Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 07:36 AM EDT

PDB ID	:	5WEL
EMDB ID	:	EMD-8820
Title	:	GluA2 bound to antagonist ZK and GSG1L in digitonin, state 2
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	2017-07-10
Resolution	:	4.40 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 (i) 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 (1)) were used in the production of this report:

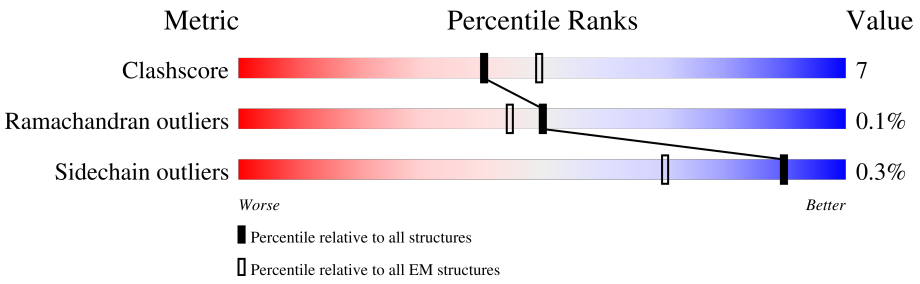
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1057	22% 76% 15% 9%
1	B	1057	10% 61% 12% 26%
1	C	1057	18% 75% 16% 9%
1	D	1057	12% 61% 12% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AJP	A	1302	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AJP	C	1302	X	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27638 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 Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	962	7555	4864	1248	1401	42	0	0
1	B	780	6125	3932	1011	1152	30	0	0
1	C	962	7555	4864	1248	1401	42	0	0
1	D	780	6125	3932	1011	1152	30	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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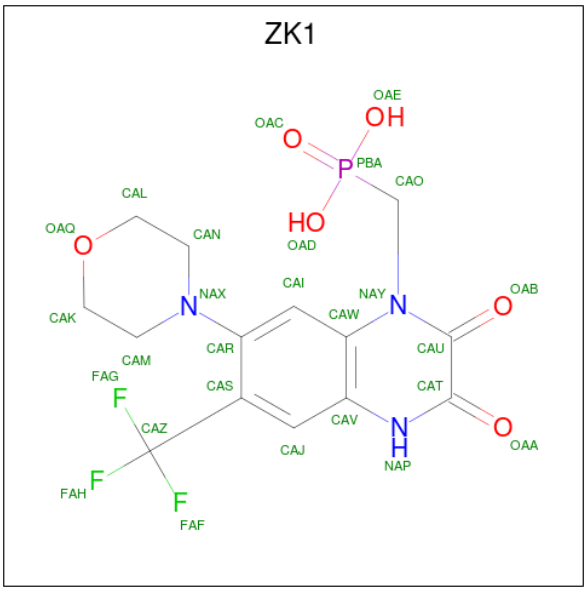
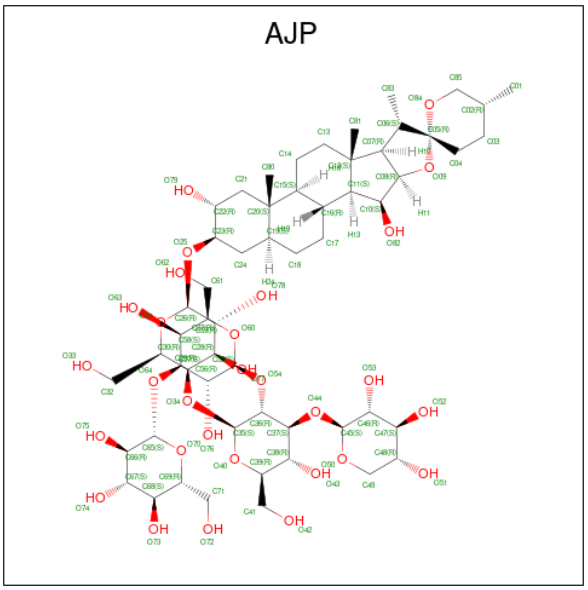
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	1151	LEU	VAL	engineered mutation	UNP D3Z7H4

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	P	
2	A	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
2	B	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
2	C	1	27	14	3	3	6	1	0
			Total	C	F	N	O	P	
2	D	1	27	14	3	3	6	1	0

- Molecule 3 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



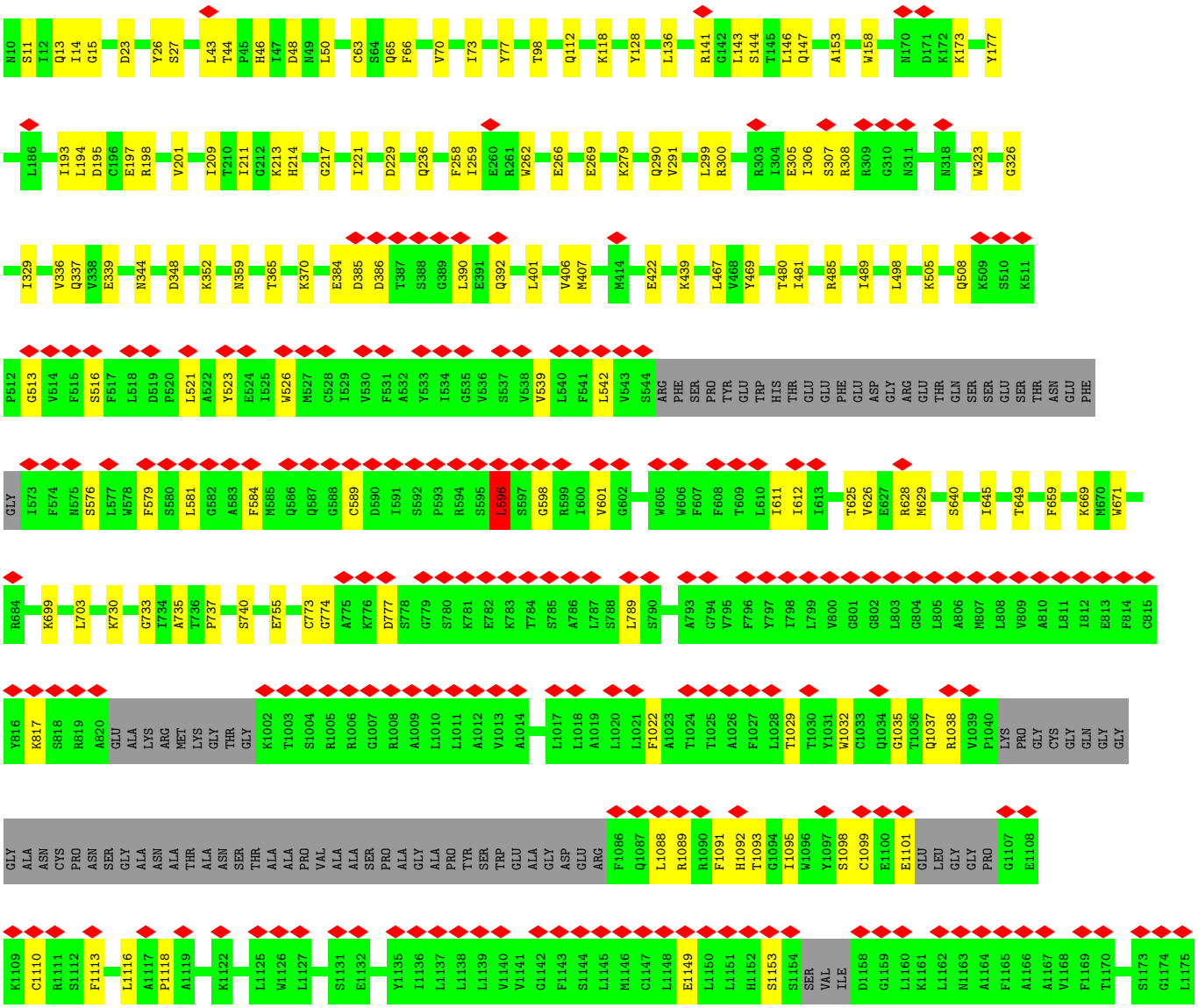
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	85	56	29	0
			Total	C	O	
3	C	1	85	56	29	0

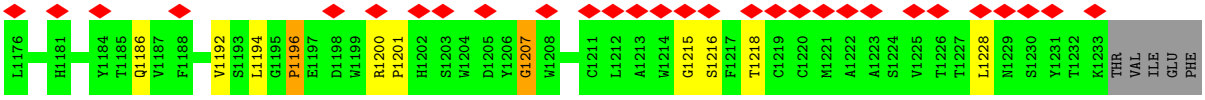
3 Residue-property plots (i)

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: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein

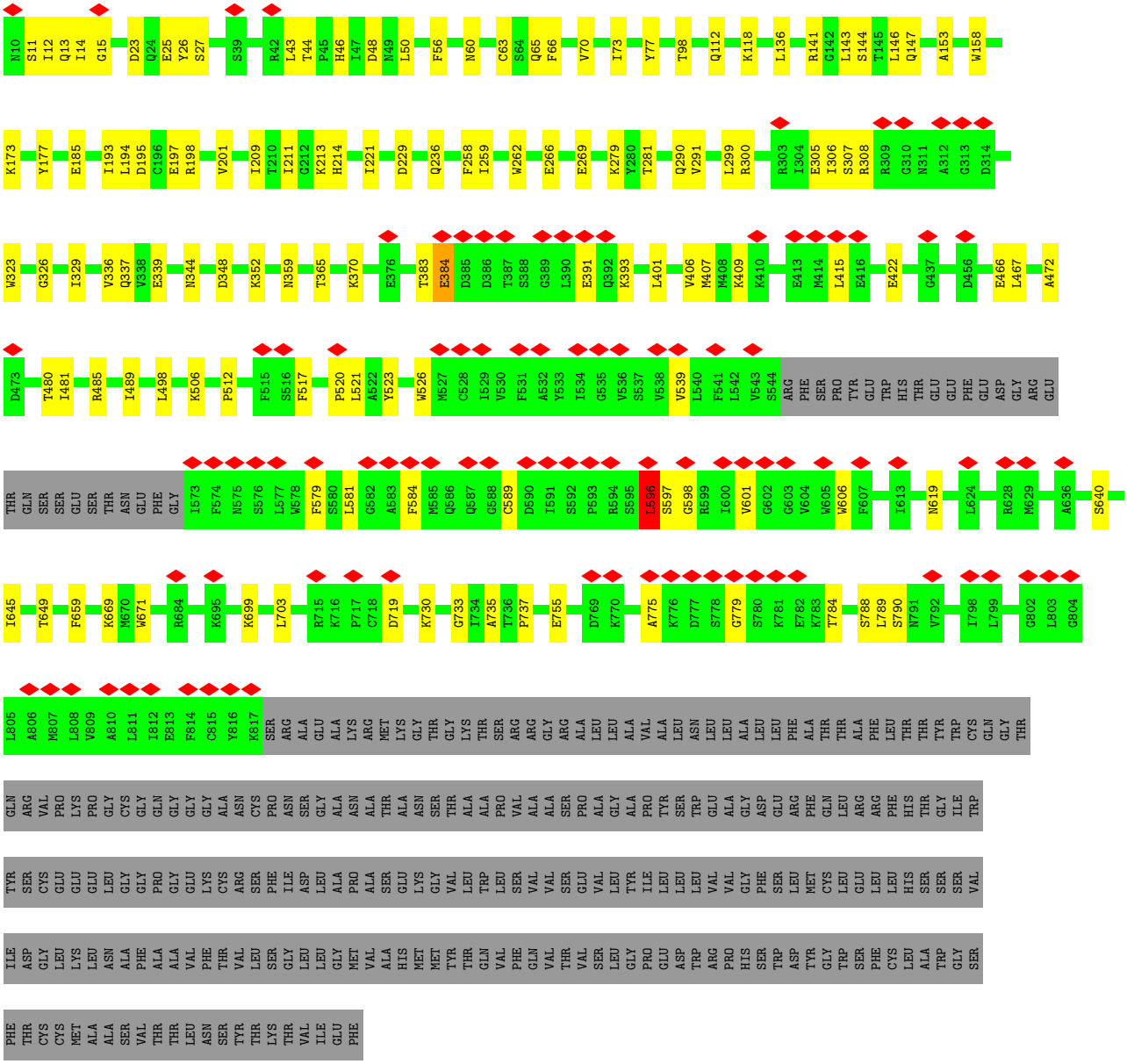
Chain A:





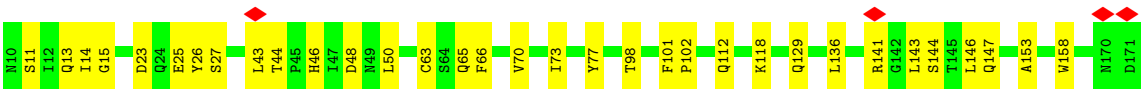
• Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein

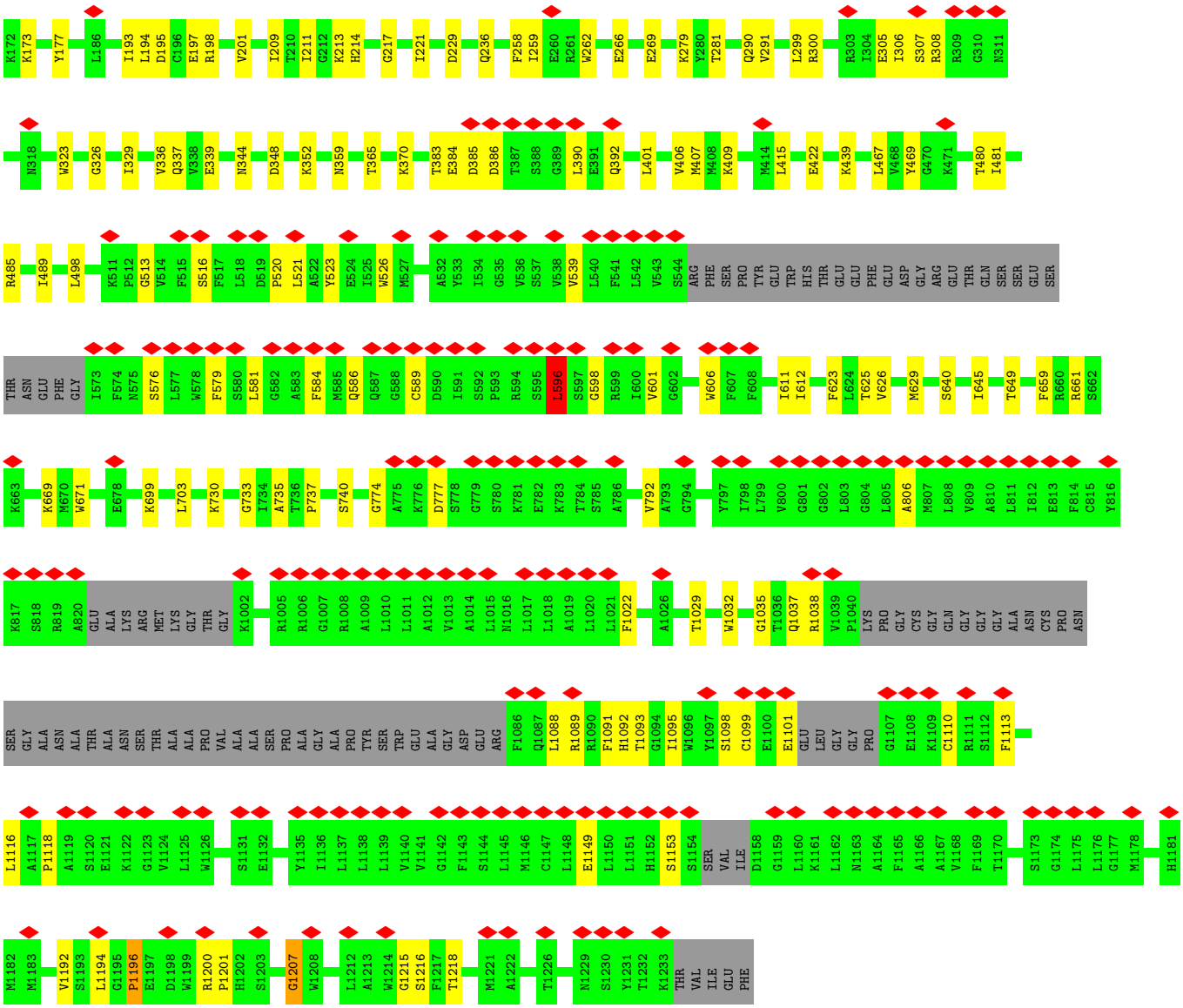
Chain B:



• Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein

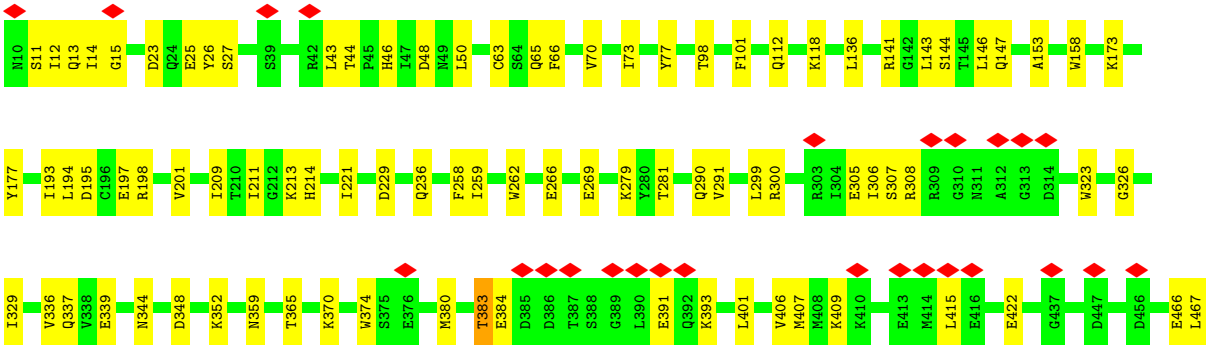
Chain C:

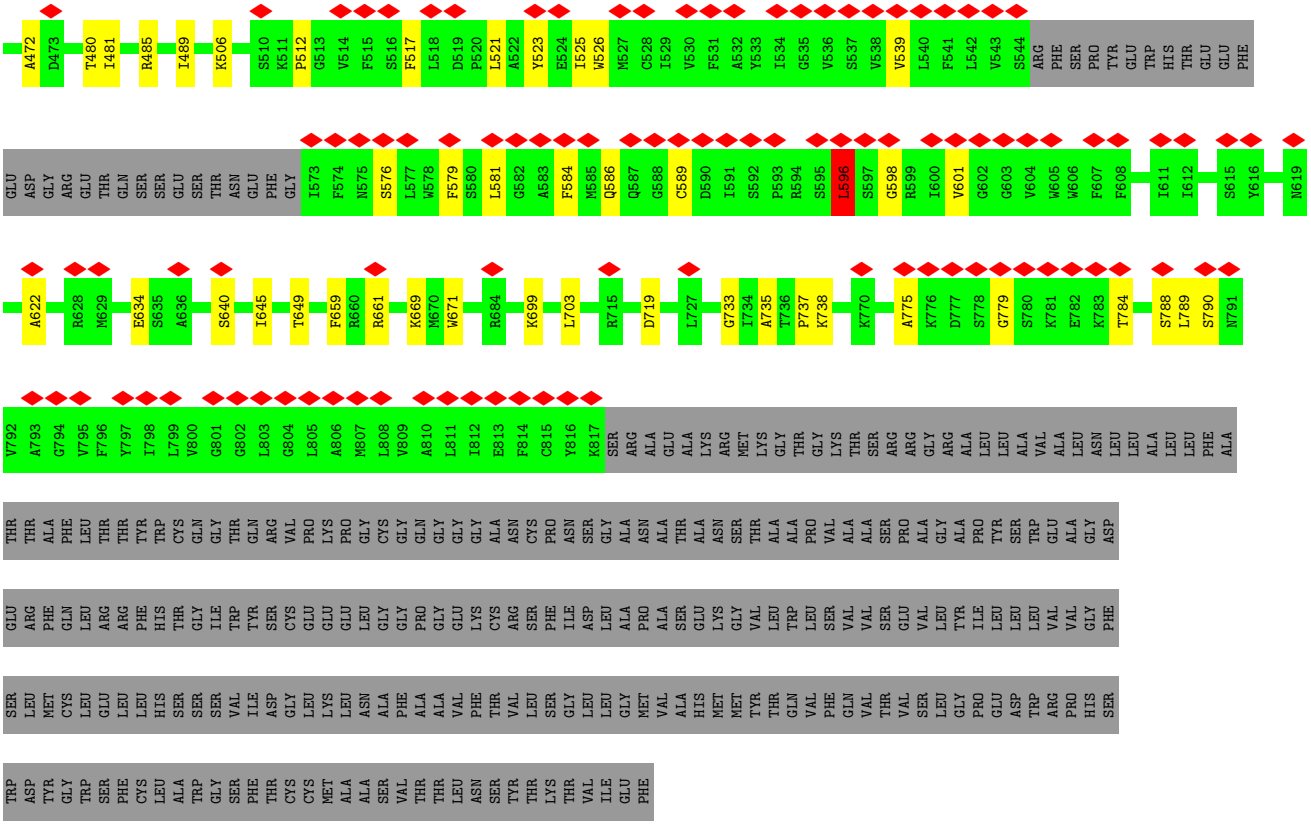




• Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein

Chain D:




A472 D473 T480 I481 R485 I489 K506 S510 K511 P512 G513 V514 F515 S516 F517 L518 D519 P520 L521 A522 Y523 E524 I525 W526 M527 C528 I529 V530 F531 A532 Y533 I534 G535 V536 S537 V538 V539 L540 F541 L542 V543 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU PHE
GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR ASN GLU PHE GLY I573 F574 N575 S576 L577 W578 F579 S580 L581 G582 A583 F584 M585 Q586 Q587 G588 C589 D590 I591 S592 P593 R594 S595 L596 S597 G598 R599 I600 V601 G602 G603 V604 W605 W606 F607 F608 I611 I612 S615 Y616 N619
A622 R628 M629 E634 S635 A636 S640 I645 T649 F659 R660 R661 K669 M670 W671 R684 K699 L703 R715 D719 L727 G733 T734 A735 T736 P737 K738 K770 A775 K776 D777 S778 G779 S780 K781 E782 K783 T784 S788 L789 S790 N791
V792 A793 G794 V795 F796 V797 I798 L799 V800 G801 G802 L803 G804 L805 A806 M807 L808 V809 A810 L811 I812 E813 F814 C815 Y816 K817 SER ARG ALA GLU ALA LYS ARG MET LYS GLY THR GLY LYS THR SER ARG ARG GLY ARG ALA LEU LEU ALA VAL ALA LEU ASN LEU LEU ALA LEU LEU PHE ALA
THR THR ALA PHE LEU THR THR TYR TRP CYS GLN GLY THR GLN ARG VAL PRO LYS PRO GLY CYS GLY GLN GLY GLY GLY ALA ASN CYS PRO ASN SER GLY ALA ASN ALA THR ALA ASN SER THR ALA ALA PRO VAL ALA ALA SER PRO ALA GLY ALA PRO TYR SER TRP GLU ALA GLY ASP
GLU ARG PHE GLN LEU ARG ARG PHE HIS THR GLY ILE TRP TYR SER CYS GLU GLU GLU LEU GLY GLY PRO GLY GLU LYS CYS ARG SER PHE ILE ASP LEU ALA PRO ALA SER GLU LYS GLY VAL LEU TRP LEU SER VAL VAL SER GLU VAL LEU TYR ILE LEU LEU LEU VAL VAL GLY PHE
SER LEU MET CYS LEU GLU LEU LEU HIS SER SER SER VAL ILE ASP GLY LEU LYS LEU ASN ALA PHE ALA ALA VAL PHE THR VAL LEU SER GLY LEU LEU GLY MET VAL ALA HIS MET MET TYR THR GLN VAL PHE GLN VAL THR VAL SER LEU GLY PRO GLU ASP TRP ARG PRO HIS SER
TRP ASP TYR GLY TRP SER PHE CYS LEU ALA TRP GLY SER PHE THR CYS CYS MET ALA ALA SER VAL THR THR LEU ASN SER TYR THR LYS THR VAL ILE GLU PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	41926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	294.0, 294.0, 294.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	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: AJP, ZK1

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	0.29	0/7718	0.51	5/10438 (0.0%)
1	B	0.29	0/6253	0.51	1/8450 (0.0%)
1	C	0.29	0/7718	0.51	4/10438 (0.0%)
1	D	0.29	0/6253	0.51	2/8450 (0.0%)
All	All	0.29	0/27942	0.51	12/37776 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	1
1	C	0	5
1	D	0	2
All	All	0	13

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	LEU	CA-CB-CG	7.89	133.44	115.30
1	C	596	LEU	CA-CB-CG	7.88	133.43	115.30
1	D	596	LEU	CA-CB-CG	7.87	133.39	115.30
1	B	596	LEU	CA-CB-CG	7.86	133.38	115.30
1	C	612	ILE	O-C-N	-6.41	112.44	122.70
1	A	390	LEU	CA-CB-CG	5.98	129.06	115.30
1	C	390	LEU	CA-CB-CG	5.98	129.06	115.30
1	C	1116	LEU	CA-CB-CG	5.96	129.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1116	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	612	ILE	O-C-N	5.56	131.60	122.70
1	A	612	ILE	CA-C-N	-5.33	105.49	117.20
1	D	634	GLU	O-C-N	5.05	130.79	122.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1196	PRO	Peptide
1	A	1207	GLY	Peptide
1	A	384	GLU	Peptide
1	A	773	CYS	Mainchain
1	A	817	LYS	Peptide
1	B	784	THR	Peptide
1	C	1196	PRO	Peptide
1	C	1207	GLY	Peptide
1	C	383	THR	Mainchain
1	C	384	GLU	Peptide
1	C	792	VAL	Mainchain
1	D	383	THR	Mainchain
1	D	784	THR	Peptide

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	7555	0	7536	105	0
1	B	6125	0	6110	77	0
1	C	7555	0	7536	109	0
1	D	6125	0	6110	76	0
2	A	27	0	13	1	0
2	B	27	0	13	2	0
2	C	27	0	13	1	0
2	D	27	0	13	1	0
3	A	85	0	0	23	0
3	C	85	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27638	0	27344	373	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 7.

All (373) 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:740:SER:HA	3:C:1302:AJP:O42	1.26	1.29
1:C:469:TYR:HB3	3:C:1302:AJP:C81	1.65	1.26
1:C:740:SER:CA	3:C:1302:AJP:O42	1.94	1.15
1:A:740:SER:HA	3:A:1302:AJP:O42	1.45	1.15
1:A:469:TYR:HB3	3:A:1302:AJP:C81	1.81	1.11
1:C:217:GLY:H	3:C:1302:AJP:C01	1.76	0.98
1:A:740:SER:CA	3:A:1302:AJP:O42	2.13	0.97
1:C:469:TYR:CB	3:C:1302:AJP:C81	2.45	0.94
1:C:217:GLY:N	3:C:1302:AJP:C01	2.32	0.93
1:C:740:SER:CB	3:C:1302:AJP:O42	2.23	0.87
1:A:128:TYR:HA	3:A:1302:AJP:C17	2.10	0.81
1:A:469:TYR:CB	3:A:1302:AJP:C81	2.63	0.77
1:B:606:TRP:HZ2	1:C:586:GLN:H	1.34	0.74
1:C:217:GLY:CA	3:C:1302:AJP:C01	2.66	0.74
1:C:469:TYR:C	3:C:1302:AJP:C80	2.56	0.73
1:C:129:GLN:NE2	3:C:1302:AJP:O78	2.23	0.71
1:A:469:TYR:C	3:A:1302:AJP:C80	2.59	0.70
1:A:596:LEU:HD22	1:A:598:GLY:H	1.57	0.70
1:B:596:LEU:HD22	1:B:598:GLY:H	1.57	0.69
1:C:596:LEU:HD22	1:C:598:GLY:H	1.57	0.69
1:D:596:LEU:HD22	1:D:598:GLY:H	1.57	0.69
1:D:337:GLN:HE21	1:D:344:ASN:HD21	1.42	0.67
1:B:337:GLN:HE21	1:B:344:ASN:HD21	1.42	0.67
1:C:217:GLY:HA2	3:C:1302:AJP:C01	2.25	0.67
1:A:337:GLN:HE21	1:A:344:ASN:HD21	1.42	0.65
1:C:337:GLN:HE21	1:C:344:ASN:HD21	1.42	0.65
1:C:1037:GLN:HE21	1:C:1200:ARG:HG2	1.63	0.64
1:A:217:GLY:H	3:A:1302:AJP:C01	2.11	0.62
1:A:740:SER:CB	3:A:1302:AJP:O42	2.46	0.62
1:A:1037:GLN:HE21	1:A:1200:ARG:HG2	1.63	0.62
1:C:740:SER:HB2	3:C:1302:AJP:O42	2.02	0.59
1:D:236:GLN:NE2	1:D:365:THR:O	2.36	0.59
1:C:236:GLN:NE2	1:C:365:THR:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1302:AJP:O33	3:A:1302:AJP:O76	2.21	0.59
3:C:1302:AJP:O33	3:C:1302:AJP:O76	2.21	0.59
1:B:236:GLN:NE2	1:B:365:THR:O	2.36	0.59
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.68	0.58
1:A:236:GLN:NE2	1:A:365:THR:O	2.36	0.58
1:A:469:TYR:HA	3:A:1302:AJP:C80	2.33	0.58
1:C:1032:TRP:N	1:C:1093:THR:O	2.35	0.58
1:D:581:LEU:HA	1:D:584:PHE:HB2	1.86	0.58
1:A:1035:GLY:HA2	1:A:1201:PRO:HB3	1.86	0.57
1:B:581:LEU:HA	1:B:584:PHE:HB2	1.86	0.57
1:C:581:LEU:HA	1:C:584:PHE:HB2	1.86	0.57
1:A:1186:GLN:NE2	1:B:790:SER:OG	2.38	0.57
1:C:1035:GLY:HA2	1:C:1201:PRO:HB3	1.86	0.57
1:A:581:LEU:HA	1:A:584:PHE:HB2	1.86	0.57
1:C:1022:PHE:HB2	1:C:1216:SER:HB3	1.87	0.56
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.69	0.56
1:A:392:GLN:HG3	1:A:439:LYS:HD3	1.86	0.56
3:A:1302:AJP:O62	3:A:1302:AJP:O64	2.23	0.56
3:A:1302:AJP:O62	3:A:1302:AJP:O75	2.22	0.56
3:C:1302:AJP:O62	3:C:1302:AJP:O75	2.22	0.56
3:C:1302:AJP:O62	3:C:1302:AJP:O64	2.23	0.56
1:A:306:ILE:HG21	1:A:329:ILE:HD11	1.88	0.56
1:B:306:ILE:HG21	1:B:329:ILE:HD11	1.88	0.56
1:C:299:LEU:HD21	1:C:329:ILE:HG12	1.88	0.56
1:D:306:ILE:HG21	1:D:329:ILE:HD11	1.88	0.55
1:A:299:LEU:HD21	1:A:329:ILE:HG12	1.88	0.55
1:C:469:TYR:CG	3:C:1302:AJP:C81	2.89	0.55
1:A:1022:PHE:HB2	1:A:1216:SER:HB3	1.87	0.55
3:C:1302:AJP:C81	3:C:1302:AJP:C83	2.85	0.55
1:A:628:ARG:HD3	1:D:622:ALA:HB1	1.89	0.55
3:A:1302:AJP:C81	3:A:1302:AJP:C83	2.85	0.55
1:B:299:LEU:HD21	1:B:329:ILE:HG12	1.88	0.55
1:D:512:PRO:HG2	1:D:790:SER:HB2	1.89	0.55
3:A:1302:AJP:C35	3:A:1302:AJP:C32	2.85	0.54
1:C:306:ILE:HG21	1:C:329:ILE:HD11	1.88	0.54
1:D:299:LEU:HD21	1:D:329:ILE:HG12	1.88	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.90	0.54
3:C:1302:AJP:C32	3:C:1302:AJP:C35	2.85	0.54
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.72	0.54
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.89	0.54
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.89	0.54
1:B:520:PRO:O	1:B:619:ASN:ND2	2.39	0.54
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.73	0.54
1:D:383:THR:HG22	1:D:384:GLU:H	1.72	0.54
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.90	0.53
1:B:512:PRO:HG2	1:B:790:SER:HB2	1.89	0.53
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.90	0.53
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.40	0.53
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.91	0.53
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.90	0.53
1:A:1029:THR:H	1:A:1095:ILE:HG22	1.74	0.53
1:B:640:SER:HB2	1:B:669:LYS:HD2	1.91	0.53
1:A:13:GLN:HA	1:A:44:THR:HB	1.91	0.53
1:A:505:LYS:NZ	1:A:508:GLN:OE1	2.35	0.53
1:D:48:ASP:HB3	1:D:50:LEU:HD13	1.91	0.52
1:A:48:ASP:HB3	1:A:50:LEU:HD13	1.91	0.52
1:B:407:MET:N	1:B:422:GLU:O	2.39	0.52
1:A:640:SER:HB2	1:A:669:LYS:HD2	1.91	0.52
1:B:48:ASP:HB3	1:B:50:LEU:HD13	1.91	0.52
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.90	0.52
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.92	0.52
1:A:539:VAL:HG11	1:A:601:VAL:HG21	1.92	0.52
1:D:13:GLN:HA	1:D:44:THR:HB	1.91	0.52
1:A:480:THR:O	1:A:485:ARG:NH1	2.41	0.52
1:B:539:VAL:HG11	1:B:601:VAL:HG21	1.92	0.52
1:C:48:ASP:HB3	1:C:50:LEU:HD13	1.91	0.52
1:D:198:ARG:HE	1:D:229:ASP:HB3	1.74	0.52
1:C:1029:THR:H	1:C:1095:ILE:HG22	1.74	0.52
1:A:1032:TRP:N	1:A:1093:THR:O	2.35	0.51
1:B:13:GLN:HA	1:B:44:THR:HB	1.92	0.51
1:B:13:GLN:HB3	1:B:70:VAL:HG12	1.92	0.51
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.40	0.51
1:D:153:ALA:HA	1:D:158:TRP:HB2	1.93	0.51
1:D:640:SER:HB2	1:D:669:LYS:HD2	1.91	0.51
1:A:198:ARG:HE	1:A:229:ASP:HB3	1.74	0.51
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.93	0.51
1:B:198:ARG:HE	1:B:229:ASP:HB3	1.74	0.51
1:C:198:ARG:HE	1:C:229:ASP:HB3	1.74	0.51
1:B:14:ILE:HG21	1:B:43:LEU:HD23	1.93	0.51
1:C:539:VAL:HG11	1:C:601:VAL:HG21	1.92	0.51
1:C:13:GLN:HA	1:C:44:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:HG21	1:C:43:LEU:HD23	1.93	0.51
1:A:14:ILE:HG21	1:A:43:LEU:HD23	1.93	0.51
1:A:258:PHE:O	1:A:262:TRP:N	2.42	0.51
3:C:1302:AJP:C02	3:C:1302:AJP:C06	2.85	0.51
1:A:173:LYS:HB2	1:A:177:TYR:HE2	1.76	0.51
3:A:1302:AJP:C02	3:A:1302:AJP:C06	2.86	0.51
1:D:539:VAL:HG11	1:D:601:VAL:HG21	1.92	0.51
1:B:23:ASP:O	1:B:27:SER:N	2.42	0.51
1:B:153:ALA:HA	1:B:158:TRP:HB2	1.93	0.51
1:C:197:GLU:O	1:C:201:VAL:N	2.38	0.51
1:D:13:GLN:HB3	1:D:70:VAL:HG12	1.92	0.51
3:A:1302:AJP:C30	3:A:1302:AJP:C56	2.89	0.51
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.92	0.51
1:D:407:MET:N	1:D:422:GLU:O	2.39	0.51
1:B:11:SER:OG	1:B:44:THR:OG1	2.30	0.50
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.92	0.50
1:C:11:SER:OG	1:C:44:THR:OG1	2.30	0.50
1:C:173:LYS:HB2	1:C:177:TYR:HE2	1.76	0.50
1:D:14:ILE:HG21	1:D:43:LEU:HD23	1.93	0.50
1:D:23:ASP:O	1:D:27:SER:N	2.42	0.50
1:B:326:GLY:HA2	1:B:329:ILE:HD12	1.92	0.50
3:C:1302:AJP:C30	3:C:1302:AJP:C56	2.89	0.50
1:A:625:THR:O	1:A:629:MET:N	2.43	0.50
1:C:193:ILE:HG12	1:C:221:ILE:HB	1.94	0.50
1:D:173:LYS:HB2	1:D:177:TYR:HE2	1.76	0.50
1:D:788:SER:OG	1:D:789:LEU:N	2.45	0.50
1:B:173:LYS:HB2	1:B:177:TYR:HE2	1.76	0.50
1:B:788:SER:OG	1:B:789:LEU:N	2.45	0.50
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.92	0.50
1:D:11:SER:OG	1:D:44:THR:OG1	2.30	0.50
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.94	0.50
1:A:11:SER:OG	1:A:44:THR:OG1	2.30	0.49
1:A:407:MET:N	1:A:422:GLU:O	2.39	0.49
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.94	0.49
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.94	0.49
1:A:1035:GLY:N	1:A:1091:PHE:O	2.42	0.49
1:C:611:ILE:HD12	1:D:517:PHE:HZ	1.77	0.49
1:A:141:ARG:NH2	1:A:195:ASP:OD1	2.40	0.49
1:C:153:ALA:HA	1:C:158:TRP:HB2	1.93	0.49
1:D:308:ARG:HH21	1:D:323:TRP:HB2	1.77	0.49
1:D:521:LEU:O	1:D:526:TRP:NE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:CA	3:A:1302:AJP:C17	2.88	0.49
1:A:153:ALA:HA	1:A:158:TRP:HB2	1.93	0.49
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.94	0.49
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.94	0.49
1:C:308:ARG:HH21	1:C:323:TRP:HB2	1.77	0.49
1:C:521:LEU:O	1:C:526:TRP:NE1	2.46	0.49
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.94	0.49
1:A:521:LEU:O	1:A:526:TRP:NE1	2.46	0.49
1:B:521:LEU:O	1:B:526:TRP:NE1	2.46	0.49
1:C:625:THR:O	1:C:629:MET:N	2.43	0.49
1:A:23:ASP:O	1:A:27:SER:N	2.42	0.49
1:A:481:ILE:HD11	1:A:733:GLY:HA3	1.94	0.49
1:B:383:THR:HG22	1:B:384:GLU:H	1.76	0.49
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.40	0.49
1:A:1035:GLY:HA3	1:A:1091:PHE:HB2	1.95	0.49
1:B:481:ILE:HD11	1:B:733:GLY:HA3	1.94	0.49
1:A:118:LYS:NZ	1:A:144:SER:OG	2.40	0.49
3:A:1302:AJP:O72	3:A:1302:AJP:O73	2.31	0.49
1:C:469:TYR:HA	3:C:1302:AJP:C80	2.42	0.49
1:B:305:GLU:OE2	1:B:307:SER:OG	2.31	0.49
1:C:481:ILE:HD11	1:C:733:GLY:HA3	1.94	0.48
3:C:1302:AJP:O72	3:C:1302:AJP:O73	2.31	0.48
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.94	0.48
1:C:258:PHE:O	1:C:262:TRP:N	2.42	0.48
1:A:348:ASP:OD1	1:A:352:LYS:N	2.47	0.48
1:C:645:ILE:HG12	1:C:699:LYS:HA	1.95	0.48
1:A:305:GLU:OE2	1:A:307:SER:OG	2.31	0.48
1:B:308:ARG:HH21	1:B:323:TRP:HB2	1.78	0.48
1:C:407:MET:N	1:C:422:GLU:O	2.39	0.48
1:D:348:ASP:OD1	1:D:352:LYS:N	2.47	0.48
1:C:606:TRP:HZ2	1:D:586:GLN:H	1.60	0.48
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.94	0.48
1:A:217:GLY:N	3:A:1302:AJP:C01	2.77	0.48
1:C:23:ASP:O	1:C:27:SER:N	2.42	0.48
2:B:1301:ZK1:HAI	2:B:1301:ZK1:HAOA	1.76	0.48
1:C:480:THR:O	1:C:485:ARG:NH1	2.41	0.48
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.96	0.48
1:A:611:ILE:HD12	1:B:517:PHE:HZ	1.79	0.48
1:B:348:ASP:OD1	1:B:352:LYS:N	2.47	0.47
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.96	0.47
1:A:308:ARG:HH21	1:A:323:TRP:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:HD22	1:B:737:PRO:HD3	1.96	0.47
1:C:305:GLU:OE2	1:C:307:SER:OG	2.31	0.47
1:D:391:GLU:HG3	1:D:393:LYS:HE3	1.96	0.47
1:D:480:THR:O	1:D:485:ARG:NH1	2.41	0.47
1:C:1035:GLY:HA3	1:C:1091:PHE:HB2	1.95	0.47
1:C:77:TYR:OH	1:C:101:PHE:O	2.24	0.47
1:C:348:ASP:OD1	1:C:352:LYS:N	2.47	0.47
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.96	0.47
1:D:506:LYS:HE3	1:D:719:ASP:HA	1.97	0.47
1:A:645:ILE:HG12	1:A:699:LYS:HA	1.96	0.47
1:B:197:GLU:O	1:B:201:VAL:N	2.38	0.47
1:B:597:SER:HB2	1:C:806:ALA:HB1	1.97	0.47
1:B:645:ILE:HG12	1:B:699:LYS:HA	1.96	0.47
1:C:1035:GLY:N	1:C:1091:PHE:O	2.42	0.47
1:D:645:ILE:HG12	1:D:699:LYS:HA	1.96	0.47
1:D:118:LYS:NZ	1:D:144:SER:OG	2.40	0.47
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.97	0.47
1:A:469:TYR:CA	3:A:1302:AJP:C80	2.92	0.47
1:B:480:THR:O	1:B:485:ARG:NH1	2.41	0.46
1:D:77:TYR:OH	1:D:101:PHE:O	2.24	0.46
1:A:774:GLY:HA3	1:A:777:ASP:HB2	1.98	0.46
1:A:1038:ARG:HA	1:A:1088:LEU:HA	1.98	0.46
1:B:77:TYR:HE1	1:B:98:THR:HG21	1.81	0.46
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.97	0.46
1:C:1038:ARG:HA	1:C:1088:LEU:HA	1.97	0.46
1:C:392:GLN:HG3	1:C:439:LYS:HD3	1.97	0.46
1:B:391:GLU:HG3	1:B:393:LYS:HE3	1.96	0.46
1:C:77:TYR:HE1	1:C:98:THR:HG21	1.80	0.46
1:D:305:GLU:OE2	1:D:307:SER:OG	2.31	0.46
1:B:775:ALA:O	1:B:779:GLY:N	2.49	0.46
1:C:1032:TRP:O	1:C:1207:GLY:N	2.49	0.46
1:A:1098:SER:HB3	1:A:1113:PHE:HB2	1.98	0.46
1:C:118:LYS:NZ	1:C:144:SER:OG	2.40	0.46
1:D:775:ALA:O	1:D:779:GLY:N	2.49	0.46
1:A:469:TYR:CG	3:A:1302:AJP:C81	2.98	0.46
1:B:112:GLN:HE21	1:B:352:LYS:HG2	1.81	0.46
1:D:197:GLU:O	1:D:201:VAL:N	2.38	0.45
1:A:1032:TRP:O	1:A:1207:GLY:N	2.49	0.45
1:C:112:GLN:HE21	1:C:352:LYS:HG2	1.81	0.45
1:D:77:TYR:HE1	1:D:98:THR:HG21	1.80	0.45
1:A:46:HIS:O	1:A:65:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:PHE:O	1:B:262:TRP:N	2.42	0.45
1:D:46:HIS:O	1:D:65:GLN:NE2	2.50	0.45
1:A:143:LEU:HD23	1:A:146:LEU:HD23	1.98	0.45
1:A:197:GLU:O	1:A:201:VAL:N	2.38	0.45
1:C:1098:SER:HB3	1:C:1113:PHE:HB2	1.98	0.45
1:D:112:GLN:HE21	1:D:352:LYS:HG2	1.81	0.45
1:D:258:PHE:O	1:D:262:TRP:N	2.42	0.45
1:A:77:TYR:HE1	1:A:98:THR:HG21	1.80	0.45
1:A:740:SER:HB2	3:A:1302:AJP:O42	2.14	0.45
1:B:46:HIS:O	1:B:65:GLN:NE2	2.50	0.45
1:C:774:GLY:HA3	1:C:777:ASP:HB2	1.98	0.45
1:C:143:LEU:HD23	1:C:146:LEU:HD23	1.98	0.45
1:D:25:GLU:OE2	1:D:281:THR:OG1	2.33	0.45
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.82	0.45
1:B:118:LYS:NZ	1:B:144:SER:OG	2.40	0.45
1:C:626:VAL:HA	1:C:629:MET:HB2	1.99	0.45
1:D:143:LEU:HD23	1:D:146:LEU:HD23	1.98	0.45
1:D:259:ILE:HA	1:D:262:TRP:HB3	2.00	0.45
1:B:579:PHE:HD1	1:B:589:CYS:HB2	1.82	0.44
1:B:755:GLU:OE2	1:C:661:ARG:NH2	2.49	0.44
1:D:14:ILE:HD13	1:D:43:LEU:HD23	1.99	0.44
1:A:112:GLN:HE21	1:A:352:LYS:HG2	1.81	0.44
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.82	0.44
1:C:579:PHE:HD1	1:C:589:CYS:HB2	1.82	0.44
1:A:755:GLU:OE2	1:D:661:ARG:NH2	2.46	0.44
1:B:14:ILE:HD13	1:B:43:LEU:HD23	1.99	0.44
1:A:1099:CYS:HA	1:A:1110:CYS:HA	2.00	0.44
1:C:46:HIS:O	1:C:65:GLN:NE2	2.50	0.44
1:C:198:ARG:HD3	1:C:279:LYS:HE2	2.00	0.44
1:A:136:LEU:HB2	1:A:194:LEU:HD23	2.00	0.44
1:A:579:PHE:HD1	1:A:589:CYS:HB2	1.82	0.44
1:C:1196:PRO:HD2	1:C:1200:ARG:HB3	2.00	0.44
1:A:266:GLU:HG2	1:A:269:GLU:H	1.83	0.44
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.82	0.44
1:C:136:LEU:HB2	1:C:194:LEU:HD23	2.00	0.44
1:D:198:ARG:HD3	1:D:279:LYS:HE2	2.00	0.44
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.99	0.43
1:A:626:VAL:HA	1:A:629:MET:HB2	1.99	0.43
1:C:266:GLU:HG2	1:C:269:GLU:H	1.83	0.43
1:A:542:LEU:HD21	1:A:1228:LEU:HD12	2.00	0.43
1:C:1192:VAL:HA	1:C:1196:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HB2	1:B:194:LEU:HD23	2.00	0.43
1:B:506:LYS:HE3	1:B:719:ASP:HA	1.99	0.43
1:D:579:PHE:HD1	1:D:589:CYS:HB2	1.82	0.43
1:B:259:ILE:HA	1:B:262:TRP:HB3	2.00	0.43
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.82	0.43
1:D:136:LEU:HB2	1:D:194:LEU:HD23	2.00	0.43
1:D:266:GLU:HG2	1:D:269:GLU:H	1.83	0.43
1:B:198:ARG:HD3	1:B:279:LYS:HE2	2.00	0.43
1:C:217:GLY:HA2	3:C:1302:AJP:C03	2.49	0.43
1:A:290:GLN:NE2	1:A:339:GLU:O	2.52	0.43
1:A:1192:VAL:HA	1:A:1196:PRO:HD3	2.00	0.43
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.99	0.43
1:C:290:GLN:NE2	1:C:339:GLU:O	2.52	0.43
1:C:359:ASN:HB3	1:C:370:LYS:HE2	2.01	0.43
1:D:359:ASN:HB3	1:D:370:LYS:HE2	2.01	0.43
2:D:1301:ZK1:HAI	2:D:1301:ZK1:HAOA	1.73	0.43
1:A:513:GLY:N	1:A:516:SER:OG	2.52	0.43
1:C:259:ILE:HA	1:C:262:TRP:HB3	2.00	0.43
1:C:1099:CYS:HA	1:C:1110:CYS:HA	2.00	0.43
1:B:290:GLN:NE2	1:B:339:GLU:O	2.52	0.42
2:C:1301:ZK1:HAI	2:C:1301:ZK1:HAOA	1.78	0.42
1:A:259:ILE:HA	1:A:262:TRP:HB3	2.00	0.42
1:C:513:GLY:N	1:C:516:SER:OG	2.52	0.42
1:D:466:GLU:O	1:D:472:ALA:N	2.47	0.42
1:A:198:ARG:HD3	1:A:279:LYS:HE2	2.00	0.42
1:B:15:GLY:HA3	1:B:73:ILE:HG23	2.02	0.42
1:C:63:CYS:HA	1:C:66:PHE:HB3	2.02	0.42
1:C:291:VAL:HG13	1:C:336:VAL:HG11	2.01	0.42
1:C:1092:HIS:HD2	1:C:1101:GLU:HB3	1.85	0.42
1:A:359:ASN:HB3	1:A:370:LYS:HE2	2.01	0.42
1:B:211:ILE:HG13	1:B:213:LYS:H	1.85	0.42
1:B:266:GLU:HG2	1:B:269:GLU:H	1.83	0.42
1:C:469:TYR:CA	3:C:1302:AJP:C80	2.97	0.42
1:C:520:PRO:HG3	1:C:623:PHE:HE2	1.83	0.42
1:A:1092:HIS:HD2	1:A:1101:GLU:HB3	1.85	0.42
1:A:1196:PRO:HD2	1:A:1200:ARG:HB3	2.00	0.42
2:A:1301:ZK1:HAI	2:A:1301:ZK1:HAOA	1.80	0.42
1:C:211:ILE:HG13	1:C:213:LYS:H	1.85	0.42
1:D:290:GLN:NE2	1:D:339:GLU:O	2.52	0.42
1:A:15:GLY:HA3	1:A:73:ILE:HG23	2.02	0.42
1:A:63:CYS:HA	1:A:66:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:HG13	1:A:336:VAL:HG11	2.02	0.42
1:A:1037:GLN:HB2	1:A:1089:ARG:HB2	2.02	0.42
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.90	0.42
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.02	0.42
1:C:23:ASP:HA	1:C:26:TYR:HB3	2.02	0.42
1:B:23:ASP:HA	1:B:26:TYR:HB3	2.02	0.42
1:B:63:CYS:HA	1:B:66:PHE:HB3	2.02	0.42
1:B:291:VAL:HG13	1:B:336:VAL:HG11	2.02	0.42
1:C:1215:GLY:HA2	1:C:1218:THR:HG22	2.02	0.42
1:D:63:CYS:HA	1:D:66:PHE:HB3	2.02	0.42
1:B:466:GLU:O	1:B:472:ALA:N	2.47	0.41
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.02	0.41
1:C:1118:PRO:HD3	1:C:1194:LEU:HD21	2.02	0.41
1:D:23:ASP:HA	1:D:26:TYR:HB3	2.01	0.41
1:B:498:LEU:N	1:B:730:LYS:O	2.49	0.41
1:B:485:ARG:NH1	2:B:1301:ZK1:OAA	2.51	0.41
1:B:359:ASN:HB3	1:B:370:LYS:HE2	2.01	0.41
1:D:12:ILE:O	1:D:44:THR:N	2.46	0.41
1:D:211:ILE:HG13	1:D:213:LYS:H	1.85	0.41
1:A:128:TYR:O	3:A:1302:AJP:C17	2.69	0.41
1:A:211:ILE:HG13	1:A:213:LYS:H	1.85	0.41
1:A:489:ILE:HD12	1:A:735:ALA:HB1	2.02	0.41
1:C:15:GLY:HA3	1:C:73:ILE:HG23	2.02	0.41
1:C:1038:ARG:HB3	1:C:1088:LEU:HD22	2.03	0.41
1:D:15:GLY:HA3	1:D:73:ILE:HG23	2.02	0.41
1:D:489:ILE:HD12	1:D:735:ALA:HB1	2.02	0.41
1:A:1035:GLY:O	1:A:1091:PHE:N	2.41	0.41
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.56	0.41
1:C:1037:GLN:HB2	1:C:1089:ARG:HB2	2.02	0.41
1:A:1215:GLY:HA2	1:A:1218:THR:HG22	2.02	0.41
1:C:498:LEU:N	1:C:730:LYS:O	2.49	0.41
1:C:576:SER:HA	1:C:579:PHE:HB2	2.03	0.41
1:C:409:LYS:HG3	1:C:415:LEU:HD12	2.03	0.41
1:D:576:SER:HA	1:D:579:PHE:HB2	2.03	0.41
1:A:23:ASP:HA	1:A:26:TYR:HB3	2.02	0.41
1:D:291:VAL:HG13	1:D:336:VAL:HG11	2.02	0.41
1:A:1149:GLU:O	1:A:1153:SER:N	2.54	0.41
1:B:25:GLU:OE2	1:B:281:THR:OG1	2.33	0.41
1:B:409:LYS:HG3	1:B:415:LEU:HD12	2.03	0.41
1:C:25:GLU:OE2	1:C:281:THR:OG1	2.33	0.41
1:A:498:LEU:N	1:A:730:LYS:O	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1149:GLU:O	1:C:1153:SER:N	2.54	0.40
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.56	0.40
1:D:489:ILE:HA	1:D:738:LYS:HB2	2.03	0.40
1:A:1118:PRO:HD3	1:A:1194:LEU:HD21	2.03	0.40
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.56	0.40
1:B:12:ILE:O	1:B:44:THR:N	2.46	0.40
1:B:56:PHE:O	1:B:60:ASN:ND2	2.55	0.40
1:C:209:ILE:HA	1:C:214:HIS:CD2	2.56	0.40
1:D:374:TRP:HD1	1:D:380:MET:HB2	1.87	0.40
1:D:409:LYS:HG3	1:D:415:LEU:HD12	2.03	0.40
1:A:576:SER:HA	1:A:579:PHE:HB2	2.03	0.40
1:B:185:GLU:HG3	1:B:213:LYS:HE3	2.04	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	950/1057 (90%)	893 (94%)	55 (6%)	2 (0%)	44	78
1	B	776/1057 (73%)	721 (93%)	54 (7%)	1 (0%)	48	83
1	C	950/1057 (90%)	889 (94%)	59 (6%)	2 (0%)	44	78
1	D	776/1057 (73%)	721 (93%)	55 (7%)	0	100	100
All	All	3452/4228 (82%)	3224 (93%)	223 (6%)	5 (0%)	50	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	GLU
1	A	385	ASP
1	A	386	ASP

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Mol	Chain	Res	Type
1	C	385	ASP
1	C	386	ASP

5.3.2 Protein sidechains (i)

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	816/888 (92%)	814 (100%)	2 (0%)	92	94
1	B	662/888 (74%)	660 (100%)	2 (0%)	91	92
1	C	816/888 (92%)	814 (100%)	2 (0%)	92	94
1	D	662/888 (74%)	660 (100%)	2 (0%)	91	92
All	All	2956/3552 (83%)	2948 (100%)	8 (0%)	90	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ARG
1	A	596	LEU
1	B	300	ARG
1	B	596	LEU
1	C	300	ARG
1	C	596	LEU
1	D	300	ARG
1	D	596	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	147	GLN
1	A	337	GLN
1	A	586	GLN
1	A	642	GLN
1	A	1037	GLN

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Mol	Chain	Res	Type
1	A	1092	HIS
1	A	1186	GLN
1	B	65	GLN
1	B	147	GLN
1	B	337	GLN
1	B	392	GLN
1	B	642	GLN
1	C	65	GLN
1	C	147	GLN
1	C	337	GLN
1	C	586	GLN
1	C	642	GLN
1	C	1037	GLN
1	C	1092	HIS
1	D	65	GLN
1	D	147	GLN
1	D	337	GLN
1	D	392	GLN
1	D	642	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)

6 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	$\#\|Z\| > 2$
3	AJP	C	1302	-	95,95,95	0.83	6 (6%)	144,149,149	1.45	20 (13%)
2	ZK1	D	1301	-	29,29,29	3.57	10 (34%)	45,45,45	1.66	10 (22%)
2	ZK1	B	1301	-	29,29,29	3.55	11 (37%)	45,45,45	1.65	10 (22%)
3	AJP	A	1302	-	95,95,95	0.84	6 (6%)	144,149,149	1.45	20 (13%)
2	ZK1	A	1301	-	29,29,29	3.53	10 (34%)	45,45,45	1.51	8 (17%)
2	ZK1	C	1301	-	29,29,29	3.53	10 (34%)	45,45,45	1.46	9 (20%)

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
3	AJP	C	1302	-	34/34/38/38	13/28/220/220	0/11/11/11
2	ZK1	D	1301	-	-	5/13/23/23	0/3/3/3
2	ZK1	B	1301	-	-	5/13/23/23	0/3/3/3
3	AJP	A	1302	-	34/34/38/38	13/28/220/220	0/11/11/11
2	ZK1	A	1301	-	-	6/13/23/23	0/3/3/3
2	ZK1	C	1301	-	-	6/13/23/23	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ZK1	OAA-CAT	9.26	1.41	1.23
2	C	1301	ZK1	OAA-CAT	9.25	1.41	1.23
2	A	1301	ZK1	OAA-CAT	9.23	1.41	1.23
2	B	1301	ZK1	OAA-CAT	9.10	1.40	1.23
2	D	1301	ZK1	OAB-CAU	8.69	1.40	1.23
2	B	1301	ZK1	OAB-CAU	8.68	1.40	1.23
2	A	1301	ZK1	OAB-CAU	8.62	1.40	1.23
2	C	1301	ZK1	OAB-CAU	8.58	1.40	1.23
2	D	1301	ZK1	PBA-OAC	7.39	1.65	1.50
2	C	1301	ZK1	PBA-OAC	7.38	1.65	1.50
2	A	1301	ZK1	PBA-OAC	7.38	1.65	1.50
2	B	1301	ZK1	PBA-OAC	7.35	1.65	1.50
2	D	1301	ZK1	CAT-NAP	5.71	1.43	1.35
2	C	1301	ZK1	CAU-CAT	-5.69	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ZK1	CAU-CAT	-5.60	1.45	1.53
2	B	1301	ZK1	CAT-NAP	5.52	1.43	1.35
2	B	1301	ZK1	CAU-CAT	-5.52	1.45	1.53
2	A	1301	ZK1	CAU-CAT	-5.50	1.45	1.53
2	A	1301	ZK1	CAT-NAP	5.47	1.43	1.35
2	C	1301	ZK1	CAT-NAP	5.28	1.43	1.35
2	B	1301	ZK1	PBA-OAE	4.68	1.65	1.55
2	D	1301	ZK1	PBA-OAE	4.64	1.65	1.55
2	A	1301	ZK1	PBA-OAE	4.61	1.65	1.55
2	C	1301	ZK1	PBA-OAE	4.61	1.65	1.55
2	D	1301	ZK1	PBA-OAD	-3.86	1.46	1.55
2	B	1301	ZK1	PBA-OAD	-3.85	1.46	1.55
2	C	1301	ZK1	PBA-OAD	-3.84	1.46	1.55
2	A	1301	ZK1	PBA-OAD	-3.82	1.46	1.55
2	D	1301	ZK1	CAJ-CAS	3.31	1.44	1.39
2	B	1301	ZK1	CAJ-CAS	3.20	1.44	1.39
2	C	1301	ZK1	CAW-NAY	3.16	1.46	1.41
2	B	1301	ZK1	CAW-NAY	3.11	1.46	1.41
2	A	1301	ZK1	CAJ-CAS	3.10	1.43	1.39
2	C	1301	ZK1	CAJ-CAS	3.06	1.43	1.39
2	A	1301	ZK1	CAW-NAY	3.05	1.46	1.41
2	D	1301	ZK1	CAW-NAY	3.03	1.46	1.41
3	A	1302	AJP	C12-C11	-2.78	1.50	1.56
3	A	1302	AJP	C16-C11	-2.72	1.50	1.54
3	C	1302	AJP	O09-C05	2.71	1.48	1.42
3	A	1302	AJP	C07-C08	-2.70	1.49	1.53
3	A	1302	AJP	O09-C05	2.68	1.48	1.42
3	C	1302	AJP	C12-C11	-2.68	1.51	1.56
3	C	1302	AJP	C07-C08	-2.67	1.49	1.53
3	C	1302	AJP	C16-C11	-2.64	1.50	1.54
2	D	1301	ZK1	PBA-CAO	2.27	1.86	1.81
2	A	1301	ZK1	PBA-CAO	2.24	1.86	1.81
2	C	1301	ZK1	PBA-CAO	2.23	1.86	1.81
2	B	1301	ZK1	PBA-CAO	2.17	1.86	1.81
3	C	1302	AJP	C20-C15	-2.17	1.52	1.56
3	A	1302	AJP	C12-C07	-2.17	1.52	1.56
3	A	1302	AJP	C20-C15	-2.17	1.52	1.56
3	C	1302	AJP	C12-C07	-2.16	1.52	1.56
2	B	1301	ZK1	CAR-NAX	2.01	1.45	1.41

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1302	AJP	C12-C11-C16	-5.37	106.42	113.90
3	A	1302	AJP	C12-C11-C16	-5.28	106.55	113.90
2	D	1301	ZK1	CAO-NAY-CAU	4.41	121.03	116.55
2	B	1301	ZK1	CAO-NAY-CAU	4.22	120.84	116.55
2	D	1301	ZK1	CAN-NAX-CAM	4.06	120.69	111.57
2	D	1301	ZK1	CAI-CAR-NAX	-3.82	117.02	122.59
2	B	1301	ZK1	CAN-NAX-CAM	3.69	119.88	111.57
3	C	1302	AJP	C06-C07-C08	-3.67	98.39	104.28
2	B	1301	ZK1	CAI-CAR-NAX	-3.64	117.29	122.59
2	A	1301	ZK1	CAV-NAP-CAT	-3.63	119.73	124.82
3	A	1302	AJP	C05-C06-C07	-3.63	98.01	103.37
3	A	1302	AJP	C06-C07-C08	-3.63	98.44	104.28
3	C	1302	AJP	C65-O64-C57	-3.60	109.45	117.98
2	B	1301	ZK1	CAV-NAP-CAT	-3.59	119.79	124.82
3	A	1302	AJP	C65-O64-C57	-3.59	109.47	117.98
2	C	1301	ZK1	CAO-NAY-CAU	3.58	120.20	116.55
3	C	1302	AJP	C05-C06-C07	-3.58	98.09	103.37
3	C	1302	AJP	C45-O44-C37	-3.57	109.52	117.98
3	A	1302	AJP	C45-O44-C37	-3.56	109.54	117.98
3	A	1302	AJP	C26-O25-C23	-3.56	109.32	115.27
3	C	1302	AJP	C26-O25-C23	-3.54	109.35	115.27
2	D	1301	ZK1	CAV-NAP-CAT	-3.53	119.88	124.82
3	A	1302	AJP	C55-O54-C36	-3.52	109.62	117.98
3	C	1302	AJP	C55-O54-C36	-3.51	109.66	117.98
2	A	1301	ZK1	CAO-NAY-CAU	3.50	120.11	116.55
3	C	1302	AJP	C20-C15-C16	-3.39	108.98	112.43
3	A	1302	AJP	C20-C15-C16	-3.38	108.99	112.43
2	C	1301	ZK1	CAN-NAX-CAM	3.38	119.17	111.57
3	C	1302	AJP	C11-C12-C07	-3.38	95.07	100.16
3	A	1302	AJP	C14-C15-C20	-3.37	110.11	113.91
3	C	1302	AJP	C14-C13-C12	-3.36	107.06	112.74
3	A	1302	AJP	C14-C13-C12	-3.34	107.10	112.74
3	A	1302	AJP	C11-C12-C07	-3.32	95.16	100.16
3	C	1302	AJP	C14-C15-C20	-3.32	110.17	113.91
2	A	1301	ZK1	CAN-NAX-CAM	3.18	118.73	111.57
3	C	1302	AJP	C35-O34-C29	-3.16	110.48	117.98
2	C	1301	ZK1	CAV-NAP-CAT	-3.16	120.40	124.82
3	A	1302	AJP	C35-O34-C29	-3.15	110.50	117.98
3	C	1302	AJP	O09-C08-C10	3.11	116.49	110.20
3	A	1302	AJP	O09-C08-C10	3.06	116.39	110.20
3	C	1302	AJP	C24-C19-C20	-3.02	109.45	112.66
3	A	1302	AJP	C24-C19-C20	-2.99	109.48	112.66
2	B	1301	ZK1	CAU-CAT-NAP	2.98	120.50	117.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1302	AJP	C83-C06-C05	-2.96	110.17	114.94
3	C	1302	AJP	C83-C06-C05	-2.95	110.19	114.94
3	A	1302	AJP	C20-C21-C22	-2.90	109.41	114.17
2	D	1301	ZK1	CAU-CAT-NAP	2.88	120.40	117.46
3	C	1302	AJP	C20-C21-C22	-2.86	109.47	114.17
3	A	1302	AJP	C04-C05-C06	-2.79	110.61	115.66
3	C	1302	AJP	C04-C05-C06	-2.74	110.69	115.66
2	A	1301	ZK1	CAU-CAT-NAP	2.64	120.16	117.46
2	C	1301	ZK1	CAI-CAR-NAX	-2.58	118.84	122.59
2	A	1301	ZK1	CAI-CAR-NAX	-2.54	118.89	122.59
2	D	1301	ZK1	CAW-NAY-CAU	-2.53	119.73	122.84
2	B	1301	ZK1	CAW-NAY-CAU	-2.47	119.79	122.84
3	A	1302	AJP	C21-C20-C19	2.46	109.58	107.23
2	A	1301	ZK1	FAG-CAZ-CAS	-2.45	108.31	112.65
2	D	1301	ZK1	CAV-CAW-NAY	2.45	120.78	118.01
3	A	1302	AJP	O09-C08-C07	-2.43	98.48	104.08
3	C	1302	AJP	O09-C08-C07	-2.41	98.53	104.08
2	C	1301	ZK1	CAU-CAT-NAP	2.41	119.92	117.46
2	C	1301	ZK1	FAG-CAZ-CAS	-2.39	108.40	112.65
2	A	1301	ZK1	CAW-NAY-CAU	-2.37	119.92	122.84
3	C	1302	AJP	C21-C20-C19	2.36	109.48	107.23
2	B	1301	ZK1	CAS-CAR-NAX	2.33	122.59	119.92
2	B	1301	ZK1	FAG-CAZ-CAS	-2.32	108.53	112.65
2	A	1301	ZK1	CAT-CAU-NAY	2.29	119.90	117.41
2	B	1301	ZK1	CAV-CAW-NAY	2.26	120.57	118.01
2	D	1301	ZK1	CAS-CAR-NAX	2.24	122.49	119.92
2	D	1301	ZK1	FAG-CAZ-CAS	-2.20	108.75	112.65
3	A	1302	AJP	C65-O70-C69	-2.18	109.47	113.72
2	C	1301	ZK1	CAW-NAY-CAU	-2.16	120.18	122.84
2	C	1301	ZK1	OAA-CAT-CAU	2.16	120.83	119.21
3	C	1302	AJP	C65-O70-C69	-2.14	109.53	113.72
2	C	1301	ZK1	CAT-CAU-NAY	2.10	119.69	117.41
2	D	1301	ZK1	CAT-CAU-NAY	2.05	119.63	117.41
2	B	1301	ZK1	CAM-NAX-CAR	2.01	120.96	116.19

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1302	AJP	C69
3	A	1302	AJP	C28
3	A	1302	AJP	C48
3	A	1302	AJP	C19

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Mol	Chain	Res	Type	Atom
3	A	1302	AJP	C20
3	A	1302	AJP	C55
3	A	1302	AJP	C27
3	A	1302	AJP	C37
3	A	1302	AJP	C22
3	A	1302	AJP	C66
3	A	1302	AJP	C07
3	A	1302	AJP	C47
3	A	1302	AJP	C59
3	A	1302	AJP	C67
3	A	1302	AJP	C23
3	A	1302	AJP	C26
3	A	1302	AJP	C15
3	A	1302	AJP	C16
3	A	1302	AJP	C56
3	A	1302	AJP	C10
3	A	1302	AJP	C68
3	A	1302	AJP	C36
3	A	1302	AJP	C30
3	A	1302	AJP	C39
3	A	1302	AJP	C02
3	A	1302	AJP	C12
3	A	1302	AJP	C57
3	A	1302	AJP	C65
3	A	1302	AJP	C35
3	A	1302	AJP	C11
3	A	1302	AJP	C46
3	A	1302	AJP	C45
3	A	1302	AJP	C05
3	A	1302	AJP	C38
3	C	1302	AJP	C69
3	C	1302	AJP	C28
3	C	1302	AJP	C48
3	C	1302	AJP	C19
3	C	1302	AJP	C20
3	C	1302	AJP	C55
3	C	1302	AJP	C27
3	C	1302	AJP	C37
3	C	1302	AJP	C22
3	C	1302	AJP	C66
3	C	1302	AJP	C07
3	C	1302	AJP	C47

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Mol	Chain	Res	Type	Atom
3	C	1302	AJP	C59
3	C	1302	AJP	C67
3	C	1302	AJP	C23
3	C	1302	AJP	C26
3	C	1302	AJP	C15
3	C	1302	AJP	C16
3	C	1302	AJP	C56
3	C	1302	AJP	C10
3	C	1302	AJP	C68
3	C	1302	AJP	C36
3	C	1302	AJP	C30
3	C	1302	AJP	C39
3	C	1302	AJP	C02
3	C	1302	AJP	C12
3	C	1302	AJP	C57
3	C	1302	AJP	C65
3	C	1302	AJP	C35
3	C	1302	AJP	C11
3	C	1302	AJP	C46
3	C	1302	AJP	C45
3	C	1302	AJP	C05
3	C	1302	AJP	C38

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ZK1	NAY-CAO-PBA-OAC
2	A	1301	ZK1	NAY-CAO-PBA-OAE
2	B	1301	ZK1	NAY-CAO-PBA-OAC
2	B	1301	ZK1	NAY-CAO-PBA-OAE
2	C	1301	ZK1	NAY-CAO-PBA-OAD
2	C	1301	ZK1	NAY-CAO-PBA-OAE
2	D	1301	ZK1	NAY-CAO-PBA-OAD
2	D	1301	ZK1	NAY-CAO-PBA-OAE
3	A	1302	AJP	C46-C45-O44-C37
3	C	1302	AJP	C46-C45-O44-C37
3	A	1302	AJP	C56-C55-O54-C36
3	C	1302	AJP	C56-C55-O54-C36
3	A	1302	AJP	C66-C65-O64-C57
3	C	1302	AJP	C66-C65-O64-C57
3	A	1302	AJP	C30-C29-O34-C35
3	C	1302	AJP	C30-C29-O34-C35

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Mol	Chain	Res	Type	Atoms
3	A	1302	AJP	O40-C39-C41-O42
3	A	1302	AJP	O70-C69-C71-O72
3	C	1302	AJP	O40-C39-C41-O42
3	C	1302	AJP	O70-C69-C71-O72
3	A	1302	AJP	O70-C65-O64-C57
3	C	1302	AJP	O70-C65-O64-C57
3	A	1302	AJP	C38-C39-C41-O42
3	C	1302	AJP	C38-C39-C41-O42
3	A	1302	AJP	O31-C30-C32-O33
3	C	1302	AJP	O31-C30-C32-O33
2	B	1301	ZK1	CAI-CAR-NAX-CAN
2	D	1301	ZK1	CAI-CAR-NAX-CAN
2	C	1301	ZK1	CAI-CAR-NAX-CAN
2	A	1301	ZK1	CAI-CAR-NAX-CAN
2	A	1301	ZK1	NAY-CAO-PBA-OAD
2	B	1301	ZK1	NAY-CAO-PBA-OAD
2	C	1301	ZK1	NAY-CAO-PBA-OAC
2	D	1301	ZK1	NAY-CAO-PBA-OAC
3	C	1302	AJP	C28-C29-O34-C35
3	A	1302	AJP	C28-C29-O34-C35
2	A	1301	ZK1	CAI-CAR-NAX-CAM
3	C	1302	AJP	C68-C69-C71-O72
3	A	1302	AJP	C68-C69-C71-O72
2	C	1301	ZK1	CAI-CAR-NAX-CAM
3	A	1302	AJP	O60-C55-O54-C36
3	C	1302	AJP	O60-C55-O54-C36
2	B	1301	ZK1	CAS-CAR-NAX-CAN
2	D	1301	ZK1	CAS-CAR-NAX-CAN
2	A	1301	ZK1	CAS-CAR-NAX-CAN
2	C	1301	ZK1	CAS-CAR-NAX-CAN
3	A	1302	AJP	C22-C23-O25-C26
3	C	1302	AJP	C22-C23-O25-C26

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1302	AJP	24	0
2	D	1301	ZK1	1	0
2	B	1301	ZK1	2	0
3	A	1302	AJP	23	0
2	A	1301	ZK1	1	0

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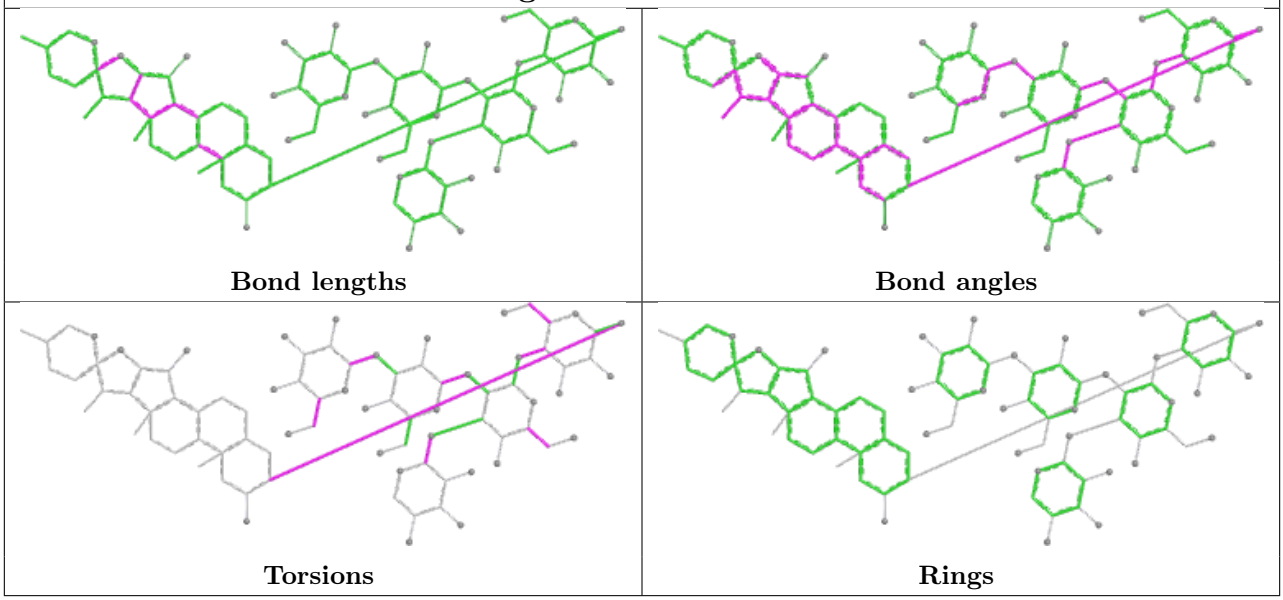
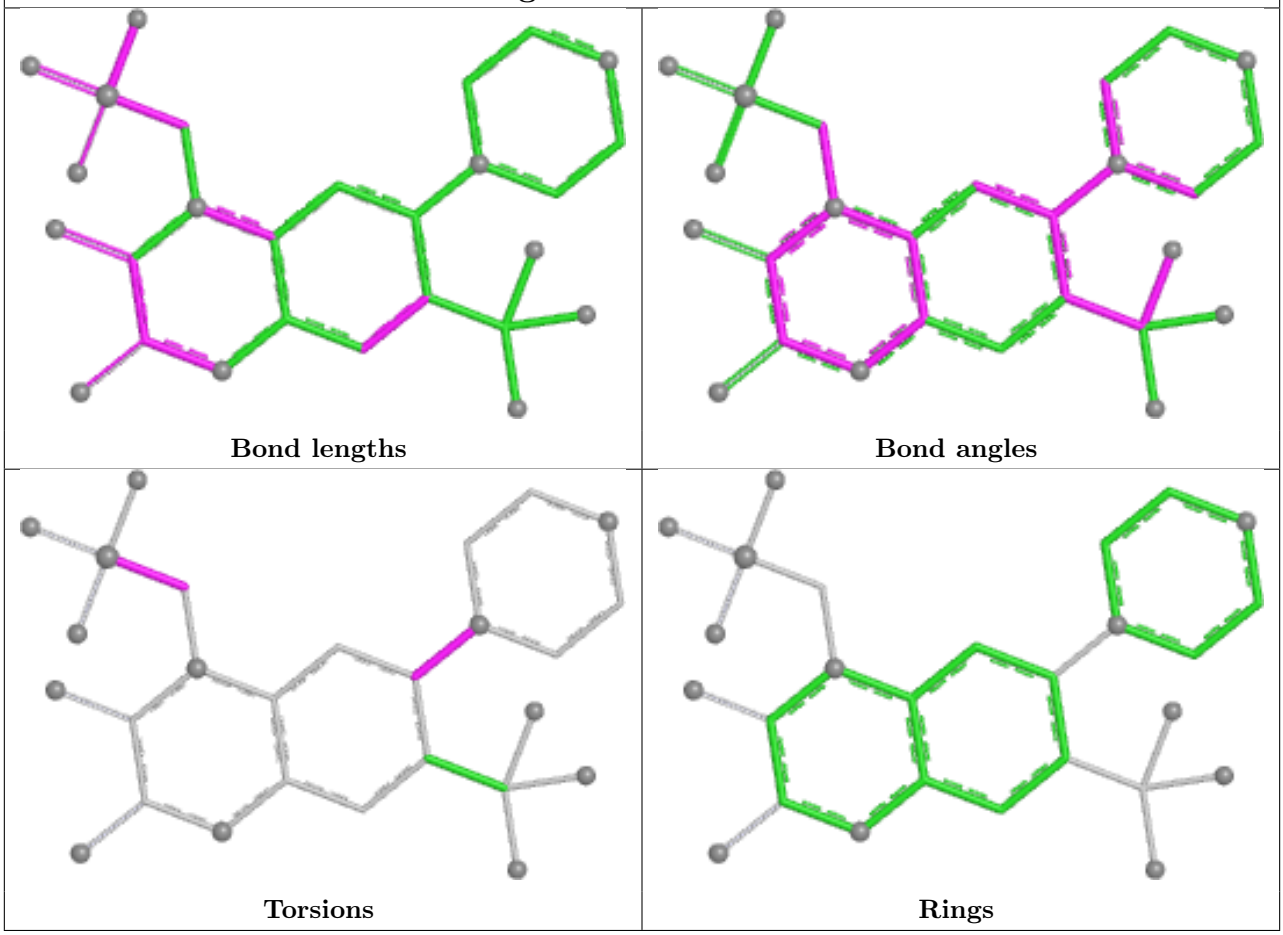
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	ZK1	1	0

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 then 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.

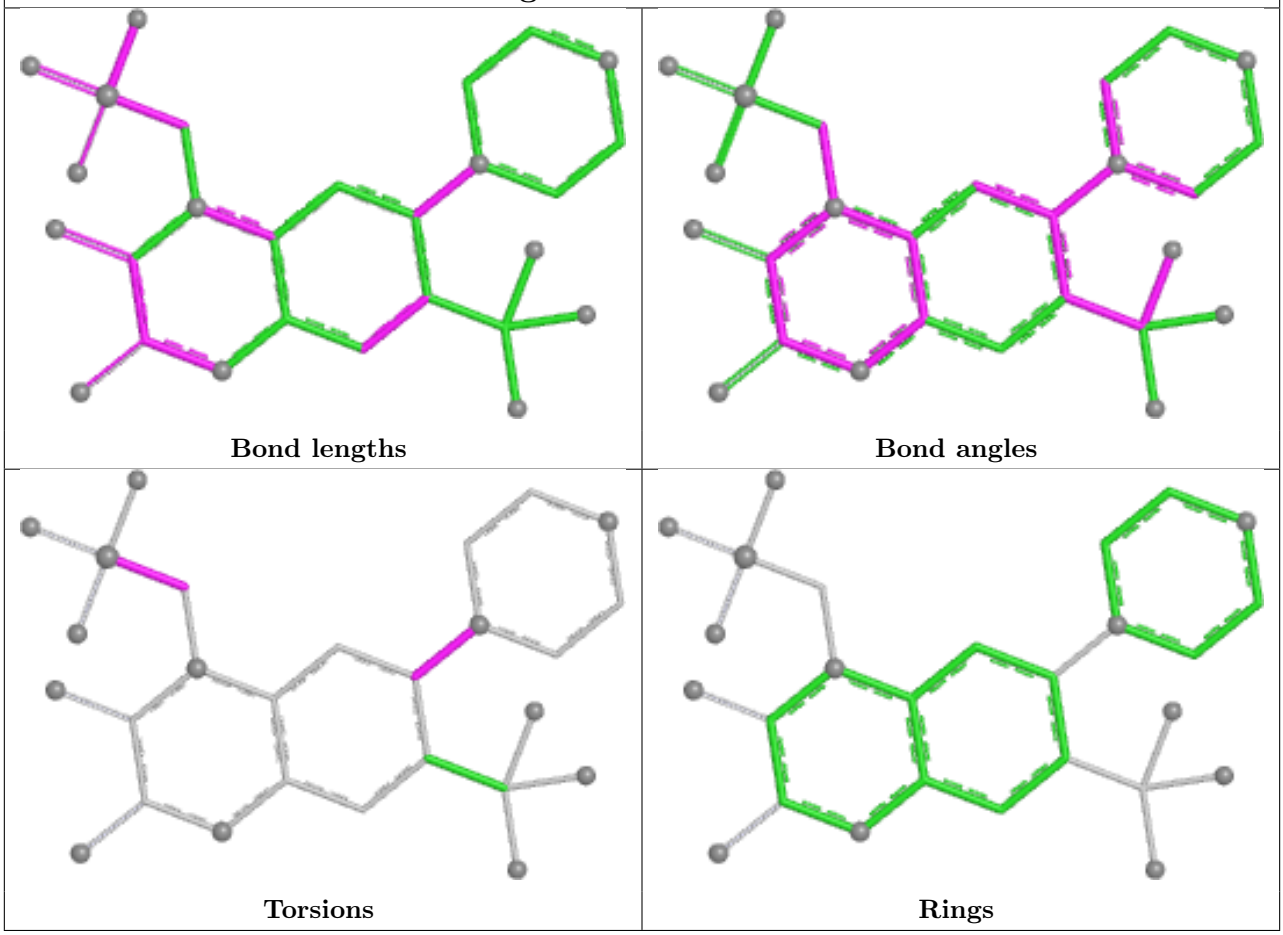
Ligand AJP C 1302



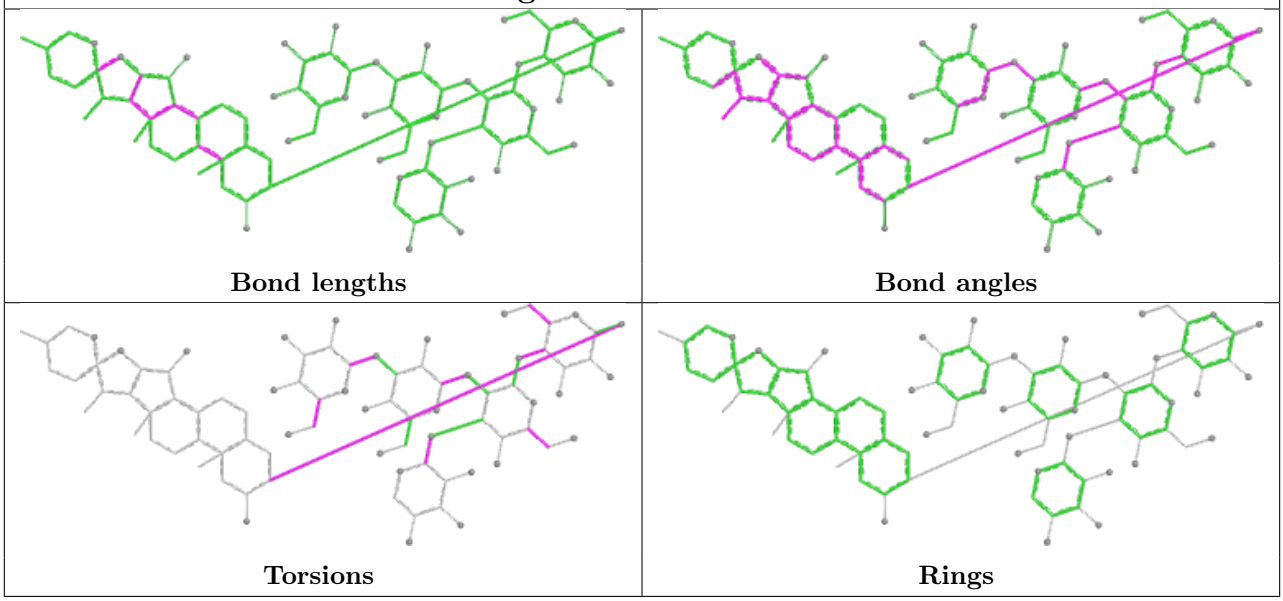
Ligand ZK1 D 1301



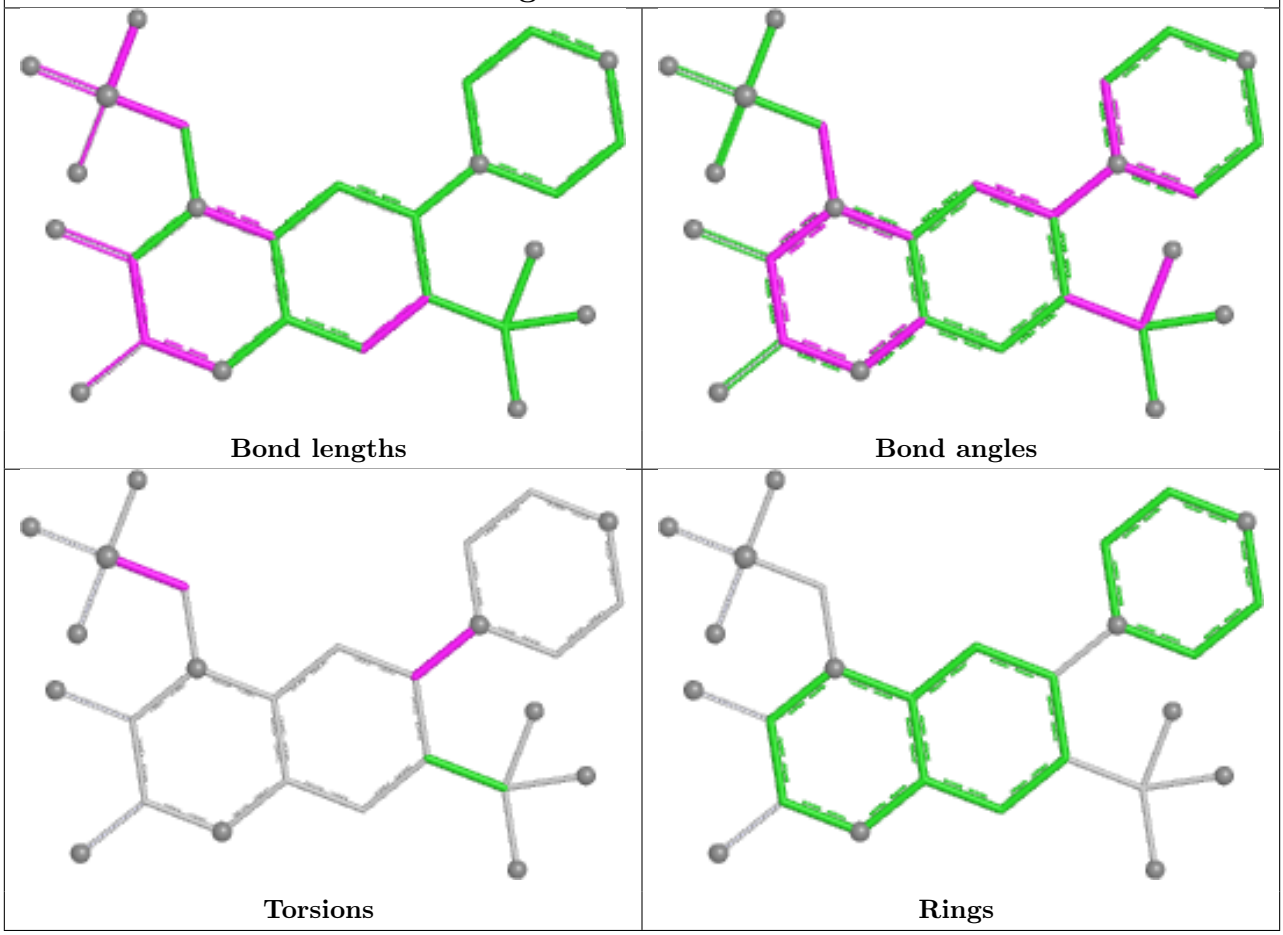
Ligand ZK1 B 1301

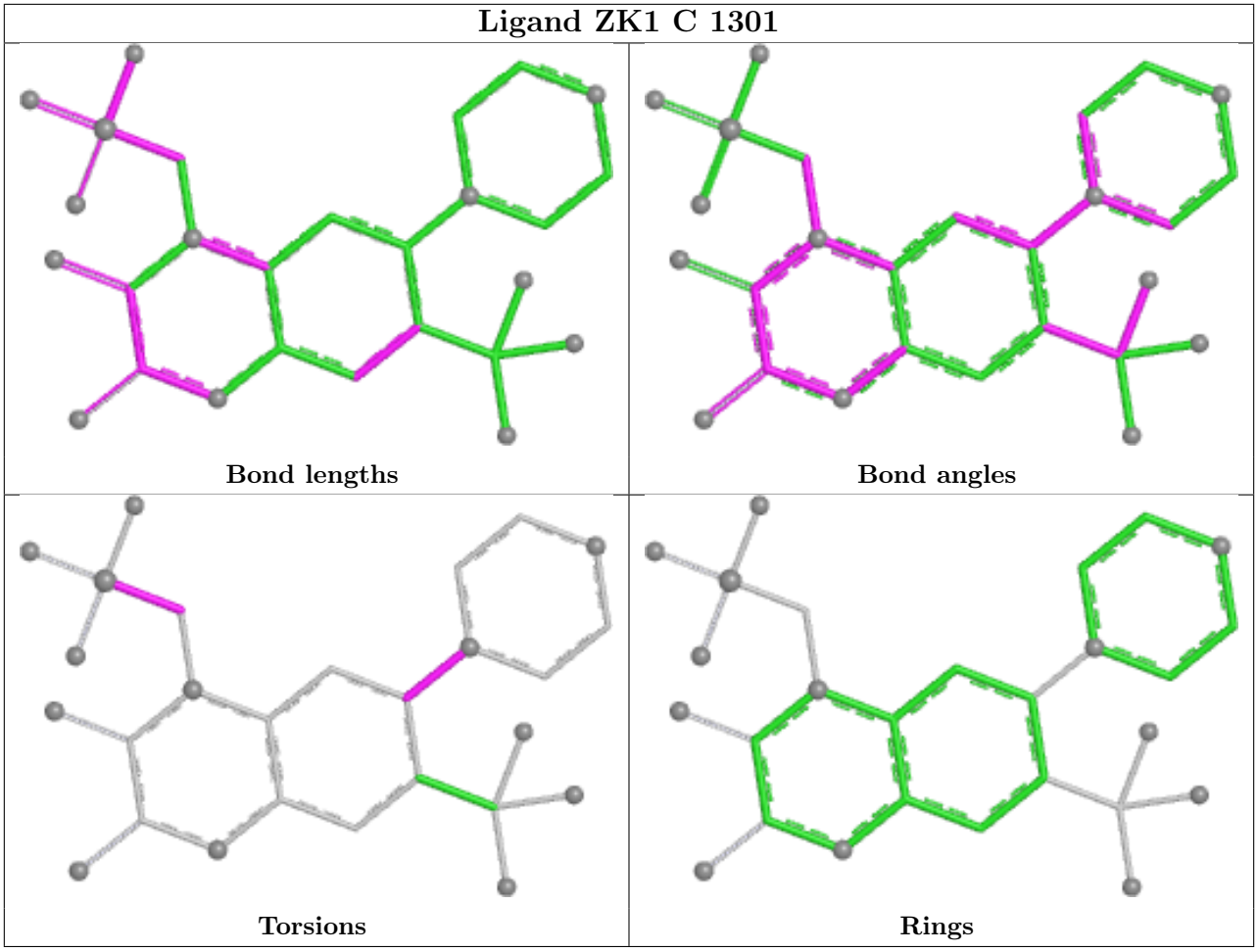


Ligand AJP A 1302



Ligand ZK1 A 1301





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.

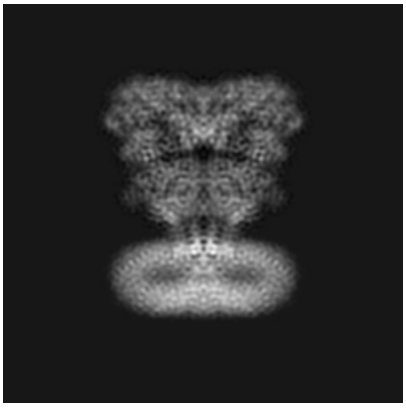
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8820. These allow visual inspection of the internal detail of the map and identification of artifacts.

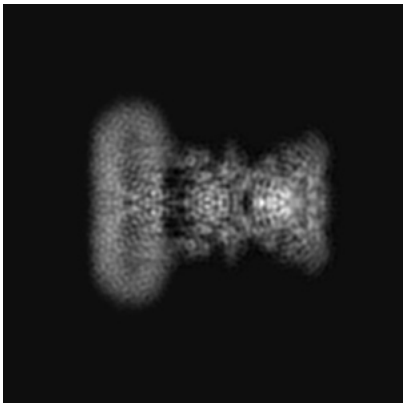
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

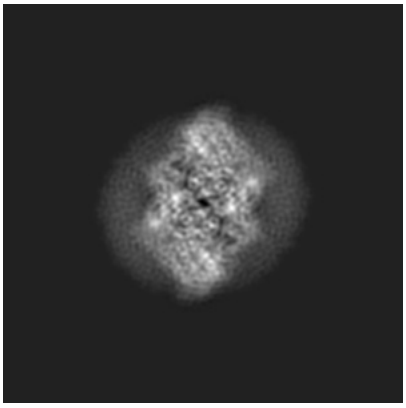
6.1.1 Primary map



X



Y

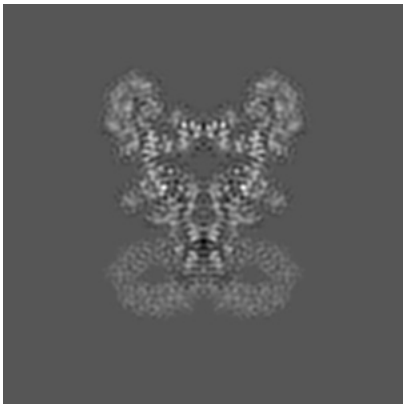


Z

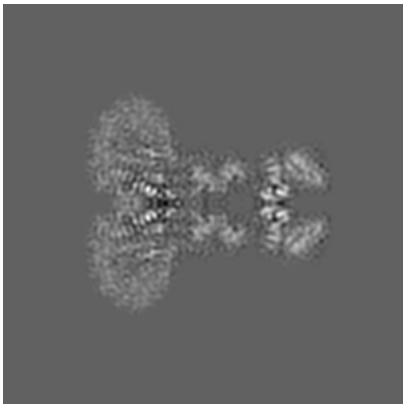
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

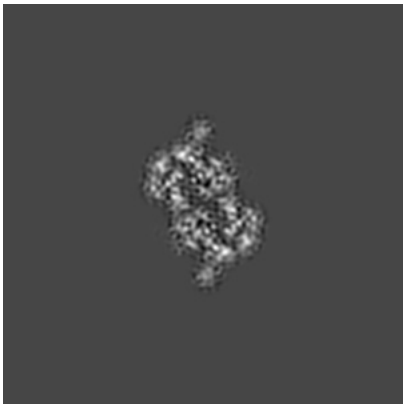
6.2.1 Primary map



X Index: 150



Y Index: 150

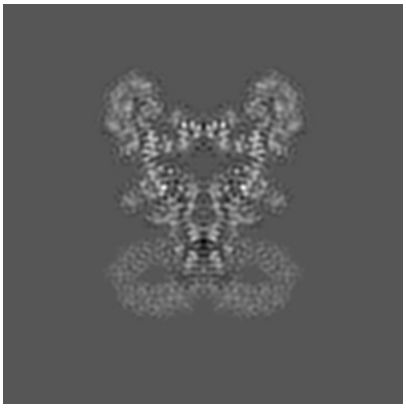


Z Index: 150

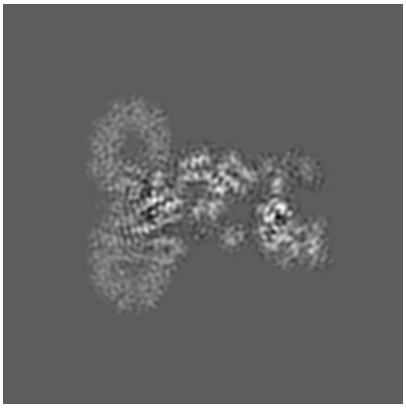
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

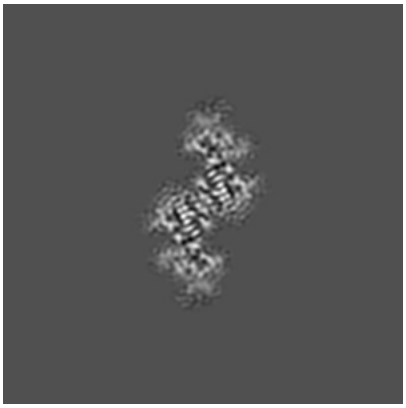
6.3.1 Primary map



X Index: 150



Y Index: 143

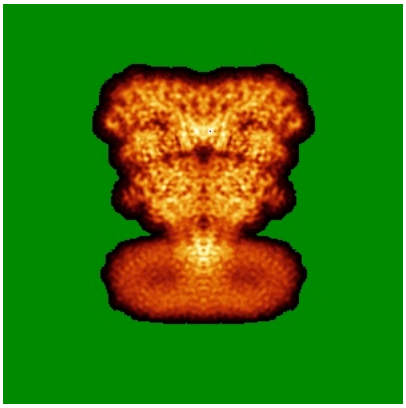


Z Index: 202

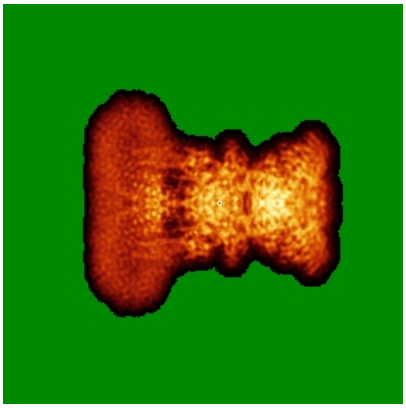
The images above show the largest variance slices of the map in three orthogonal directions.

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

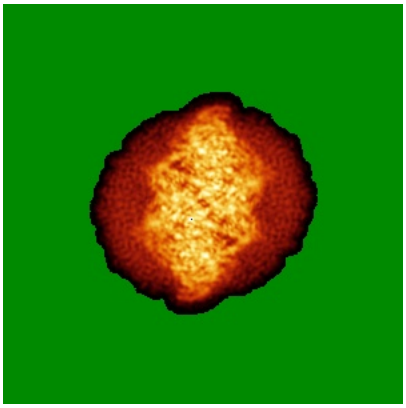
6.4.1 Primary map



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

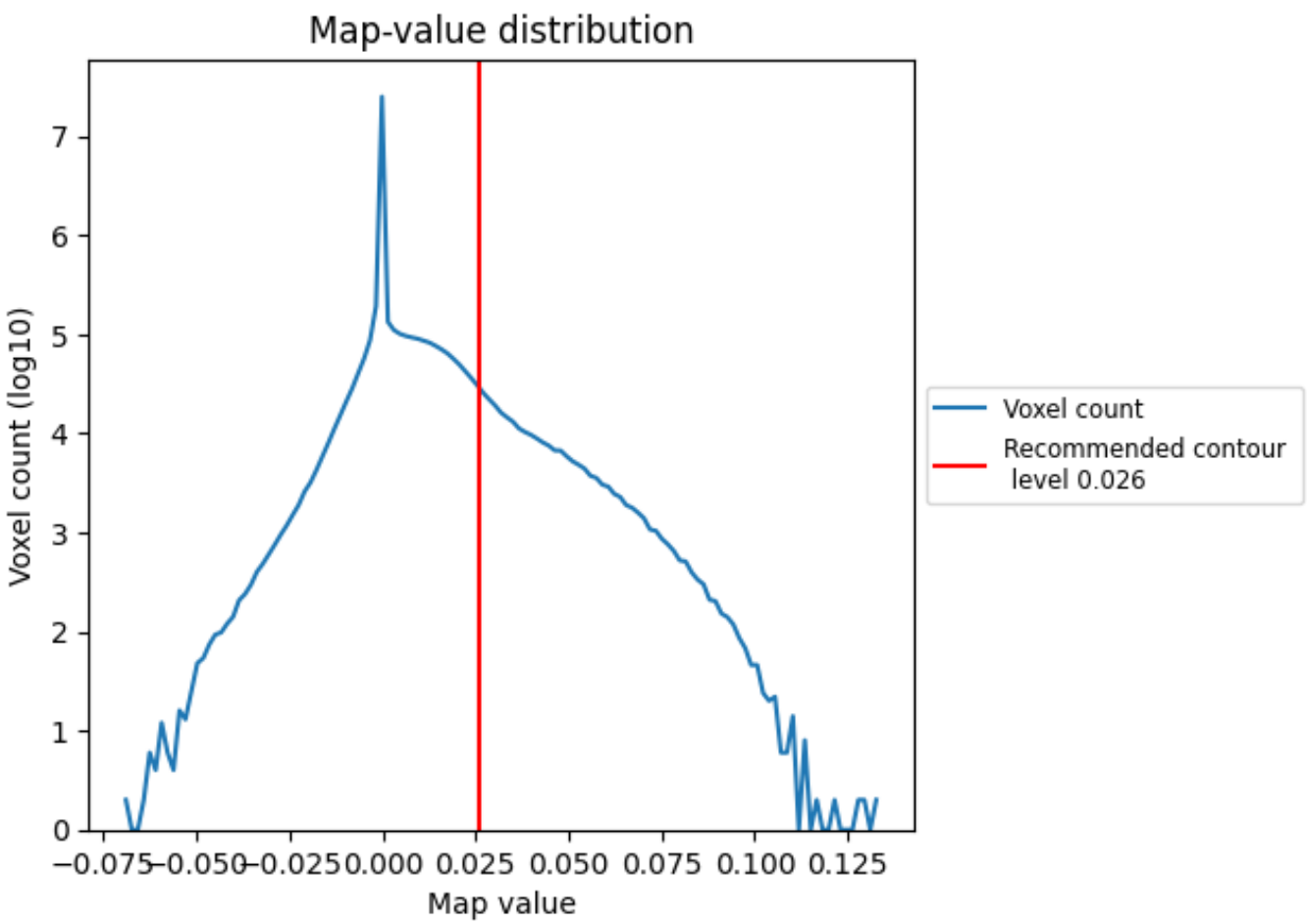
6.6 Mask visualisation (i)

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

7 Map analysis (i)

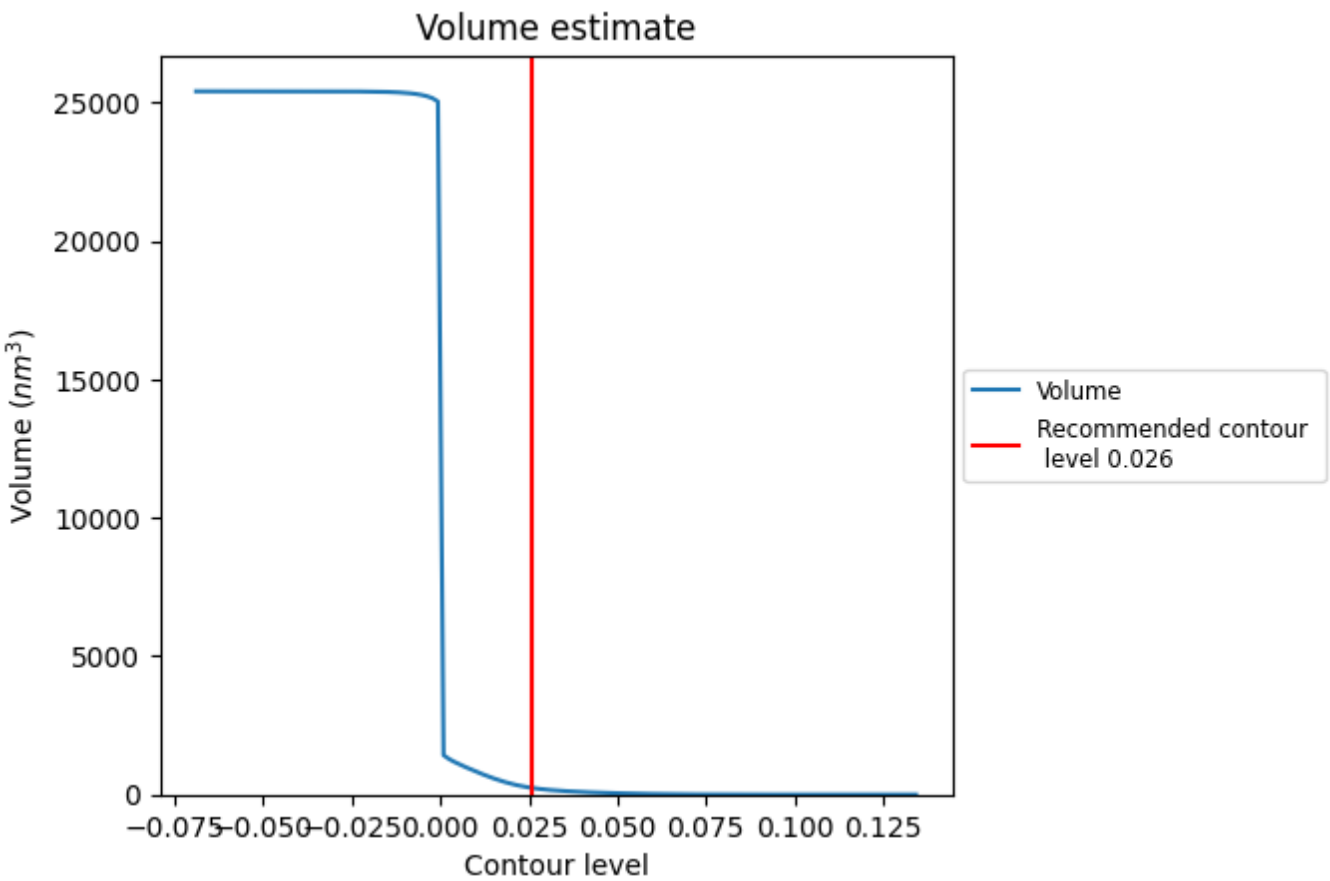
This section contains the results of statistical analysis of the map.

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.

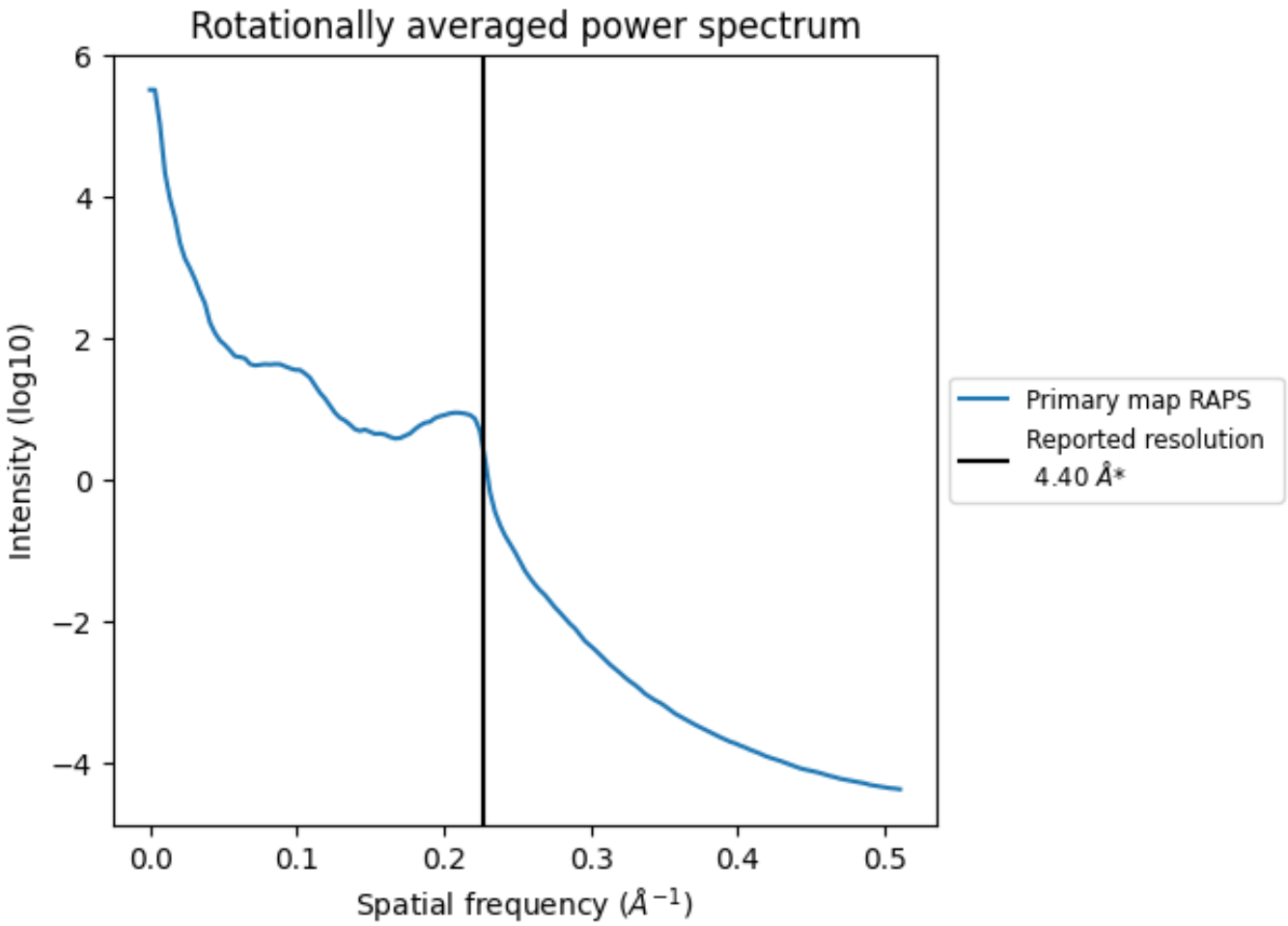
7.2 Volume estimate (i)



The volume at the recommended contour level is 238 nm^3; this corresponds to an approximate mass of 215 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 0.227 Å^{-1}

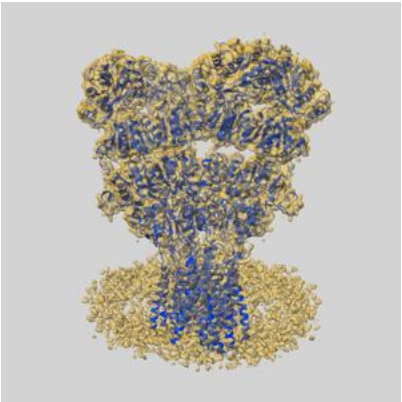
8 Fourier-Shell correlation (i)

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

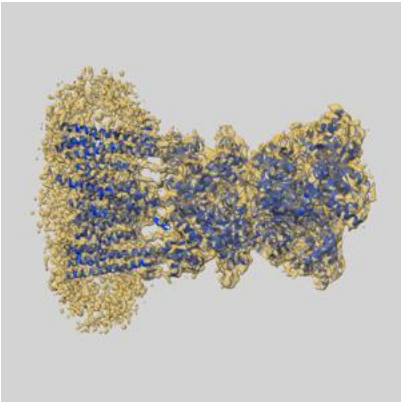
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8820 and PDB model 5WEL. Per-residue inclusion information can be found in section 3 on page 8.

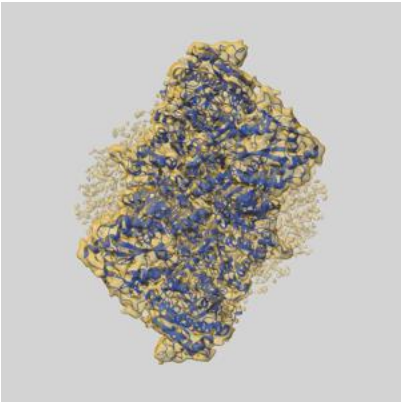
9.1 Map-model overlay (i)



X



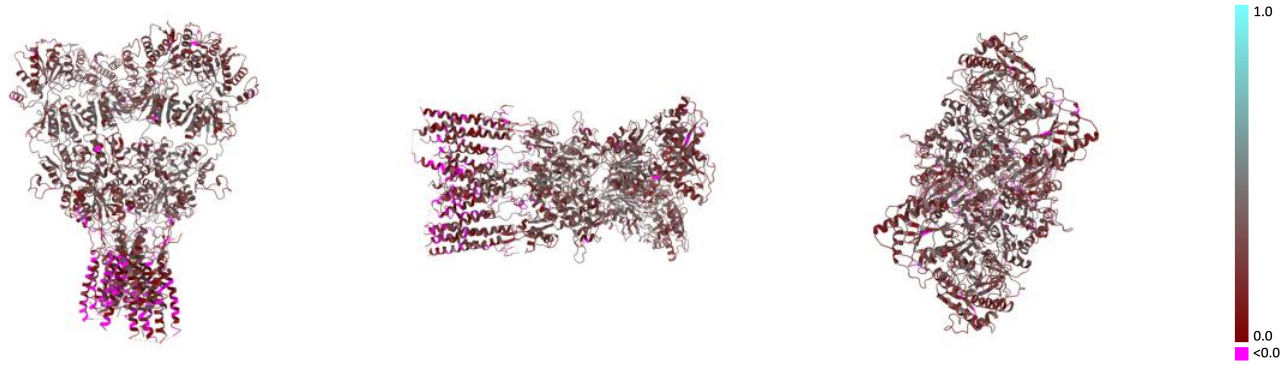
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

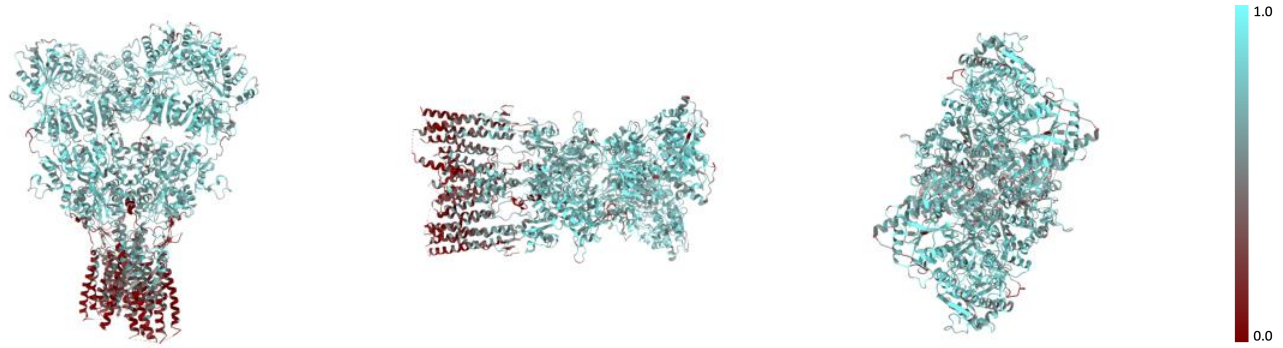
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

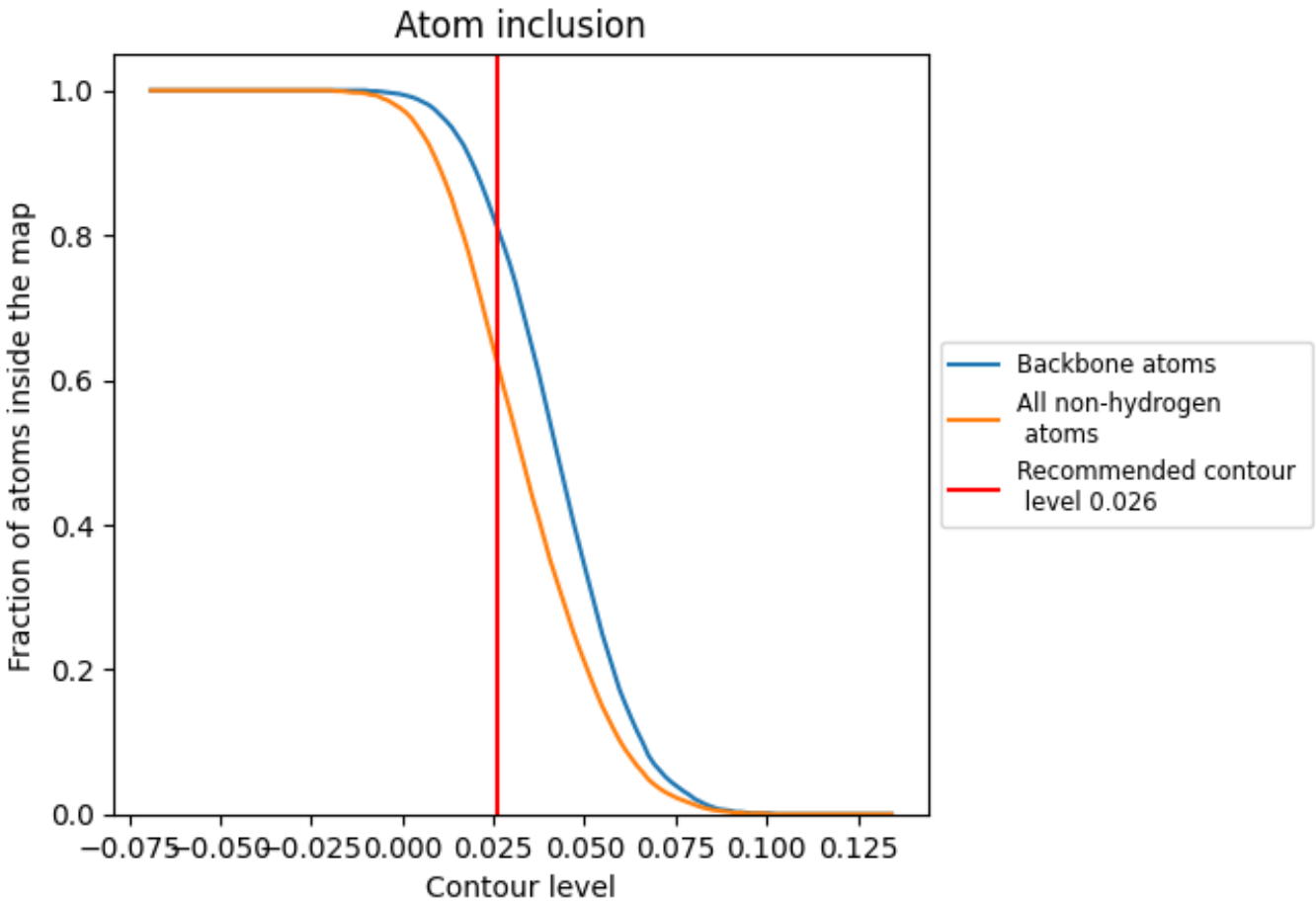
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.2540
A	0.5930	0.2370
B	0.6630	0.2740
C	0.6140	0.2600
D	0.6410	0.2470