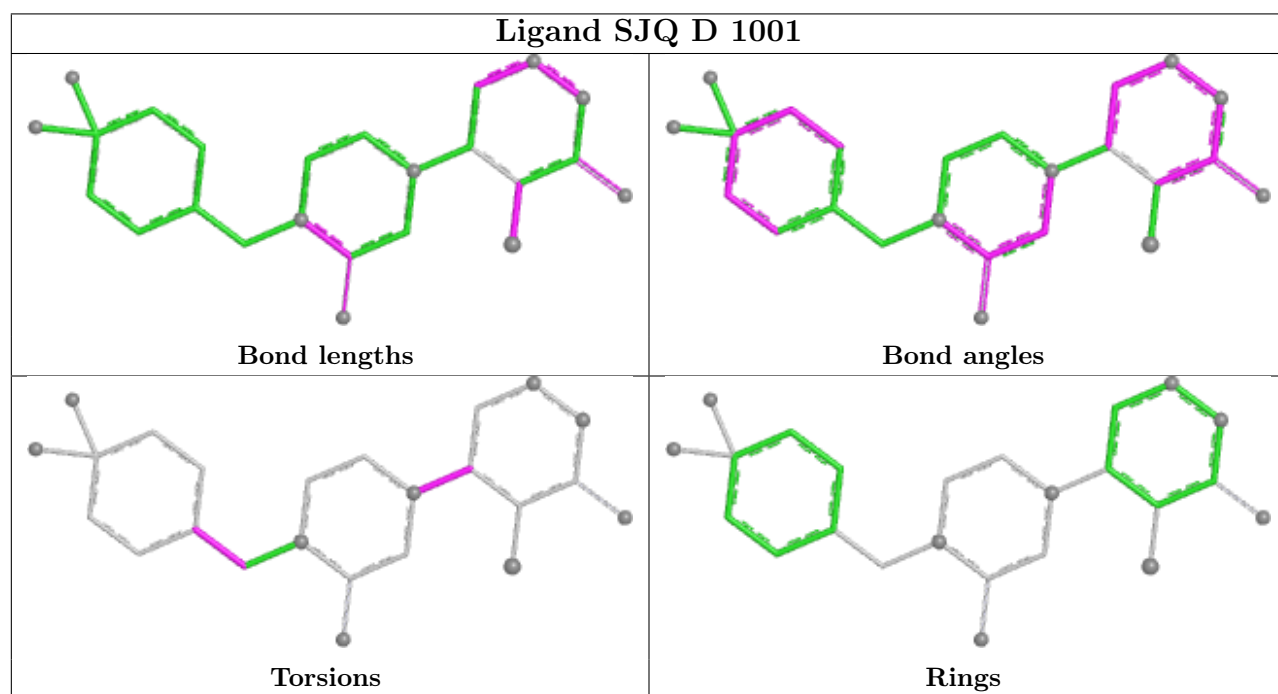
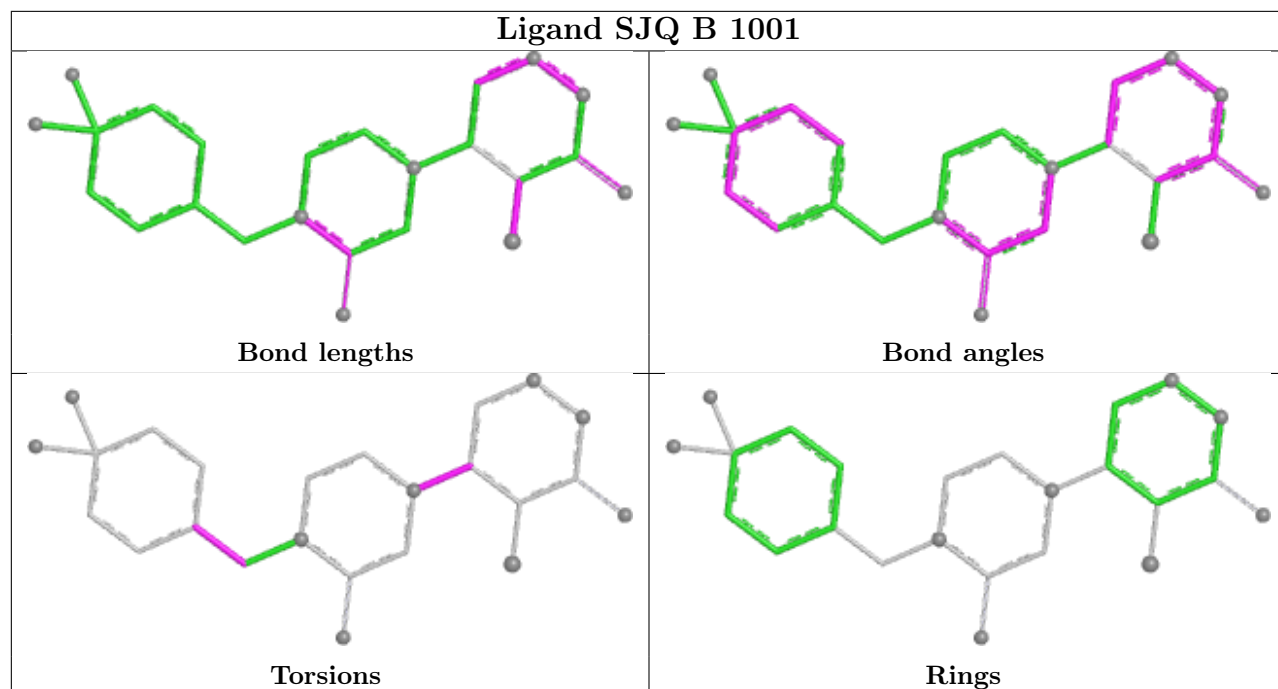
There are no ring outliers.

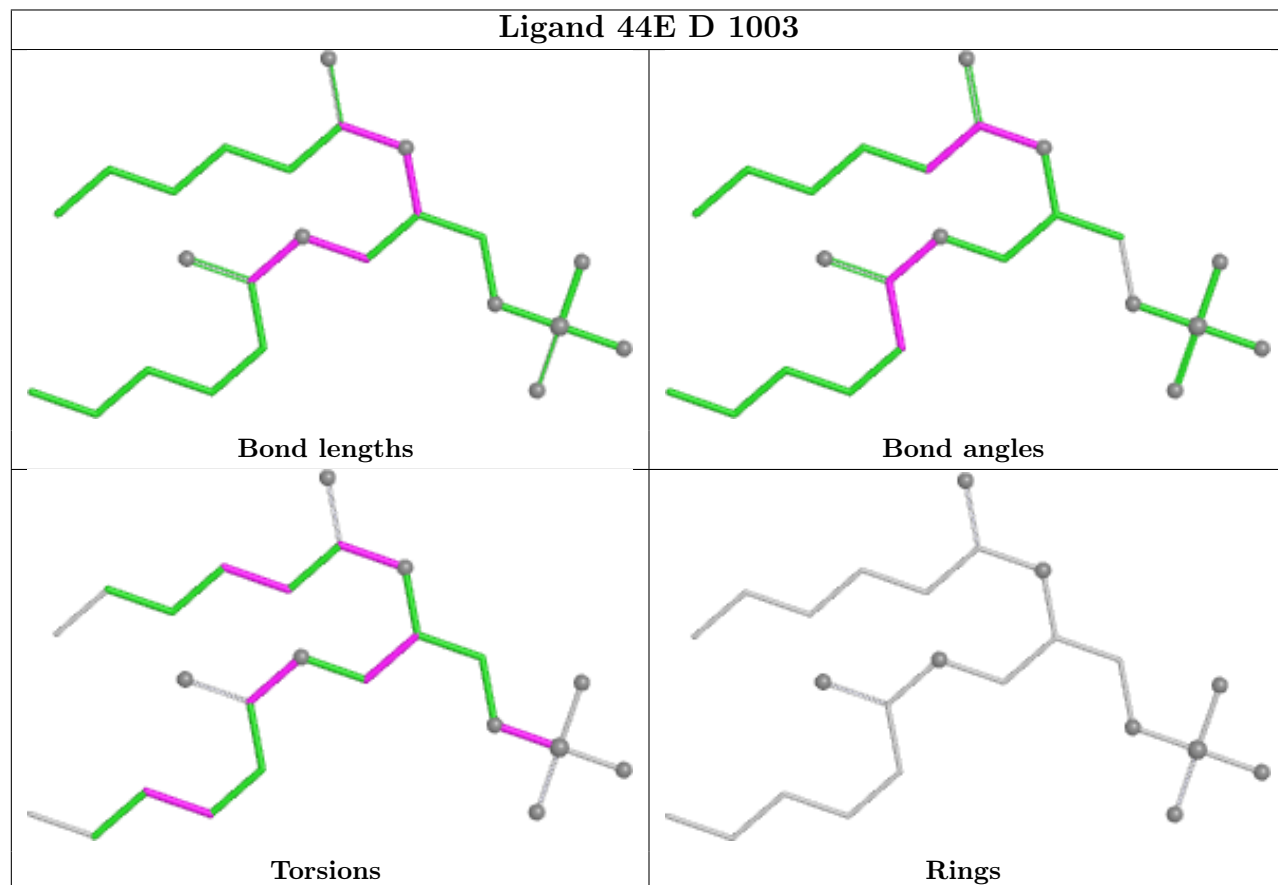
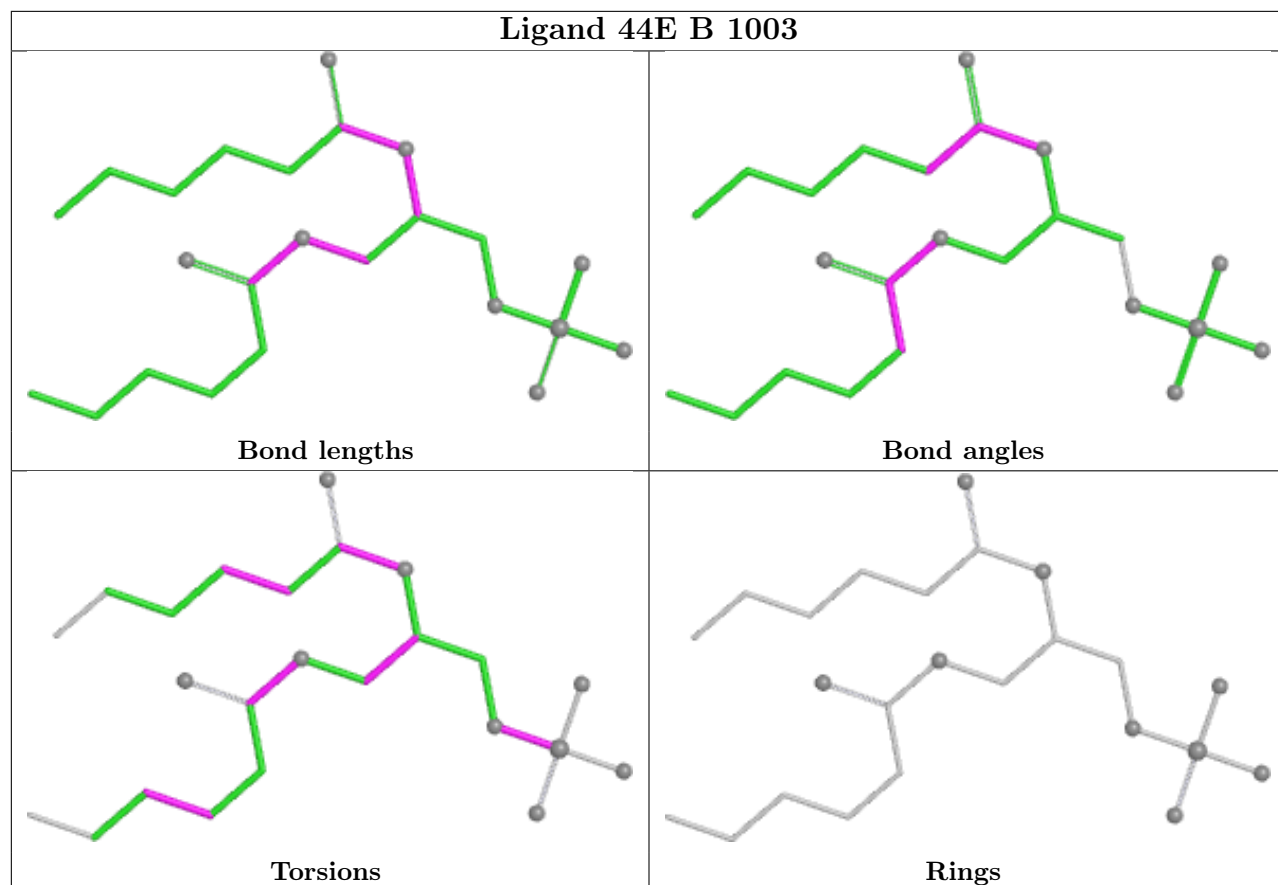
4 monomers are involved in 4 short contacts:

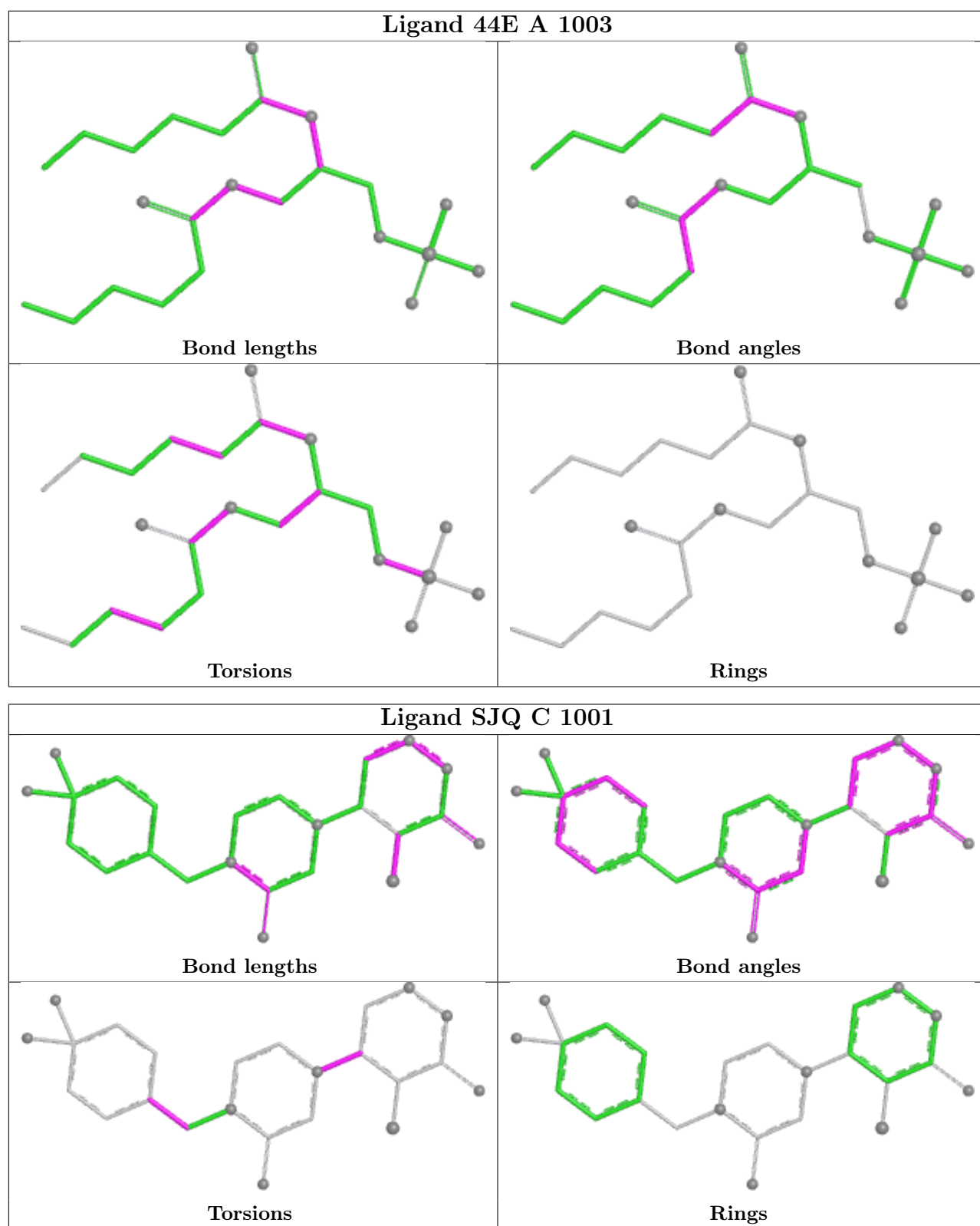
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SJQ	1	0
2	B	1001	SJQ	1	0
2	D	1001	SJQ	1	0
2	C	1001	SJQ	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

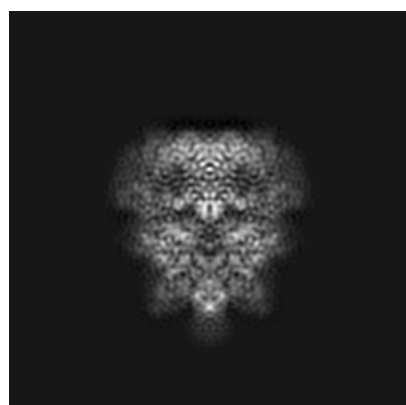
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11957. These allow visual inspection of the internal detail of the map and identification of artifacts.

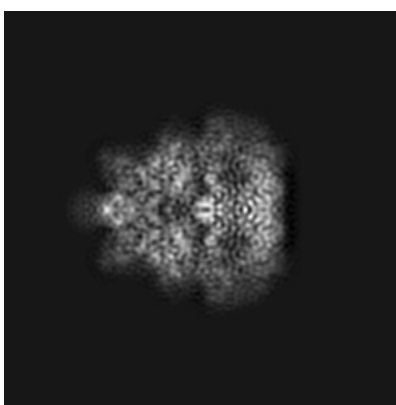
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

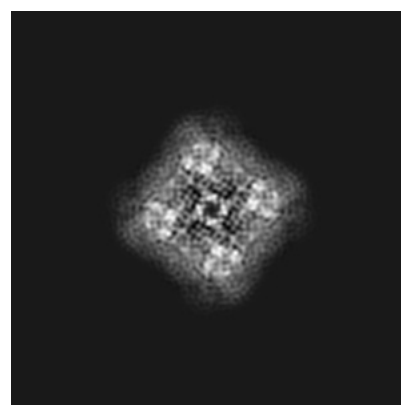
6.1.1 Primary map



X



Y

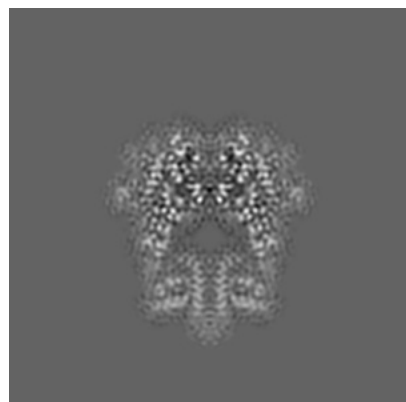


Z

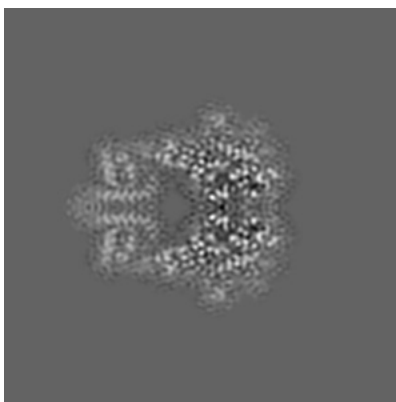
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144



Y Index: 144

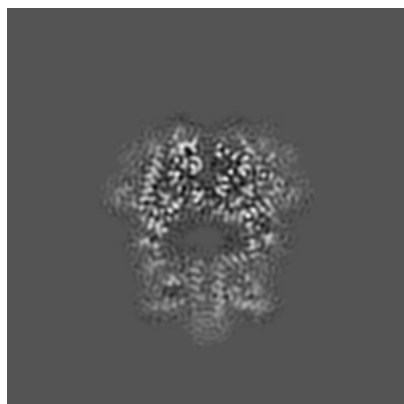


Z Index: 144

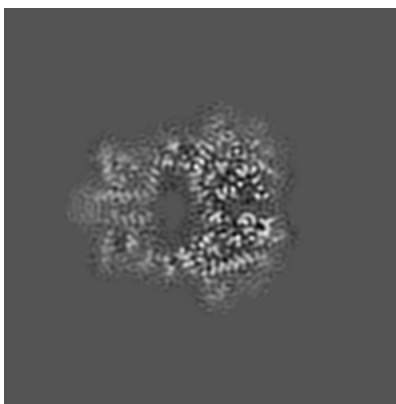
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

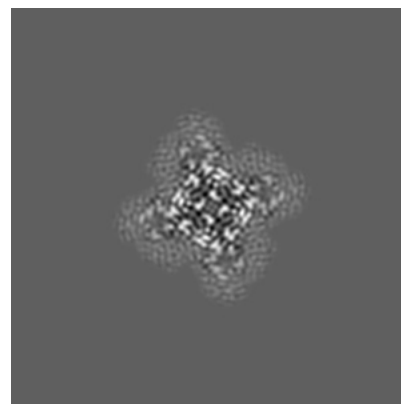
6.3.1 Primary map



X Index: 142



Y Index: 146

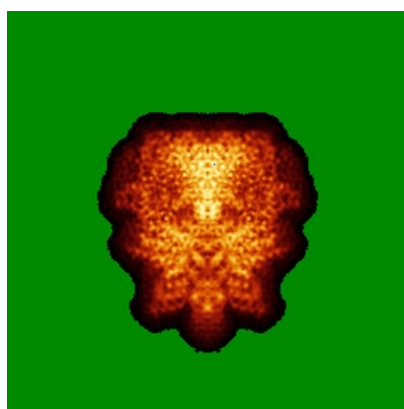


Z Index: 179

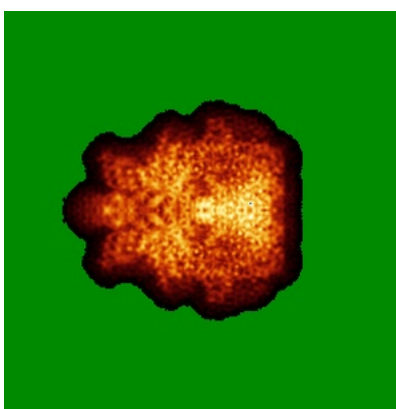
The images above show the largest variance slices of the map in three orthogonal directions.

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

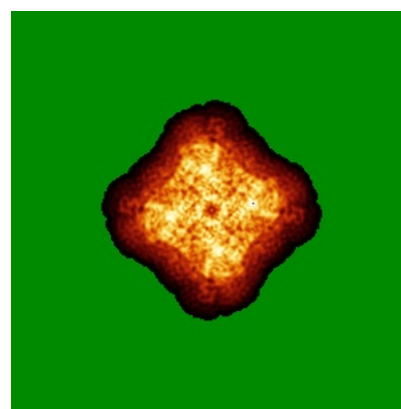
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0093. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

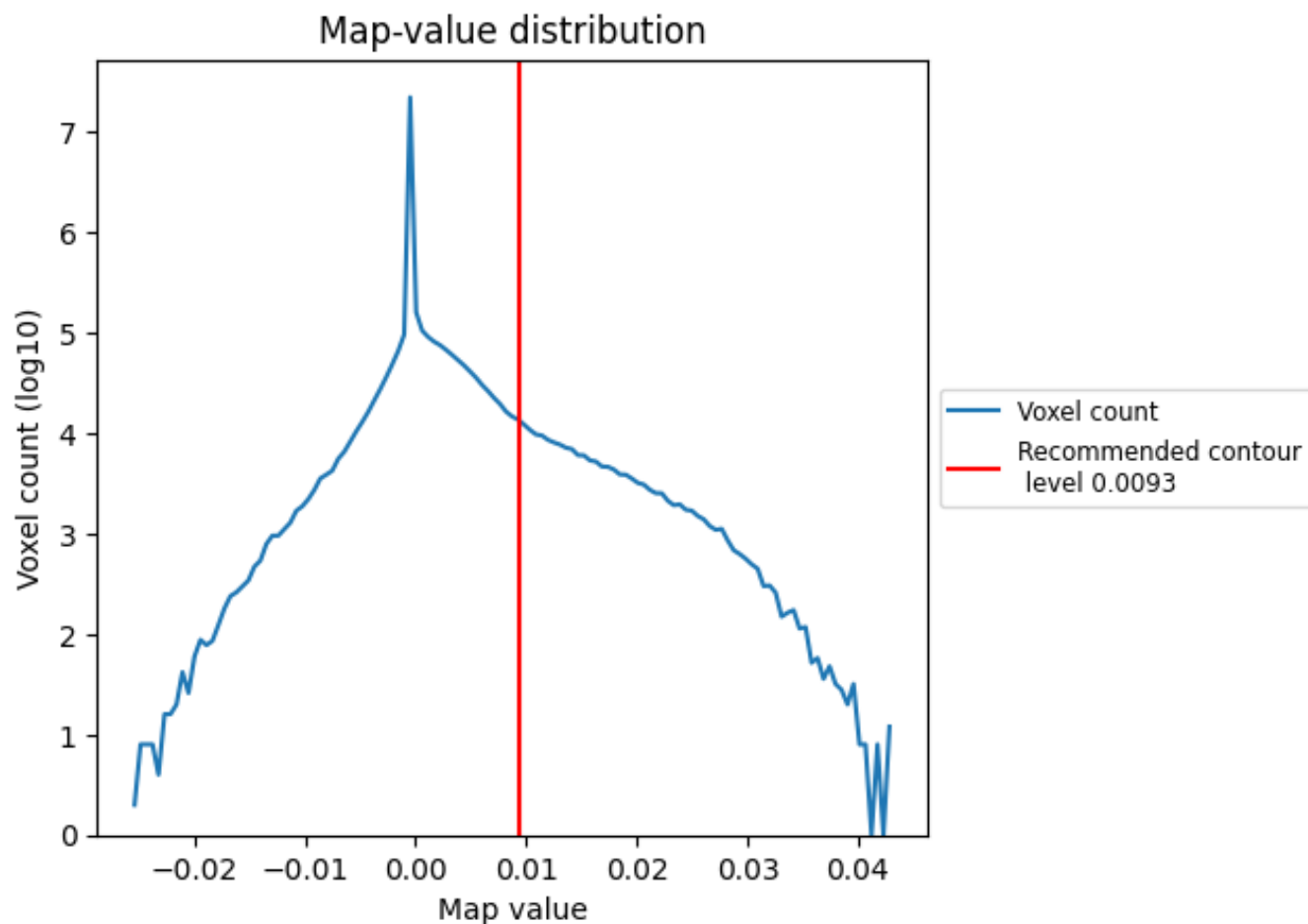
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

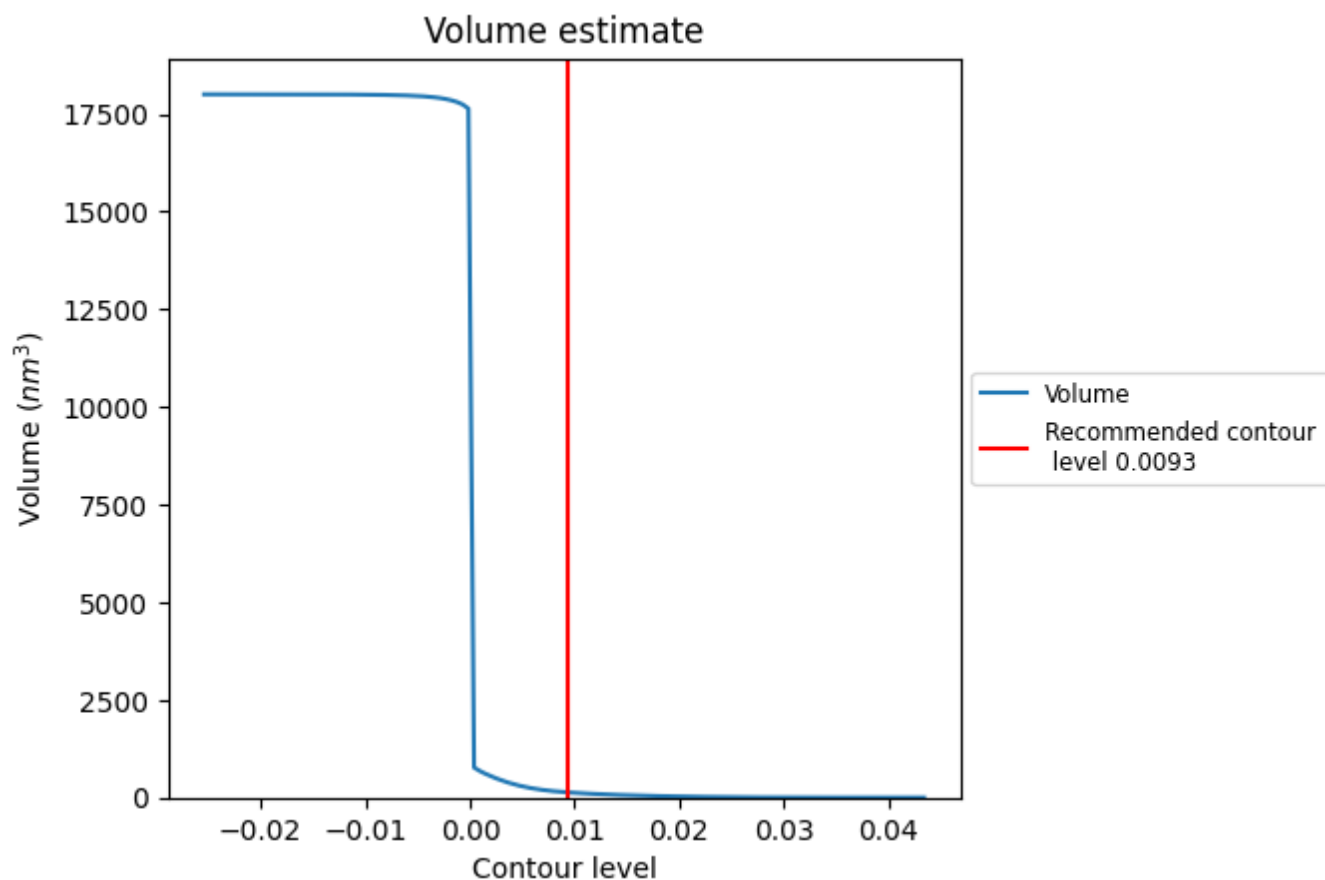
This section contains the results of statistical analysis of the map.

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.

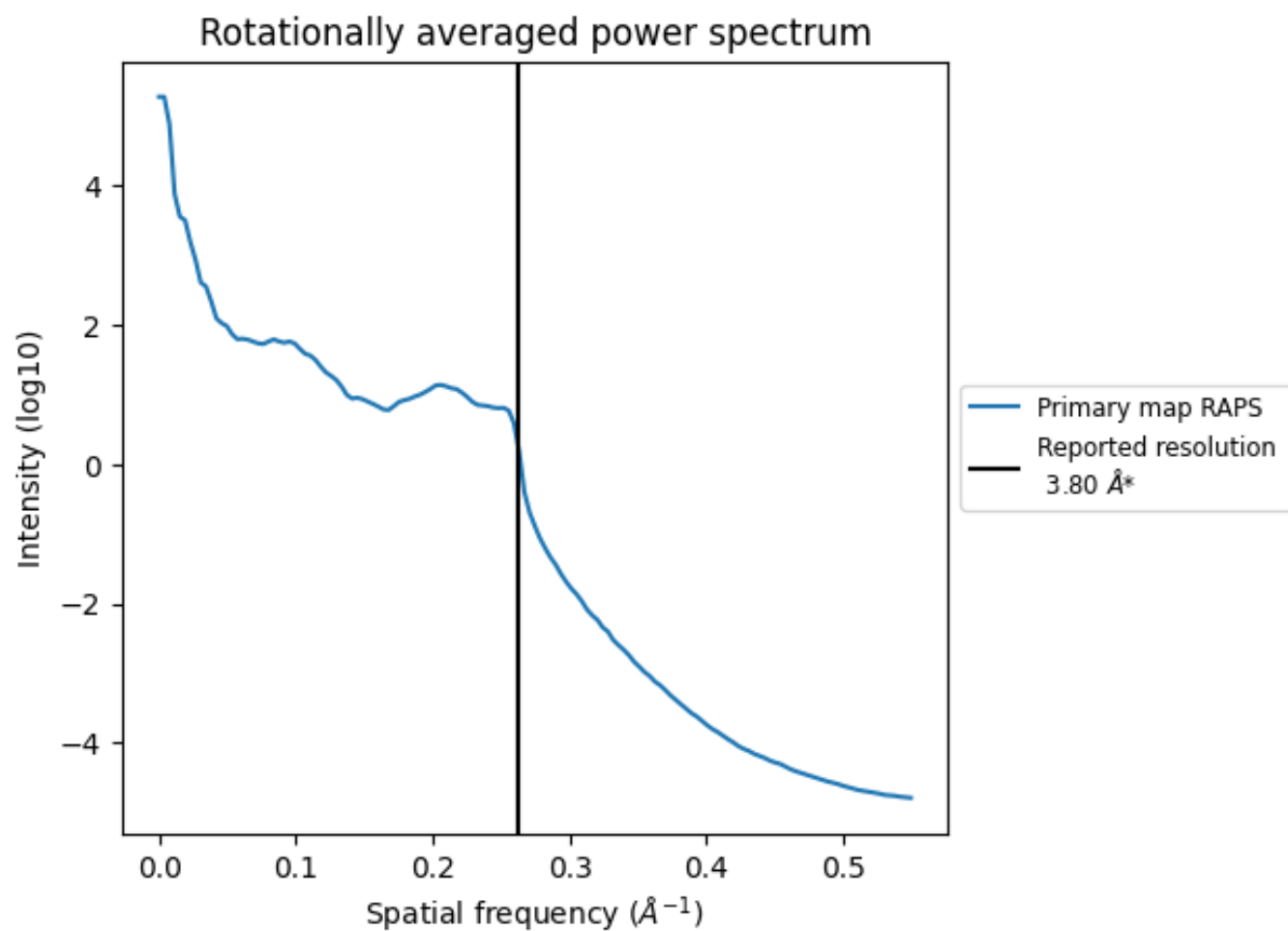
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

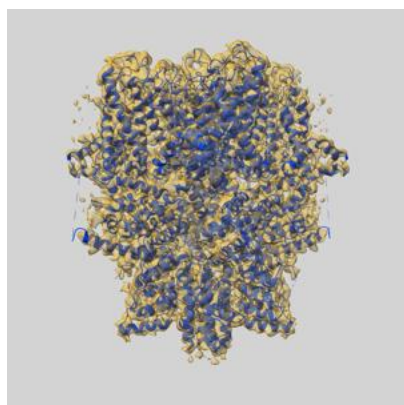
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

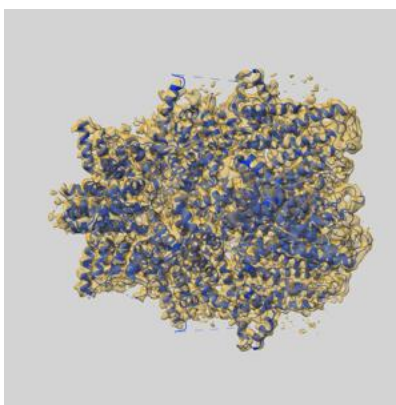
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11957 and PDB model 7B05. Per-residue inclusion information can be found in section [3](#) on page [6](#).

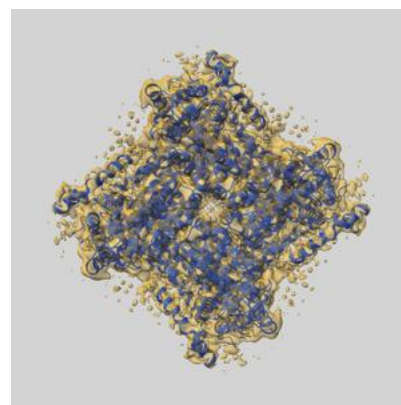
9.1 Map-model overlay [i](#)



X



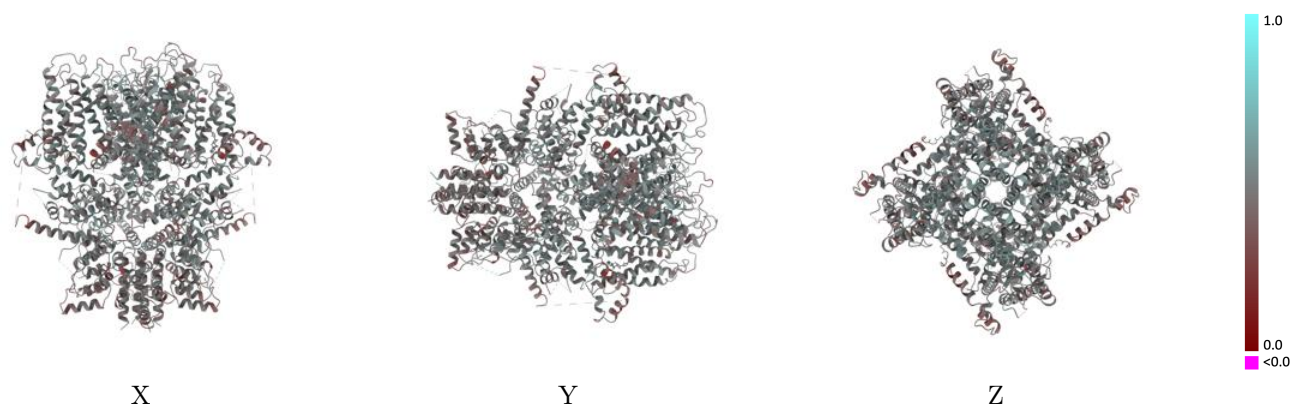
Y



Z

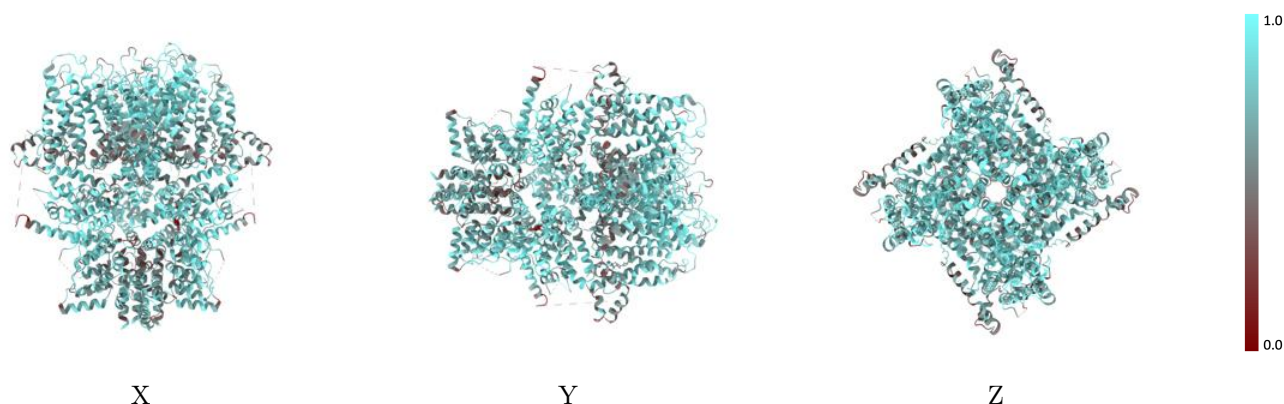
The images above show the 3D surface view of the map at the recommended contour level 0.0093 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



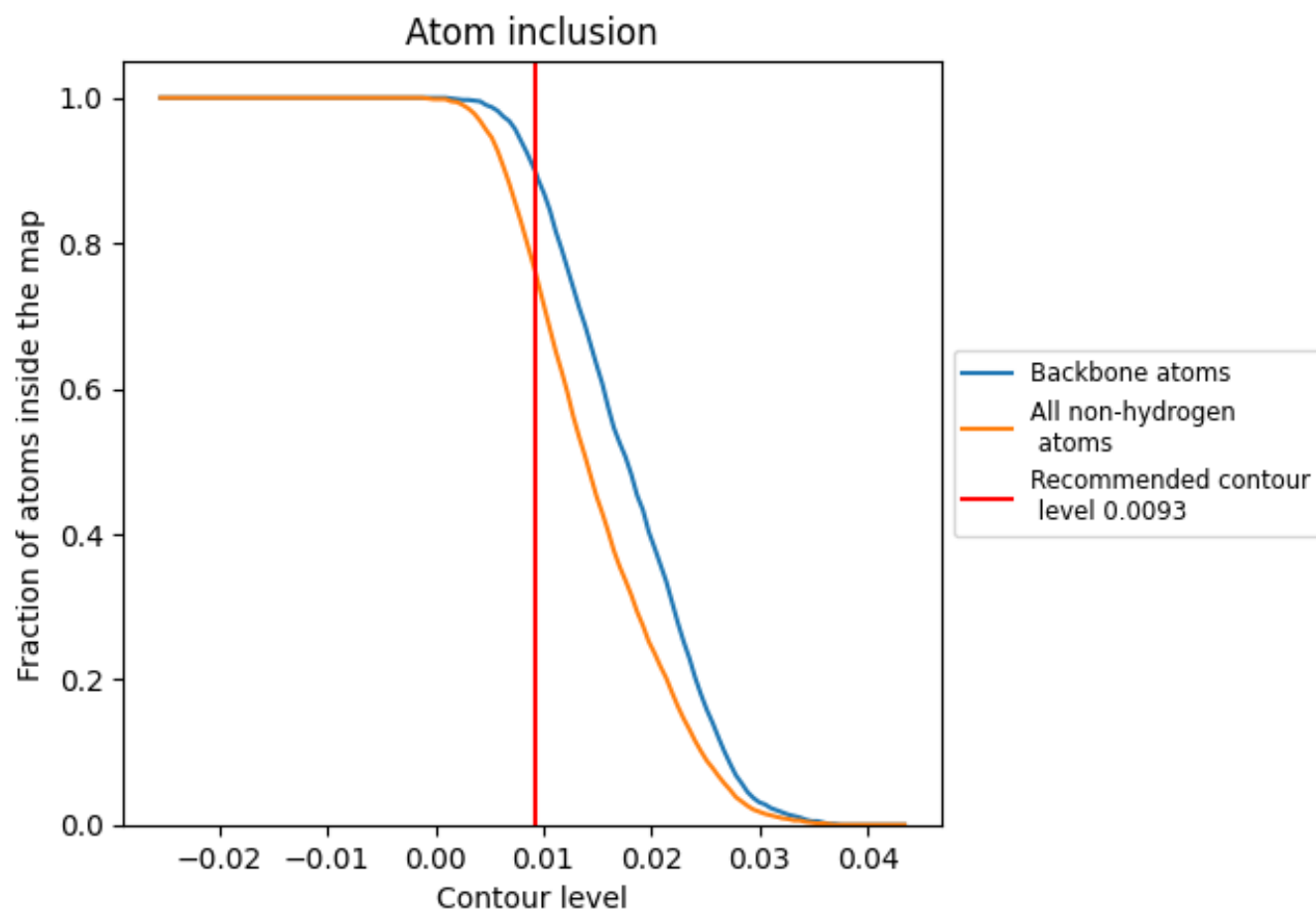
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0093).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.0093) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.4760
A	0.7580	0.4770
B	0.7580	0.4760
C	0.7580	0.4770
D	0.7580	0.4760

