



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:29 PM UTC

PDB ID : 7DD7 / pdb_00007dd7
EMDB ID : EMD-30647
Title : Structure of Calcium-Sensing Receptor in complex with Evocalcet
Authors : Wen, T.L.; Yang, X.; Shen, Y.Q.
Deposited on : 2020-10-27
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

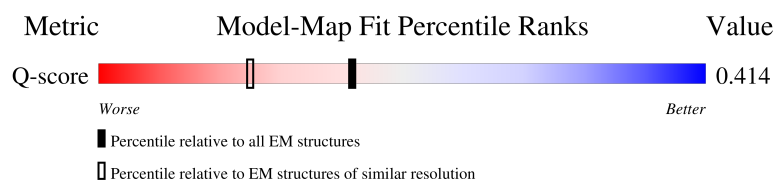
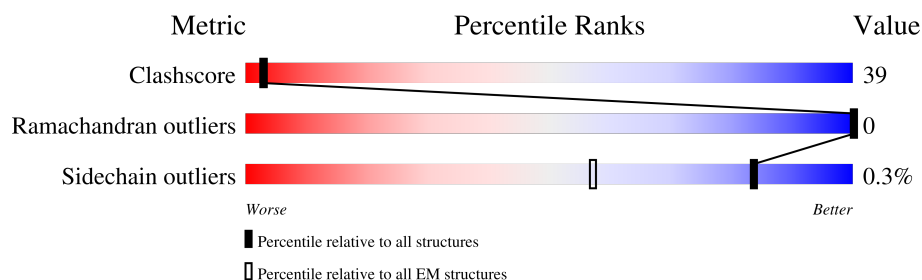
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

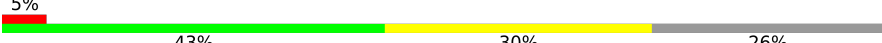
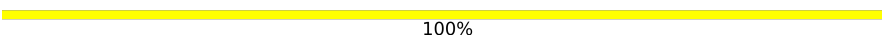
The reported resolution of this entry is 3.20 Å.

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	15020 (2.70 - 3.70)

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	1069	
1	B	1069	
2	C	2	
2	D	2	

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Mol	Chain	Length	Quality of chain
2	E	2	 50%50%
2	F	2	 100%

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
7	H43	A	1108	-	-	X	-
7	H43	B	1110	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12737 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 Calcium-Sensing Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	791	Total	C	N	O	S	0	0
			6212	4032	1004	1141	35		
1	B	792	Total	C	N	O	S	0	0
			6235	4048	1007	1145	35		

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Cl	0
			1	1	
3	B	1	Total	Cl	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

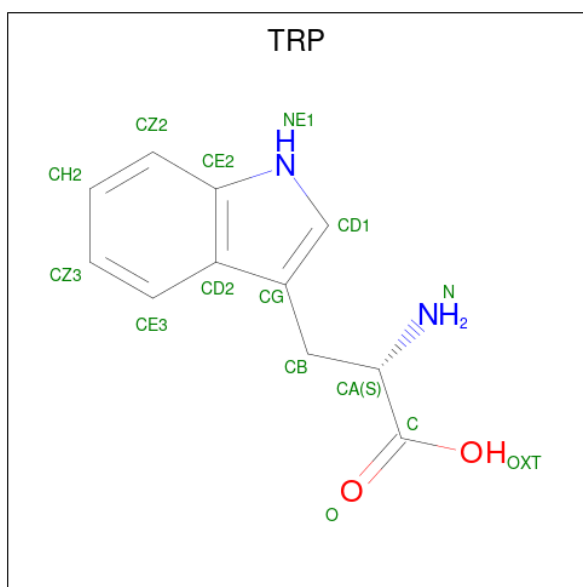
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	4	Total	Ca	0
			4	4	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



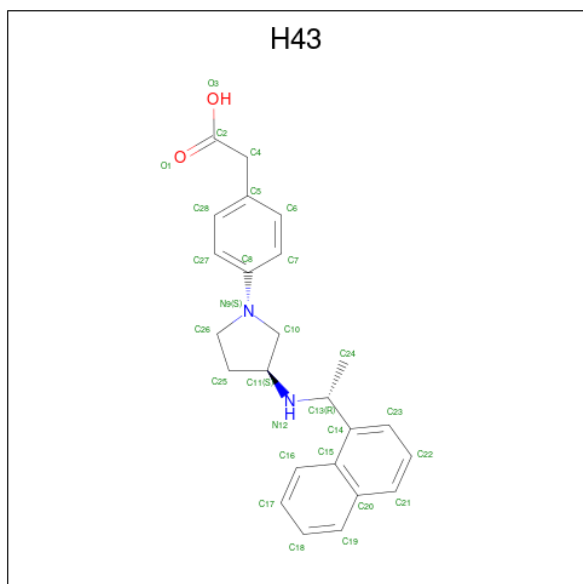
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	11	2	2	
6	B	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 7 is 2-[4-[(3S)-3-[[[(1R)-1-naphthalen-1-ylethyl]amino]pyrrolidin-1-yl]phenyl]ethanoic acid (CCD ID: H43) (formula: $C_{24}H_{26}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			28	24	2	2	

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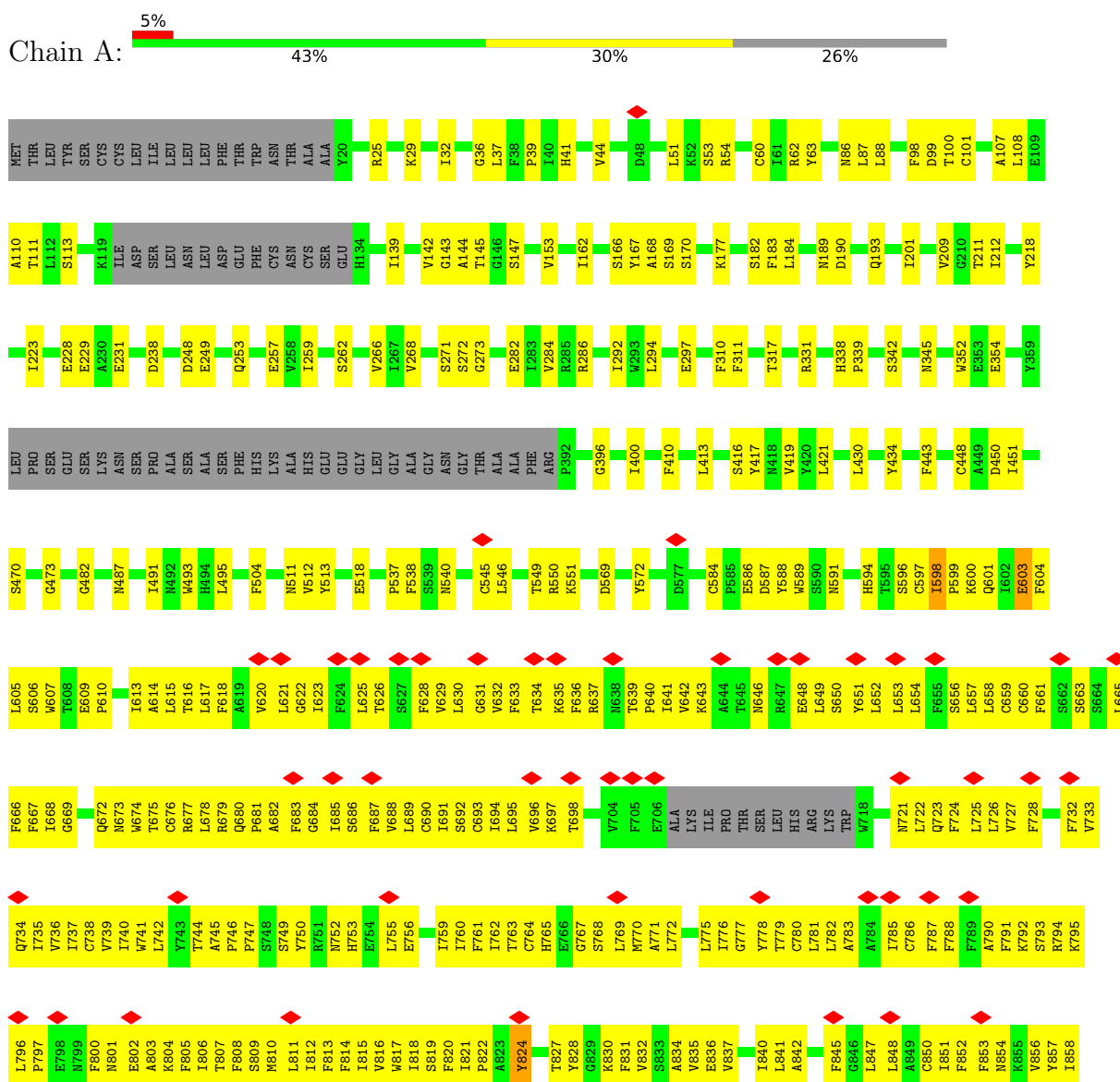
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	B	1	28	24	2	2	0

3 Residue-property plots

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

• Molecule 1: Calcium-Sensing Receptor



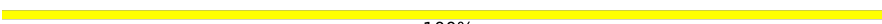
VAL
THR
GLU
ASN
THR
VAL
HIS
SER
GLU
SER
ALA
LEU
GLU
VAL
PHE
GLN

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	2.385	Depositor
Minimum map value	-1.457	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	304.2, 304.2, 304.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.014, 1.014, 1.014	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: NAG, CL, H43, CA

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	0.34	0/6371	0.51	4/8652 (0.0%)
1	B	0.34	2/6395 (0.0%)	0.48	2/8683 (0.0%)
All	All	0.34	2/12766 (0.0%)	0.50	6/17335 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	GLN	N-CA	5.59	1.53	1.46
1	B	601	GLN	CA-C	5.46	1.60	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	GLU	N-CA-C	8.73	122.61	109.25
1	A	598	ILE	CA-C-N	7.90	127.96	119.90
1	A	598	ILE	C-N-CA	7.90	127.96	119.90
1	A	598	ILE	N-CA-C	-7.09	102.43	109.02
1	B	601	GLN	N-CA-C	5.17	117.19	109.59
1	B	701	VAL	N-CA-C	-5.01	104.78	111.05

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	6212	0	6022	501	0
1	B	6235	0	6055	478	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
6	A	15	0	9	2	0
6	B	15	0	9	1	0
7	A	28	0	0	11	0
7	B	28	0	0	12	0
All	All	12737	0	12273	975	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 39.

All (975) 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:B:601:GLN:O	1:B:759:ILE:CG2	1.77	1.30
1:A:683:PHE:HE2	1:A:840:ILE:CG2	1.48	1.26
1:A:60:CYS:SG	1:A:101:CYS:CB	2.24	1.24
1:A:60:CYS:SG	1:A:101:CYS:HB3	1.76	1.24
1:B:601:GLN:O	1:B:759:ILE:HG23	1.33	1.22
1:B:601:GLN:C	1:B:759:ILE:HG23	1.66	1.21
1:A:776:ILE:HG23	7:A:1108:H43:C18	1.71	1.20
1:B:776:ILE:HG23	7:B:1110:H43:C18	1.71	1.19
1:A:545:CYS:SG	1:A:549:THR:HG21	1.87	1.13
1:A:683:PHE:CE2	1:A:840:ILE:CG2	2.34	1.11
1:B:734:GLN:HE21	1:B:775:LEU:HD12	1.05	1.10
1:A:683:PHE:HE2	1:A:840:ILE:HG22	1.07	1.08
1:A:677:ARG:HE	1:A:746:PRO:HB2	1.09	1.07
1:B:677:ARG:HE	1:B:746:PRO:HB2	1.09	1.07
1:B:430:LEU:O	1:B:433:ILE:HG22	1.51	1.07
1:B:809:SER:O	1:B:812:ILE:HG22	1.57	1.03
1:A:338:HIS:HD2	1:A:339:PRO:HD2	1.22	1.03
1:A:683:PHE:CE2	1:A:840:ILE:HG22	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:O	6:A:1107:TRP:HB2	1.59	1.01
1:B:601:GLN:O	1:B:759:ILE:HG22	1.57	1.00
1:B:588:TYR:CZ	1:B:599:PRO:HG3	1.98	0.99
1:B:734:GLN:NE2	1:B:775:LEU:HD12	1.78	0.99
1:B:541:CYS:HB3	1:B:561:CYS:HB3	1.42	0.99
1:B:615:LEU:HD21	1:B:837:VAL:HG21	1.42	0.99
1:B:683:PHE:HE2	1:B:840:ILE:HG22	1.24	0.98
1:A:615:LEU:HD21	1:A:837:VAL:HG21	1.42	0.98
1:B:430:LEU:O	1:B:433:ILE:CG2	2.13	0.97
1:A:630:LEU:O	1:A:637:ARG:NH2	1.98	0.96
1:B:634:THR:HA	1:B:637:ARG:HB2	1.48	0.96
1:A:797:PRO:HA	1:A:801:ASN:HB2	1.47	0.96
1:A:809:SER:O	1:A:812:ILE:HG12	1.65	0.96
1:B:630:LEU:O	1:B:637:ARG:NH2	1.98	0.95
1:B:659:CYS:HG	1:B:686:SER:HG	1.09	0.95
1:B:615:LEU:HD11	1:B:837:VAL:HG22	1.48	0.95
1:A:615:LEU:HD11	1:A:837:VAL:HG22	1.48	0.94
1:A:546:LEU:O	1:A:549:THR:HG22	1.66	0.94
1:A:634:THR:HA	1:A:637:ARG:HB2	1.48	0.94
1:B:797:PRO:HA	1:B:801:ASN:HB2	1.47	0.93
1:B:840:ILE:HG13	1:B:841:LEU:H	1.34	0.92
1:A:572:TYR:CD2	1:A:597:CYS:SG	2.62	0.92
1:A:572:TYR:HE2	1:A:584:CYS:HB3	1.33	0.92
1:A:417:TYR:CZ	1:A:421:LEU:HD11	2.05	0.92
1:B:601:GLN:HB3	1:B:759:ILE:CG1	2.00	0.91
1:A:603:GLU:HB3	1:A:761:PHE:HA	1.52	0.91
1:B:603:GLU:HB3	1:B:761:PHE:HA	1.52	0.91
1:B:800:PHE:HB2	1:B:802:GLU:OE2	1.70	0.91
1:A:659:CYS:HG	1:A:686:SER:HG	1.17	0.91
1:B:683:PHE:CD2	7:B:1110:H43:C23	2.54	0.91
1:A:734:GLN:HE21	1:A:775:LEU:HD12	1.33	0.91
1:A:818:ILE:O	1:A:821:ILE:HG22	1.71	0.91
1:A:800:PHE:HB2	1:A:802:GLU:OE2	1.71	0.90
1:B:601:GLN:HB3	1:B:759:ILE:HG23	1.50	0.90
1:B:807:THR:HA	1:B:810:MET:HE3	1.54	0.90
1:A:569:ASP:OD1	1:A:594:HIS:HE1	1.52	0.90
1:B:601:GLN:HB3	1:B:759:ILE:CG2	2.01	0.90
1:A:732:PHE:O	1:A:736:VAL:HG23	1.72	0.90
1:A:840:ILE:HG13	1:A:841:LEU:H	1.34	0.90
1:A:569:ASP:OD1	1:A:594:HIS:CE1	2.25	0.89
1:A:807:THR:HA	1:A:810:MET:HE3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:ARG:HD2	1:B:651:TYR:CE1	2.08	0.89
1:B:824:TYR:HE2	1:B:836:GLU:HG3	1.37	0.89
1:A:634:THR:OG1	1:A:637:ARG:NH2	2.06	0.89
1:B:634:THR:OG1	1:B:637:ARG:NH2	2.06	0.89
1:B:818:ILE:O	1:B:821:ILE:HG22	1.71	0.88
1:B:732:PHE:O	1:B:736:VAL:HG23	1.72	0.88
1:A:338:HIS:CD2	1:A:339:PRO:HD2	2.09	0.88
1:A:650:SER:O	1:A:654:LEU:HG	1.74	0.88
1:A:637:ARG:HD2	1:A:651:TYR:CE1	2.08	0.87
1:B:650:SER:O	1:B:654:LEU:HG	1.74	0.87
1:A:819:SER:HB3	1:B:819:SER:HB3	1.55	0.87
1:B:732:PHE:O	1:B:735:ILE:HG22	1.75	0.87
1:B:430:LEU:C	1:B:433:ILE:HG22	2.00	0.87
1:B:637:ARG:HD2	1:B:651:TYR:HE1	1.41	0.86
1:B:683:PHE:CE2	1:B:840:ILE:HG22	2.09	0.86
1:A:417:TYR:O	1:A:421:LEU:HD13	1.75	0.85
1:A:736:VAL:O	1:A:739:VAL:HG22	1.76	0.85
1:B:840:ILE:HG13	1:B:841:LEU:N	1.90	0.85
1:B:601:GLN:CB	1:B:759:ILE:HG23	2.05	0.85
1:A:732:PHE:O	1:A:735:ILE:HG22	1.75	0.85
1:A:618:PHE:O	1:A:621:LEU:HG	1.77	0.85
1:B:694:ILE:O	1:B:697:LYS:HB3	1.77	0.85
1:B:736:VAL:O	1:B:739:VAL:HG22	1.76	0.84
1:B:541:CYS:CB	1:B:561:CYS:HB3	2.07	0.84
1:B:683:PHE:CE2	1:B:840:ILE:CG2	2.60	0.84
1:B:618:PHE:O	1:B:621:LEU:HG	1.77	0.84
1:A:637:ARG:HD2	1:A:651:TYR:HE1	1.41	0.84
1:B:804:LYS:HE3	1:B:805:PHE:HE1	1.43	0.84
1:A:804:LYS:HE3	1:A:805:PHE:HE1	1.43	0.83
1:A:677:ARG:NE	1:A:746:PRO:HB2	1.91	0.83
1:A:840:ILE:HG13	1:A:841:LEU:N	1.90	0.83
1:B:812:ILE:O	1:B:816:VAL:HG23	1.78	0.83
1:A:60:CYS:HG	1:A:101:CYS:CB	1.83	0.83
1:B:589:TRP:O	1:B:597:CYS:HB3	1.77	0.83
1:B:606:SER:OG	1:B:609:GLU:HB2	1.78	0.83
1:B:677:ARG:NE	1:B:746:PRO:HB2	1.91	0.82
1:A:812:ILE:O	1:A:816:VAL:HG23	1.78	0.82
1:A:630:LEU:HD21	1:A:654:LEU:HB3	1.61	0.82
1:A:626:THR:HG22	1:A:848:LEU:CD2	2.09	0.82
1:A:753:HIS:HB3	1:A:760:ILE:HG12	1.59	0.82
1:B:753:HIS:HB3	1:B:760:ILE:HG12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:SER:OG	1:A:609:GLU:HB2	1.78	0.82
1:A:695:LEU:HD12	1:A:786:CYS:HB2	1.62	0.82
1:A:628:PHE:O	1:A:632:VAL:HG23	1.81	0.81
1:B:626:THR:HG22	1:B:848:LEU:CD2	2.09	0.81
1:A:657:LEU:HD23	1:A:848:LEU:HB2	1.63	0.81
1:B:630:LEU:HD21	1:B:654:LEU:HB3	1.61	0.81
1:B:695:LEU:HD12	1:B:786:CYS:HB2	1.62	0.81
1:A:694:ILE:O	1:A:697:LYS:HB3	1.81	0.81
1:B:628:PHE:O	1:B:632:VAL:HG23	1.81	0.80
1:A:733:VAL:O	1:A:736:VAL:HB	1.81	0.80
1:A:851:ILE:HG23	1:A:852:PHE:CD1	2.17	0.80
1:B:601:GLN:CA	1:B:759:ILE:HG23	2.10	0.80
1:A:750:TYR:HE2	1:A:765:HIS:HB2	1.47	0.79
1:A:790:ALA:O	1:A:803:ALA:HB1	1.83	0.79
1:B:633:PHE:HB3	1:B:637:ARG:HE	1.46	0.79
1:B:733:VAL:O	1:B:736:VAL:HB	1.81	0.79
1:A:633:PHE:HB3	1:A:637:ARG:HE	1.46	0.79
1:B:851:ILE:HG23	1:B:852:PHE:CD1	2.17	0.79
1:A:640:PRO:HA	1:A:643:LYS:CB	2.12	0.79
1:B:790:ALA:O	1:B:803:ALA:HB1	1.83	0.79
1:B:778:TYR:CE1	1:B:782:LEU:HD11	2.18	0.79
1:B:657:LEU:HD23	1:B:848:LEU:HB2	1.63	0.79
1:B:778:TYR:O	1:B:782:LEU:HG	1.83	0.79
1:A:545:CYS:SG	1:A:549:THR:CG2	2.69	0.79
1:A:778:TYR:CE1	1:A:782:LEU:HD11	2.18	0.78
1:B:640:PRO:HA	1:B:643:LYS:CB	2.13	0.78
1:A:653:LEU:HG	1:A:693:CYS:HB3	1.65	0.78
1:B:653:LEU:HG	1:B:693:CYS:HB3	1.65	0.78
1:A:572:TYR:CE2	1:A:597:CYS:SG	2.76	0.78
1:A:778:TYR:O	1:A:782:LEU:HG	1.83	0.78
1:A:734:GLN:HA	1:A:737:ILE:CD1	2.14	0.78
1:B:734:GLN:HA	1:B:737:ILE:CD1	2.14	0.78
1:A:572:TYR:CE2	1:A:584:CYS:HB3	2.17	0.77
1:B:750:TYR:HE2	1:B:765:HIS:HB2	1.47	0.77
1:B:683:PHE:HE2	1:B:840:ILE:CG2	1.95	0.77
1:B:814:PHE:O	1:B:818:ILE:HG13	1.85	0.76
1:A:609:GLU:OE2	1:A:830:LYS:NZ	2.15	0.76
1:B:609:GLU:OE2	1:B:830:LYS:NZ	2.15	0.76
1:A:814:PHE:O	1:A:818:ILE:HG13	1.85	0.76
1:A:659:CYS:SG	1:A:686:SER:OG	2.42	0.76
1:A:622:GLY:O	1:A:626:THR:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:GLN:HB3	1:B:759:ILE:HG12	1.66	0.75
1:A:683:PHE:CE2	1:A:840:ILE:HB	2.21	0.75
1:A:193:GLN:HE22	1:A:297:GLU:HB2	1.49	0.75
1:A:646:ASN:OD1	1:A:649:LEU:N	2.15	0.75
1:A:60:CYS:SG	1:A:101:CYS:HB2	2.24	0.75
1:B:622:GLY:O	1:B:626:THR:HG23	1.86	0.75
1:B:836:GLU:OE2	7:B:1110:H43:C24	2.35	0.75
1:B:213:ALA:HB2	1:B:223:ILE:HG13	1.68	0.74
1:A:733:VAL:HG11	1:A:778:TYR:CE2	2.22	0.74
1:B:601:GLN:HB3	1:B:759:ILE:CD1	2.17	0.74
1:A:776:ILE:HG23	7:A:1108:H43:C17	2.17	0.74
1:B:733:VAL:HG11	1:B:778:TYR:CE2	2.22	0.74
1:A:661:PHE:HZ	1:A:845:PHE:HA	1.52	0.74
1:A:688:VAL:HG12	1:A:779:THR:HG23	1.70	0.73
1:B:776:ILE:HG23	7:B:1110:H43:C17	2.17	0.73
1:B:741:TRP:NE1	1:B:768:SER:OG	2.21	0.73
1:A:683:PHE:HE2	1:A:840:ILE:CB	2.01	0.73
1:B:734:GLN:HA	1:B:737:ILE:HD13	1.71	0.73
1:A:32:ILE:HG23	1:A:139:ILE:HD13	1.68	0.73
1:B:601:GLN:HB3	1:B:759:ILE:HD13	1.70	0.73
1:A:683:PHE:CE2	1:A:840:ILE:CB	2.72	0.73
1:B:661:PHE:HZ	1:B:845:PHE:HA	1.52	0.73
1:A:815:ILE:HG13	1:A:816:VAL:N	2.04	0.73
1:B:722:LEU:HD12	1:B:723:GLN:N	2.04	0.72
1:B:750:TYR:CE2	1:B:765:HIS:HB2	2.24	0.72
1:A:741:TRP:NE1	1:A:768:SER:OG	2.21	0.72
1:A:750:TYR:CE2	1:A:765:HIS:HB2	2.24	0.72
1:B:688:VAL:HG12	1:B:779:THR:HG23	1.70	0.72
1:B:614:ALA:O	1:B:617:LEU:HG	1.90	0.72
1:B:815:ILE:HG13	1:B:816:VAL:N	2.04	0.72
1:B:417:TYR:CE2	1:B:421:LEU:HD11	2.24	0.72
1:B:637:ARG:HG2	1:B:637:ARG:HH11	1.55	0.72
1:A:683:PHE:HE1	1:A:687:PHE:HB2	1.55	0.71
1:A:734:GLN:HA	1:A:737:ILE:HD13	1.71	0.71
1:B:417:TYR:O	1:B:421:LEU:HD13	1.89	0.71
1:A:809:SER:O	1:A:812:ILE:CG1	2.38	0.71
1:A:614:ALA:O	1:A:617:LEU:HG	1.90	0.71
1:A:697:LYS:HZ3	1:A:851:ILE:HD11	1.55	0.71
1:A:791:PHE:O	1:A:794:ARG:N	2.19	0.71
1:B:674:TRP:O	1:B:678:LEU:HD13	1.91	0.71
1:A:44:VAL:HA	1:A:60:CYS:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HB3	1:A:416:SER:OG	1.91	0.71
1:B:604:PHE:CG	1:B:762:ILE:HD11	2.26	0.71
1:A:722:LEU:HD12	1:A:723:GLN:N	2.04	0.71
1:A:801:ASN:O	1:A:804:LYS:HG2	1.90	0.71
1:B:801:ASN:O	1:B:804:LYS:HG2	1.90	0.71
1:A:637:ARG:HG2	1:A:637:ARG:HH11	1.55	0.71
1:A:513:TYR:HE2	2:C:1:NAG:HN2	1.38	0.70
1:A:683:PHE:CE2	1:A:840:ILE:HG21	2.23	0.70
1:A:656:SER:CB	1:A:689:LEU:HD22	2.22	0.70
1:B:755:LEU:HD23	1:B:755:LEU:H	1.57	0.70
1:B:772:LEU:O	1:B:776:ILE:HG12	1.92	0.70
1:A:604:PHE:CG	1:A:762:ILE:HD11	2.26	0.70
1:A:615:LEU:HD11	1:A:837:VAL:CG2	2.21	0.70
1:A:189:ASN:OD1	1:A:190:ASP:N	2.25	0.69
1:A:674:TRP:O	1:A:678:LEU:HD13	1.91	0.69
1:B:656:SER:CB	1:B:689:LEU:HD22	2.22	0.69
1:B:791:PHE:O	1:B:794:ARG:N	2.19	0.69
1:B:860:LEU:HD12	1:B:861:PHE:HB2	1.74	0.69
1:A:656:SER:HB3	1:A:689:LEU:HD22	1.74	0.69
1:B:603:GLU:HG2	1:B:761:PHE:CD1	2.27	0.69
1:B:656:SER:HB3	1:B:689:LEU:HD22	1.74	0.69
1:A:603:GLU:HG2	1:A:761:PHE:CD1	2.27	0.69
1:B:646:ASN:OD1	1:B:649:LEU:N	2.15	0.69
1:B:733:VAL:O	1:B:737:ILE:HD12	1.93	0.69
1:A:184:LEU:CD2	1:A:482:GLY:HA2	2.22	0.69
1:A:691:ILE:HD11	1:A:783:ALA:HA	1.75	0.69
1:A:733:VAL:O	1:A:737:ILE:HD12	1.93	0.69
1:A:860:LEU:HD12	1:A:861:PHE:HB2	1.74	0.69
1:A:691:ILE:HD11	1:A:783:ALA:CA	2.23	0.69
1:A:253:GLN:NE2	1:A:282:GLU:OE2	2.26	0.69
1:A:253:GLN:OE1	1:A:286:ARG:NH1	2.26	0.69
1:A:755:LEU:H	1:A:755:LEU:HD23	1.57	0.69
1:B:601:GLN:C	1:B:759:ILE:CG2	2.46	0.69
1:A:653:LEU:HD22	1:A:694:ILE:HG13	1.75	0.68
1:A:190:ASP:OD1	1:A:190:ASP:O	2.12	0.68
1:A:417:TYR:CE1	1:A:421:LEU:HD11	2.28	0.68
1:A:772:LEU:O	1:A:776:ILE:HG12	1.92	0.68
1:B:768:SER:OG	1:B:771:ALA:HB3	1.94	0.68
1:B:511:ASN:ND2	2:E:1:NAG:O5	2.26	0.68
1:B:615:LEU:HD11	1:B:837:VAL:CG2	2.21	0.67
1:B:691:ILE:HD11	1:B:783:ALA:CA	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ARG:CG	1:A:747:PRO:HG2	2.24	0.67
1:B:811:LEU:O	1:B:815:ILE:HG23	1.95	0.67
1:B:653:LEU:HD22	1:B:694:ILE:HG13	1.75	0.67
1:A:677:ARG:HG2	1:A:747:PRO:HG2	1.77	0.67
1:B:691:ILE:HD11	1:B:783:ALA:HA	1.75	0.67
1:A:604:PHE:CB	1:A:762:ILE:HD11	2.25	0.67
1:A:806:ILE:O	1:A:809:SER:OG	2.12	0.67
1:B:677:ARG:CG	1:B:747:PRO:HG2	2.24	0.67
1:B:806:ILE:O	1:B:809:SER:OG	2.12	0.67
1:A:342:SER:HB2	1:A:345:ASN:HB3	1.77	0.67
1:A:768:SER:OG	1:A:771:ALA:HB3	1.94	0.67
1:B:541:CYS:SG	1:B:561:CYS:HB3	2.35	0.67
1:B:633:PHE:CB	1:B:637:ARG:HE	2.08	0.67
1:A:811:LEU:O	1:A:815:ILE:HG23	1.95	0.66
1:B:604:PHE:CB	1:B:762:ILE:HD11	2.25	0.66
1:B:667:PHE:H	1:B:668:ILE:HD12	1.60	0.66
1:A:633:PHE:CB	1:A:637:ARG:HE	2.08	0.66
1:A:667:PHE:H	1:A:668:ILE:HD12	1.60	0.66
1:B:677:ARG:HG2	1:B:747:PRO:HG2	1.77	0.66
1:A:620:VAL:O	1:A:623:ILE:HG22	1.96	0.66
1:A:653:LEU:CD2	1:A:693:CYS:HB2	2.26	0.66
1:A:815:ILE:HA	1:A:818:ILE:HD12	1.78	0.66
1:B:341:LYS:O	1:B:341:LYS:HG2	1.96	0.66
1:A:677:ARG:HD2	1:A:747:PRO:O	1.96	0.66
1:B:653:LEU:CD2	1:B:693:CYS:HB2	2.26	0.66
1:B:815:ILE:HA	1:B:818:ILE:HD12	1.78	0.66
1:A:604:PHE:HB3	1:A:762:ILE:HD11	1.78	0.65
1:A:683:PHE:CG	7:A:1108:H43:C22	2.79	0.65
1:A:809:SER:HB3	1:A:850:CYS:SG	2.36	0.65
1:A:683:PHE:CD2	7:A:1108:H43:C23	2.80	0.65
1:B:604:PHE:HB3	1:B:762:ILE:HD11	1.78	0.65
1:B:620:VAL:O	1:B:623:ILE:HG22	1.96	0.65
1:B:777:GLY:HA2	1:B:780:CYS:SG	2.37	0.65
1:B:588:TYR:CE1	1:B:599:PRO:HG3	2.32	0.65
1:B:809:SER:HB3	1:B:850:CYS:SG	2.36	0.65
1:A:793:SER:O	1:A:796:LEU:HD13	1.97	0.65
1:B:147:SER:OG	6:B:1109:TRP:O	2.15	0.65
1:B:677:ARG:HD2	1:B:747:PRO:O	1.96	0.65
1:A:653:LEU:CD2	1:A:694:ILE:HG13	2.27	0.64
1:A:787:PHE:HA	1:A:810:MET:CE	2.27	0.64
1:B:727:VAL:HG23	1:B:728:PHE:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:LEU:HG	1:B:693:CYS:CB	2.27	0.64
1:B:793:SER:O	1:B:796:LEU:HD13	1.97	0.64
1:B:804:LYS:HE3	1:B:805:PHE:CE1	2.29	0.64
1:A:777:GLY:HA2	1:A:780:CYS:SG	2.37	0.64
1:A:170:SER:HG	6:A:1107:TRP:N	1.96	0.64
1:A:734:GLN:HE21	1:A:775:LEU:CD1	2.08	0.64
1:B:836:GLU:OE2	7:B:1110:H43:C25	2.45	0.64
1:A:727:VAL:HG23	1:A:728:PHE:CD1	2.32	0.64
1:B:787:PHE:HA	1:B:810:MET:CE	2.27	0.64
1:B:193:GLN:HE22	1:B:297:GLU:HB2	1.62	0.64
1:A:190:ASP:OD1	1:A:193:GLN:HB3	1.98	0.64
1:A:653:LEU:HG	1:A:693:CYS:CB	2.27	0.64
1:B:602:ILE:HD11	1:B:762:ILE:HG23	1.79	0.64
1:B:604:PHE:HB3	1:B:762:ILE:CG1	2.28	0.64
1:B:653:LEU:CD2	1:B:694:ILE:HG13	2.27	0.64
1:A:44:VAL:HG12	1:A:60:CYS:SG	2.38	0.64
1:A:591:ASN:ND2	1:A:596:SER:O	2.31	0.63
1:A:653:LEU:HD11	1:A:694:ILE:HA	1.79	0.63
1:B:724:PHE:O	1:B:727:VAL:HG22	1.98	0.63
1:A:617:LEU:HA	1:A:620:VAL:HG12	1.80	0.63
1:B:617:LEU:HA	1:B:620:VAL:HG12	1.80	0.63
1:B:653:LEU:HD11	1:B:694:ILE:HA	1.79	0.63
1:A:724:PHE:O	1:A:727:VAL:HG22	1.98	0.63
1:A:637:ARG:HG2	1:A:637:ARG:NH1	2.13	0.63
1:B:654:LEU:HD21	1:B:852:PHE:HZ	1.63	0.63
1:A:626:THR:HG22	1:A:848:LEU:HD22	1.81	0.63
1:A:653:LEU:HD21	1:A:694:ILE:H	1.63	0.63
1:A:654:LEU:HD21	1:A:852:PHE:HZ	1.63	0.63
1:B:634:THR:CA	1:B:637:ARG:HB2	2.27	0.63
1:A:588:TYR:CD1	1:A:599:PRO:HA	2.34	0.63
1:A:604:PHE:HB3	1:A:762:ILE:CG1	2.28	0.63
1:B:777:GLY:O	1:B:781:LEU:HD23	1.99	0.63
1:A:804:LYS:HE3	1:A:805:PHE:CE1	2.29	0.62
1:B:653:LEU:HD21	1:B:694:ILE:H	1.63	0.62
1:A:824:TYR:HE2	1:A:836:GLU:HG3	1.64	0.62
1:B:209:VAL:HG12	1:B:266:VAL:HB	1.82	0.62
1:B:683:PHE:CE1	1:B:687:PHE:HB2	2.34	0.62
1:A:618:PHE:HA	1:A:621:LEU:CD2	2.30	0.62
1:B:626:THR:HG22	1:B:848:LEU:HD22	1.81	0.62
1:B:854:ASN:O	1:B:858:ILE:HG23	1.99	0.62
1:B:683:PHE:HE1	1:B:687:PHE:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:LEU:O	1:B:785:ILE:HG12	2.00	0.62
1:A:777:GLY:O	1:A:781:LEU:HD23	1.99	0.62
1:A:417:TYR:CE2	1:A:421:LEU:HD11	2.34	0.61
1:A:782:LEU:O	1:A:785:ILE:HG12	2.00	0.61
1:A:854:ASN:O	1:A:858:ILE:HG23	1.99	0.61
1:B:434:TYR:HB2	1:B:451:ILE:HD12	1.82	0.61
1:A:591:ASN:HB3	1:A:598:ILE:HG13	1.80	0.61
1:B:802:GLU:O	1:B:806:ILE:HG12	2.00	0.61
1:A:812:ILE:HA	1:A:815:ILE:HG12	1.82	0.61
1:B:618:PHE:HA	1:B:621:LEU:CD2	2.30	0.61
1:A:852:PHE:O	1:A:856:VAL:HG22	2.01	0.61
1:A:802:GLU:O	1:A:806:ILE:HG12	2.00	0.61
1:A:807:THR:HA	1:A:810:MET:CE	2.29	0.61
1:A:821:ILE:N	1:A:822:PRO:HD2	2.16	0.61
1:A:821:ILE:HG23	1:A:822:PRO:HD3	1.83	0.61
1:B:852:PHE:O	1:B:856:VAL:HG22	2.01	0.61
1:B:856:VAL:O	1:B:860:LEU:HG	2.00	0.61
1:B:648:GLU:OE1	1:B:648:GLU:HA	2.01	0.61
1:B:189:ASN:OD1	1:B:190:ASP:N	2.30	0.61
1:B:821:ILE:N	1:B:822:PRO:HD2	2.16	0.61
1:A:741:TRP:CH2	1:A:772:LEU:HG	2.36	0.60
1:A:88:LEU:HD21	1:A:430:LEU:HB3	1.83	0.60
1:B:776:ILE:HD12	7:B:1110:H43:C17	2.32	0.60
1:B:206:TRP:CD1	1:B:539:SER:HG	2.19	0.60
1:B:679:ARG:O	1:B:682:ALA:HB3	2.02	0.60
1:B:733:VAL:HG12	1:B:734:GLN:OE1	2.01	0.60
1:B:812:ILE:HA	1:B:815:ILE:HG12	1.82	0.60
1:A:776:ILE:HD12	7:A:1108:H43:C17	2.32	0.60
1:B:741:TRP:CH2	1:B:772:LEU:HG	2.36	0.60
1:A:733:VAL:HG12	1:A:734:GLN:OE1	2.01	0.60
1:A:856:VAL:O	1:A:860:LEU:HG	2.00	0.60
1:A:648:GLU:OE1	1:A:648:GLU:HA	2.01	0.60
1:B:797:PRO:HA	1:B:801:ASN:CB	2.28	0.60
1:A:776:ILE:CG2	7:A:1108:H43:C18	2.65	0.60
1:B:809:SER:O	1:B:812:ILE:CG2	2.43	0.60
1:B:832:VAL:O	1:B:835:VAL:HG12	2.01	0.60
1:A:832:VAL:O	1:A:835:VAL:HG12	2.02	0.60
1:B:588:TYR:CD1	1:B:599:PRO:HA	2.37	0.60
1:B:794:ARG:C	1:B:795:LYS:HD3	2.27	0.60
1:A:797:PRO:HA	1:A:801:ASN:CB	2.28	0.59
1:B:601:GLN:CB	1:B:759:ILE:HG12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ILE:HG13	1:B:642:VAL:H	1.67	0.59
1:B:653:LEU:HD21	1:B:694:ILE:N	2.17	0.59
1:B:776:ILE:CG2	7:B:1110:H43:C18	2.65	0.59
1:A:653:LEU:HD21	1:A:694:ILE:N	2.17	0.59
1:A:858:ILE:HG13	1:A:859:ILE:N	2.18	0.59
1:B:626:THR:O	1:B:630:LEU:HD23	2.02	0.59
1:A:626:THR:HG22	1:A:848:LEU:HD21	1.84	0.59
1:B:807:THR:HA	1:B:810:MET:CE	2.29	0.59
1:A:641:ILE:HG13	1:A:642:VAL:N	2.16	0.59
1:B:626:THR:HG22	1:B:848:LEU:HD21	1.85	0.59
1:A:518:GLU:O	1:A:518:GLU:HG2	2.03	0.59
1:A:794:ARG:C	1:A:795:LYS:HD3	2.27	0.59
1:B:821:ILE:HG23	1:B:822:PRO:HD3	1.83	0.59
1:A:626:THR:O	1:A:630:LEU:HD23	2.02	0.59
1:A:679:ARG:O	1:A:682:ALA:HB3	2.01	0.59
1:A:836:GLU:OE2	7:A:1108:H43:C25	2.51	0.59
1:A:257:GLU:OE1	1:A:286:ARG:NH2	2.35	0.59
1:A:697:LYS:NZ	1:A:851:ILE:HD11	2.17	0.59
1:A:756:GLU:HA	1:A:756:GLU:OE1	2.03	0.59
1:B:637:ARG:HG2	1:B:637:ARG:NH1	2.13	0.59
1:A:588:TYR:CA	1:A:600:LYS:HG3	2.33	0.59
1:B:688:VAL:O	1:B:691:ILE:HG22	2.03	0.59
1:B:756:GLU:OE1	1:B:756:GLU:HA	2.03	0.59
1:A:491:ILE:HD12	1:A:504:PHE:HB3	1.84	0.58
1:A:688:VAL:O	1:A:691:ILE:HG22	2.03	0.58
1:A:802:GLU:HA	1:A:802:GLU:OE1	2.03	0.58
1:B:802:GLU:OE1	1:B:802:GLU:HA	2.03	0.58
1:B:769:LEU:HG	1:B:770:MET:H	1.68	0.58
1:A:641:ILE:HG13	1:A:642:VAL:H	1.67	0.58
1:A:734:GLN:NE2	1:A:775:LEU:HA	2.18	0.58
1:B:769:LEU:H	1:B:769:LEU:HD23	1.68	0.58
1:A:665:LEU:HD22	1:A:666:PHE:CE1	2.38	0.58
1:B:665:LEU:HD22	1:B:666:PHE:CE1	2.38	0.58
1:B:734:GLN:NE2	1:B:775:LEU:HA	2.18	0.58
1:B:858:ILE:HG13	1:B:859:ILE:N	2.18	0.58
1:A:769:LEU:HD23	1:A:769:LEU:H	1.68	0.58
1:A:769:LEU:HG	1:A:770:MET:H	1.68	0.58
1:B:39:PRO:HG3	1:B:145:THR:HG21	1.85	0.58
1:B:430:LEU:HA	1:B:433:ILE:HG22	1.86	0.58
1:A:693:CYS:O	1:A:696:VAL:HG12	2.04	0.58
1:B:641:ILE:HG13	1:B:642:VAL:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:CG1	1:A:60:CYS:SG	2.91	0.58
1:A:819:SER:CB	1:B:819:SER:HB3	2.30	0.58
1:B:738:CYS:SG	1:B:739:VAL:N	2.77	0.58
1:A:248:ASP:CG	1:A:249:GLU:H	2.12	0.58
1:B:661:PHE:HZ	1:B:845:PHE:CA	2.17	0.58
1:A:634:THR:CA	1:A:637:ARG:HB2	2.27	0.58
1:B:601:GLN:CB	1:B:759:ILE:HD13	2.32	0.58
1:A:684:GLY:O	1:A:688:VAL:HG13	2.04	0.57
1:B:528:LEU:O	1:B:528:LEU:HD12	2.04	0.57
1:B:684:GLY:O	1:B:688:VAL:HG13	2.04	0.57
1:B:430:LEU:CA	1:B:433:ILE:HG22	2.33	0.57
1:B:683:PHE:CG	7:B:1110:H43:C22	2.87	0.57
1:A:633:PHE:O	1:A:637:ARG:N	2.37	0.57
1:B:62:ARG:NH2	1:B:277:GLU:OE1	2.37	0.57
1:B:700:ARG:CB	1:B:703:LEU:CB	2.82	0.57
1:A:738:CYS:SG	1:A:739:VAL:N	2.77	0.57
1:B:684:GLY:O	1:B:688:VAL:HG22	2.05	0.57
1:A:331:ARG:NH1	1:A:410:PHE:O	2.37	0.57
1:A:654:LEU:HD21	1:A:852:PHE:CZ	2.40	0.57
1:A:683:PHE:CD2	1:A:840:ILE:HG21	2.39	0.57
1:A:769:LEU:HG	1:A:770:MET:N	2.19	0.57
1:B:633:PHE:O	1:B:637:ARG:N	2.37	0.57
1:A:734:GLN:HA	1:A:737:ILE:HD12	1.87	0.57
1:A:820:PHE:C	1:A:822:PRO:HD2	2.29	0.57
1:B:851:ILE:C	1:B:852:PHE:HD1	2.13	0.57
1:A:851:ILE:C	1:A:852:PHE:HD1	2.13	0.56
1:B:541:CYS:SG	1:B:561:CYS:CB	2.93	0.56
1:B:820:PHE:C	1:B:822:PRO:HD2	2.29	0.56
1:B:602:ILE:HD12	1:B:760:ILE:O	2.05	0.56
1:B:654:LEU:HD21	1:B:852:PHE:CZ	2.40	0.56
1:B:693:CYS:O	1:B:696:VAL:HG12	2.04	0.56
1:B:769:LEU:HG	1:B:770:MET:N	2.19	0.56
1:B:776:ILE:HD12	7:B:1110:H43:C18	2.36	0.56
1:B:603:GLU:O	1:B:762:ILE:HG12	2.05	0.56
1:B:617:LEU:O	1:B:620:VAL:HG12	2.05	0.56
1:A:184:LEU:HD23	1:A:482:GLY:CA	2.36	0.56
1:A:603:GLU:CB	1:A:761:PHE:HD1	2.19	0.56
1:A:621:LEU:HD12	1:A:622:GLY:N	2.21	0.56
1:A:683:PHE:HD1	1:A:683:PHE:O	1.89	0.56
1:A:211:THR:HB	1:A:223:ILE:HD11	1.87	0.56
1:B:603:GLU:CB	1:B:761:PHE:HD1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:PRO:HA	1:B:613:ILE:HD12	1.88	0.56
1:B:793:SER:OG	1:B:796:LEU:HD13	2.06	0.56
1:A:684:GLY:O	1:A:688:VAL:HG22	2.05	0.56
1:B:621:LEU:HD12	1:B:622:GLY:N	2.20	0.56
1:A:776:ILE:HD12	7:A:1108:H43:C18	2.36	0.56
1:A:793:SER:OG	1:A:796:LEU:HD13	2.06	0.56
1:B:610:PRO:O	1:B:613:ILE:HB	2.06	0.56
1:B:685:ILE:HG13	1:B:686:SER:N	2.21	0.56
1:A:41:HIS:ND1	1:A:62:ARG:O	2.29	0.56
1:A:685:ILE:HG13	1:A:686:SER:N	2.21	0.56
1:B:430:LEU:O	1:B:433:ILE:HG23	2.03	0.56
1:A:617:LEU:O	1:A:620:VAL:HG12	2.05	0.55
1:A:661:PHE:HZ	1:A:845:PHE:CA	2.17	0.55
1:A:603:GLU:O	1:A:762:ILE:HG12	2.05	0.55
1:A:683:PHE:CG	7:A:1108:H43:C23	2.89	0.55
1:B:685:ILE:HA	1:B:688:VAL:CG2	2.37	0.55
1:A:610:PRO:HA	1:A:613:ILE:HD12	1.88	0.55
1:B:417:TYR:CZ	1:B:421:LEU:HD11	2.41	0.55
1:A:610:PRO:O	1:A:613:ILE:HB	2.06	0.55
1:B:778:TYR:CD1	1:B:782:LEU:HD11	2.42	0.55
1:A:677:ARG:HH21	1:A:746:PRO:HG3	1.72	0.55
1:A:800:PHE:CE2	1:A:858:ILE:HD13	2.41	0.55
1:B:491:ILE:HD12	1:B:504:PHE:HB3	1.89	0.55
1:A:685:ILE:HA	1:A:688:VAL:CG2	2.37	0.55
1:A:797:PRO:CA	1:A:801:ASN:HB2	2.30	0.55
1:B:601:GLN:CG	1:B:759:ILE:HD13	2.37	0.55
1:B:800:PHE:CE2	1:B:858:ILE:HD13	2.42	0.55
1:A:209:VAL:HG12	1:A:266:VAL:HB	1.88	0.54
1:B:604:PHE:HB3	1:B:762:ILE:CD1	2.37	0.54
1:B:821:ILE:CG2	1:B:822:PRO:HD3	2.38	0.54
1:B:840:ILE:CG1	1:B:841:LEU:N	2.69	0.54
1:A:177:LYS:NZ	1:A:183:PHE:O	2.35	0.54
1:B:296:SER:OG	1:B:297:GLU:N	2.40	0.54
1:A:572:TYR:HD2	1:A:597:CYS:SG	2.26	0.54
1:B:677:ARG:HH21	1:B:746:PRO:HG3	1.72	0.54
1:A:37:LEU:HB2	1:A:144:ALA:H	1.73	0.54
1:A:614:ALA:HA	1:A:617:LEU:HD21	1.89	0.54
1:A:656:SER:HB2	1:A:689:LEU:HD22	1.89	0.54
1:A:434:TYR:HB2	1:A:451:ILE:HD12	1.89	0.54
1:A:487:ASN:OD1	1:A:512:VAL:HG12	2.06	0.54
1:A:821:ILE:CG2	1:A:822:PRO:HD3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:CD2	1:A:482:GLY:CA	2.85	0.54
1:A:587:ASP:HA	1:A:600:LYS:HD3	1.89	0.54
1:A:778:TYR:CD1	1:A:782:LEU:HD11	2.42	0.54
1:A:604:PHE:HB3	1:A:762:ILE:CD1	2.37	0.54
1:B:683:PHE:CD2	7:B:1110:H43:C22	2.91	0.54
1:B:824:TYR:CE2	1:B:836:GLU:HG3	2.29	0.54
1:B:734:GLN:HA	1:B:737:ILE:HD12	1.87	0.53
1:A:819:SER:HB3	1:B:819:SER:CB	2.32	0.53
1:A:587:ASP:C	1:A:600:LYS:HD3	2.33	0.53
1:B:817:TRP:HA	1:B:817:TRP:CE3	2.41	0.53
1:A:605:LEU:CD2	1:A:830:LYS:HG3	2.39	0.53
1:B:656:SER:HB2	1:B:689:LEU:HD22	1.89	0.53
1:A:677:ARG:HH21	1:A:746:PRO:CG	2.22	0.53
1:A:685:ILE:HA	1:A:688:VAL:HG22	1.91	0.53
1:B:666:PHE:CD2	1:B:679:ARG:HA	2.44	0.53
1:A:691:ILE:HG23	1:A:692:SER:N	2.24	0.53
1:A:212:ILE:HD11	1:A:259:ILE:HD11	1.91	0.53
1:A:605:LEU:HD23	1:A:830:LYS:HG3	1.91	0.53
1:A:683:PHE:CE1	1:A:687:PHE:HB2	2.40	0.53
1:A:795:LYS:C	1:A:796:LEU:HD12	2.34	0.53
1:B:605:LEU:CD2	1:B:830:LYS:HG3	2.39	0.53
1:B:685:ILE:HA	1:B:688:VAL:HG22	1.91	0.53
1:A:827:THR:HB	1:A:832:VAL:HG23	1.91	0.53
1:B:212:ILE:HD11	1:B:259:ILE:HD11	1.90	0.53
1:B:299:TRP:HA	1:B:302:SER:HB2	1.91	0.53
1:B:614:ALA:HA	1:B:617:LEU:HD21	1.90	0.53
1:B:741:TRP:HE1	1:B:771:ALA:CB	2.22	0.53
1:A:271:SER:OG	1:A:272:SER:N	2.42	0.53
1:B:859:ILE:HG22	1:B:859:ILE:O	2.09	0.53
1:A:666:PHE:CD2	1:A:679:ARG:HA	2.44	0.52
1:A:668:ILE:HG22	1:A:668:ILE:O	2.10	0.52
1:B:588:TYR:OH	1:B:599:PRO:HG3	2.09	0.52
1:B:677:ARG:HH21	1:B:746:PRO:CG	2.22	0.52
1:A:311:PHE:HE2	1:A:495:LEU:HB2	1.74	0.52
1:A:776:ILE:CG2	7:A:1108:H43:C17	2.87	0.52
1:B:601:GLN:HB3	1:B:759:ILE:CB	2.38	0.52
1:B:806:ILE:C	1:B:810:MET:HE2	2.34	0.52
1:A:741:TRP:HE1	1:A:771:ALA:CB	2.22	0.52
1:B:683:PHE:CE2	1:B:840:ILE:HB	2.45	0.52
1:B:824:TYR:CE1	1:B:832:VAL:HG13	2.45	0.52
1:A:615:LEU:HD21	1:A:837:VAL:CG2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ILE:C	1:A:810:MET:HE2	2.34	0.52
1:B:605:LEU:HD23	1:B:830:LYS:HG3	1.91	0.52
1:B:589:TRP:C	1:B:597:CYS:HB3	2.34	0.52
1:B:795:LYS:C	1:B:796:LEU:HD12	2.34	0.52
1:A:841:LEU:HD23	1:A:842:ALA:N	2.25	0.52
1:B:860:LEU:HD12	1:B:861:PHE:N	2.24	0.52
1:A:443:PHE:HD2	1:A:448:CYS:HA	1.74	0.52
1:A:614:ALA:HA	1:A:617:LEU:CD2	2.40	0.52
1:A:660:CYS:O	1:A:663:SER:HB2	2.10	0.52
1:B:614:ALA:HA	1:B:617:LEU:CD2	2.40	0.52
1:B:668:ILE:HG22	1:B:668:ILE:O	2.10	0.52
1:B:691:ILE:HG23	1:B:692:SER:N	2.24	0.52
1:A:184:LEU:HD22	1:A:482:GLY:HA2	1.92	0.52
1:A:860:LEU:HD12	1:A:861:PHE:N	2.24	0.52
1:B:538:PHE:HD1	2:F:1:NAG:H82	1.75	0.52
1:B:688:VAL:HG12	1:B:779:THR:CG2	2.40	0.52
1:B:797:PRO:CA	1:B:801:ASN:HB2	2.30	0.52
1:A:740:ILE:O	1:A:744:THR:HG23	2.10	0.52
1:A:859:ILE:HG22	1:A:859:ILE:O	2.09	0.52
1:B:821:ILE:HG23	1:B:822:PRO:CD	2.40	0.52
1:B:841:LEU:HD23	1:B:842:ALA:N	2.25	0.52
1:B:740:ILE:O	1:B:744:THR:HG23	2.10	0.51
1:B:787:PHE:HA	1:B:810:MET:HE1	1.91	0.51
2:F:1:NAG:O6	2:F:2:NAG:N2	2.43	0.51
1:B:626:THR:OG1	1:B:658:LEU:HG	2.10	0.51
1:A:691:ILE:CD1	1:A:783:ALA:HB2	2.41	0.51
1:B:755:LEU:HG	1:B:761:PHE:HE2	1.75	0.51
1:B:827:THR:HB	1:B:832:VAL:HG23	1.91	0.51
1:A:603:GLU:HG2	1:A:761:PHE:HD1	1.72	0.51
1:A:741:TRP:CZ2	1:A:771:ALA:HB3	2.46	0.51
1:B:588:TYR:CZ	1:B:599:PRO:CG	2.84	0.51
1:B:653:LEU:HD11	1:B:694:ILE:CA	2.41	0.51
1:B:848:LEU:O	1:B:851:ILE:HG22	2.11	0.51
1:B:858:ILE:HG13	1:B:859:ILE:HG13	1.93	0.51
1:A:653:LEU:HD11	1:A:694:ILE:CA	2.41	0.51
1:A:400:ILE:HD12	1:A:400:ILE:H	1.76	0.51
1:A:653:LEU:HD21	1:A:693:CYS:HB2	1.93	0.51
1:A:806:ILE:C	1:A:809:SER:HG	2.13	0.51
1:A:317:THR:HG1	1:A:493:TRP:CG	2.29	0.51
1:A:615:LEU:HD22	1:A:837:VAL:HG11	1.93	0.51
1:A:683:PHE:HE1	1:A:687:PHE:CB	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:PHE:HA	1:A:810:MET:HE1	1.91	0.51
1:A:858:ILE:HG13	1:A:859:ILE:HG13	1.93	0.51
1:B:660:CYS:O	1:B:663:SER:HB2	2.10	0.51
1:A:588:TYR:HA	1:A:600:LYS:HG3	1.92	0.50
1:A:821:ILE:HG23	1:A:822:PRO:CD	2.40	0.50
1:B:617:LEU:HD12	1:B:618:PHE:N	2.25	0.50
1:B:745:ALA:O	1:B:767:GLY:HA3	2.11	0.50
1:B:790:ALA:CB	1:B:807:THR:HG23	2.41	0.50
1:A:609:GLU:O	1:A:613:ILE:HD12	2.11	0.50
1:B:399:ASN:HB3	1:B:402:SER:OG	2.12	0.50
1:B:430:LEU:HA	1:B:433:ILE:CG2	2.40	0.50
1:B:588:TYR:CE2	1:B:599:PRO:HD3	2.46	0.50
1:A:755:LEU:HG	1:A:761:PHE:HE2	1.76	0.50
1:A:790:ALA:CB	1:A:807:THR:HG23	2.41	0.50
1:B:615:LEU:HD22	1:B:837:VAL:HG11	1.93	0.50
1:B:741:TRP:CZ2	1:B:771:ALA:HB3	2.46	0.50
1:B:776:ILE:CG2	7:B:1110:H43:C17	2.87	0.50
1:A:617:LEU:HD12	1:A:618:PHE:N	2.25	0.50
1:A:626:THR:OG1	1:A:658:LEU:HG	2.10	0.50
1:A:695:LEU:O	1:A:698:THR:HG23	2.11	0.50
1:B:609:GLU:O	1:B:613:ILE:HD12	2.11	0.50
1:B:691:ILE:CD1	1:B:783:ALA:HB2	2.41	0.50
1:B:613:ILE:O	1:B:616:THR:HG22	2.12	0.50
1:A:745:ALA:O	1:A:767:GLY:HA3	2.11	0.50
1:B:637:ARG:HD2	1:B:651:TYR:CZ	2.46	0.50
1:B:639:THR:O	1:B:641:ILE:HG12	2.12	0.50
1:A:804:LYS:HG3	1:A:805:PHE:HD1	1.77	0.50
1:A:827:THR:HG22	1:A:828:TYR:N	2.27	0.50
1:B:200:ILE:HD11	1:B:490:ILE:HD13	1.93	0.50
1:A:39:PRO:HG3	1:A:145:THR:HG21	1.94	0.50
1:A:417:TYR:O	1:A:421:LEU:CD1	2.52	0.50
1:A:689:LEU:HD23	1:A:693:CYS:SG	2.51	0.50
1:A:848:LEU:O	1:A:851:ILE:HG22	2.11	0.50
1:B:685:ILE:O	1:B:688:VAL:HG22	2.12	0.50
1:A:605:LEU:O	1:A:669:GLY:HA2	2.12	0.50
1:A:657:LEU:CD2	1:A:848:LEU:HB2	2.39	0.50
1:B:689:LEU:HD23	1:B:693:CYS:SG	2.52	0.50
1:B:756:GLU:HG3	1:B:759:ILE:H	1.77	0.50
1:A:184:LEU:HD23	1:A:482:GLY:HA3	1.92	0.49
1:A:778:TYR:HE1	1:A:782:LEU:HD11	1.75	0.49
1:B:603:GLU:HG2	1:B:761:PHE:HD1	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:O	1:B:669:GLY:HA2	2.12	0.49
1:B:637:ARG:CD	1:B:651:TYR:HE1	2.21	0.49
1:B:804:LYS:HG3	1:B:805:PHE:HD1	1.77	0.49
1:B:840:ILE:O	1:B:841:LEU:C	2.55	0.49
1:A:756:GLU:HG3	1:A:759:ILE:H	1.77	0.49
1:A:629:VAL:HG12	1:A:633:PHE:HE2	1.78	0.49
1:A:688:VAL:HG12	1:A:779:THR:CG2	2.40	0.49
1:B:653:LEU:HD21	1:B:693:CYS:HB2	1.93	0.49
1:B:734:GLN:HE22	1:B:775:LEU:HA	1.78	0.49
1:A:60:CYS:HG	1:A:101:CYS:HB2	1.67	0.49
1:A:613:ILE:O	1:A:616:THR:HG22	2.12	0.49
1:A:639:THR:O	1:A:641:ILE:HG12	2.12	0.49
1:A:683:PHE:CD1	7:A:1108:H43:C22	2.95	0.49
1:A:687:PHE:HE2	1:A:779:THR:HG22	1.78	0.49
1:A:723:GLN:O	1:A:726:LEU:HB2	2.13	0.49
1:A:840:ILE:O	1:A:841:LEU:C	2.55	0.49
1:B:538:PHE:CZ	1:B:540:ASN:HB2	2.47	0.49
1:B:629:VAL:HG12	1:B:633:PHE:HE2	1.78	0.49
1:B:657:LEU:CD2	1:B:848:LEU:HB2	2.39	0.49
1:A:694:ILE:O	1:A:697:LYS:CB	2.57	0.49
1:B:591:ASN:HB2	1:B:596:SER:O	2.12	0.49
1:B:629:VAL:HG12	1:B:633:PHE:CE2	2.47	0.49
1:B:741:TRP:HH2	1:B:772:LEU:HD23	1.77	0.49
1:A:815:ILE:HG13	1:A:816:VAL:H	1.77	0.49
1:B:545:CYS:HB2	1:B:577:ASP:HA	1.94	0.49
1:B:804:LYS:HG3	1:B:805:PHE:CD1	2.48	0.49
1:A:685:ILE:O	1:A:688:VAL:HG22	2.12	0.49
1:A:734:GLN:HE22	1:A:775:LEU:HA	1.77	0.49
1:A:741:TRP:HH2	1:A:772:LEU:HD23	1.78	0.49
1:A:790:ALA:HB3	1:A:807:THR:CG2	2.43	0.49
1:B:827:THR:HG22	1:B:828:TYR:N	2.27	0.49
1:A:36:GLY:HA2	1:A:142:VAL:O	2.12	0.49
1:A:685:ILE:C	1:A:688:VAL:HG22	2.38	0.49
1:A:677:ARG:HH21	1:A:746:PRO:CB	2.25	0.48
1:A:677:ARG:HG3	1:A:747:PRO:HG2	1.94	0.48
1:B:723:GLN:O	1:B:726:LEU:HB2	2.13	0.48
1:A:110:ALA:O	1:A:113:SER:OG	2.19	0.48
1:B:809:SER:OG	1:B:810:MET:N	2.46	0.48
1:A:182:SER:O	1:A:182:SER:OG	2.27	0.48
1:A:637:ARG:CD	1:A:651:TYR:HE1	2.20	0.48
1:B:659:CYS:SG	1:B:686:SER:OG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:VAL:O	1:B:736:VAL:CB	2.59	0.48
1:A:629:VAL:HG12	1:A:633:PHE:CE2	2.47	0.48
1:A:812:ILE:HG13	1:A:813:PHE:N	2.27	0.48
1:B:601:GLN:CB	1:B:759:ILE:CD1	2.90	0.48
1:B:683:PHE:CE2	1:B:840:ILE:CB	2.97	0.48
1:B:683:PHE:O	1:B:684:GLY:C	2.57	0.48
1:B:685:ILE:C	1:B:688:VAL:HG22	2.38	0.48
1:B:824:TYR:CE1	1:B:832:VAL:CG1	2.96	0.48
1:A:268:VAL:HG22	1:A:294:LEU:HD12	1.94	0.48
1:A:804:LYS:HG3	1:A:805:PHE:CD1	2.48	0.48
1:B:694:ILE:O	1:B:697:LYS:CB	2.56	0.48
1:A:51:LEU:HB2	1:B:461:LYS:HD3	1.95	0.48
1:B:618:PHE:HA	1:B:621:LEU:HD23	1.95	0.48
1:B:674:TRP:H	1:B:674:TRP:CD1	2.32	0.48
1:B:806:ILE:C	1:B:809:SER:HG	2.15	0.48
1:A:111:THR:HG21	1:A:153:VAL:HG13	1.96	0.48
1:A:683:PHE:O	1:A:684:GLY:C	2.57	0.48
1:A:860:LEU:HD12	1:A:861:PHE:CB	2.43	0.48
1:B:737:ILE:HD12	1:B:737:ILE:H	1.78	0.48
1:B:796:LEU:HD12	1:B:796:LEU:N	2.29	0.48
1:B:665:LEU:HD22	1:B:666:PHE:HE1	1.78	0.48
1:A:621:LEU:HD12	1:A:621:LEU:C	2.39	0.48
1:A:737:ILE:HD12	1:A:737:ILE:H	1.79	0.48
1:A:840:ILE:CG1	1:A:841:LEU:H	2.16	0.48
1:B:677:ARG:HH21	1:B:746:PRO:CB	2.26	0.48
1:B:790:ALA:HB3	1:B:807:THR:CG2	2.43	0.48
1:A:639:THR:C	1:A:641:ILE:H	2.22	0.48
1:B:676:CYS:SG	1:B:677:ARG:N	2.87	0.48
1:A:60:CYS:CB	1:A:101:CYS:SG	3.02	0.47
1:A:676:CYS:SG	1:A:677:ARG:N	2.87	0.47
1:A:809:SER:OG	1:A:810:MET:N	2.46	0.47
1:B:722:LEU:O	1:B:726:LEU:HD23	2.14	0.47
1:B:621:LEU:HD12	1:B:621:LEU:C	2.39	0.47
1:B:687:PHE:HE2	1:B:779:THR:HG22	1.78	0.47
1:A:674:TRP:H	1:A:674:TRP:CD1	2.32	0.47
1:B:639:THR:C	1:B:641:ILE:H	2.22	0.47
1:B:677:ARG:HG3	1:B:747:PRO:HG2	1.94	0.47
1:B:804:LYS:O	1:B:807:THR:OG1	2.29	0.47
1:A:733:VAL:O	1:A:736:VAL:CB	2.59	0.47
1:A:722:LEU:O	1:A:726:LEU:HD23	2.14	0.47
1:B:741:TRP:NE1	1:B:768:SER:HG	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ARG:HD2	1:A:651:TYR:CZ	2.46	0.47
1:A:668:ILE:HD12	1:A:668:ILE:N	2.30	0.47
1:B:668:ILE:HD12	1:B:668:ILE:N	2.30	0.47
1:B:672:GLN:O	1:B:673:ASN:C	2.58	0.47
1:B:685:ILE:CA	1:B:688:VAL:HG22	2.45	0.47
1:B:860:LEU:HD12	1:B:861:PHE:CB	2.43	0.47
1:A:618:PHE:HA	1:A:621:LEU:HD23	1.95	0.47
1:A:685:ILE:CA	1:A:688:VAL:HG22	2.45	0.47
1:A:834:ALA:O	1:A:837:VAL:HG12	2.15	0.47
1:A:248:ASP:CG	1:A:249:GLU:N	2.72	0.47
1:A:587:ASP:CA	1:A:600:LYS:HD3	2.45	0.47
1:A:804:LYS:O	1:A:807:THR:OG1	2.29	0.47
1:B:677:ARG:HG2	1:B:747:PRO:CG	2.45	0.47
1:A:25:ARG:HD3	1:A:98:PHE:HE1	1.80	0.46
1:A:272:SER:OG	1:A:273:GLY:N	2.48	0.46
1:B:615:LEU:CD2	1:B:837:VAL:HG11	2.45	0.46
1:B:666:PHE:CB	1:B:679:ARG:CB	2.93	0.46
1:A:586:GLU:O	1:A:600:LYS:HD3	2.15	0.46
1:A:588:TYR:C	1:A:600:LYS:HG3	2.40	0.46
1:B:841:LEU:HD23	1:B:841:LEU:C	2.40	0.46
1:A:201:ILE:HD13	1:A:209:VAL:HG11	1.98	0.46
1:B:828:TYR:O	1:B:832:VAL:HG23	2.16	0.46
1:A:666:PHE:CB	1:A:679:ARG:CB	2.93	0.46
1:A:753:HIS:CB	1:A:760:ILE:HG12	2.39	0.46
1:A:796:LEU:HD12	1:A:796:LEU:N	2.29	0.46
1:A:828:TYR:O	1:A:832:VAL:CG2	2.64	0.46
1:A:615:LEU:CD2	1:A:837:VAL:HG11	2.45	0.46
1:A:672:GLN:O	1:A:673:ASN:C	2.58	0.46
1:B:513:TYR:HE2	2:E:1:NAG:HN2	1.64	0.46
1:B:615:LEU:HD21	1:B:837:VAL:CG2	2.29	0.46
1:B:44:VAL:HA	1:B:60:CYS:HA	1.96	0.46
1:B:794:ARG:O	1:B:801:ASN:ND2	2.49	0.46
1:B:860:LEU:CD1	1:B:861:PHE:HB2	2.45	0.46
1:A:636:PHE:HB3	1:A:639:THR:OG1	2.16	0.46
1:A:676:CYS:SG	1:A:749:SER:HB3	2.56	0.46
1:A:695:LEU:C	1:A:697:LYS:N	2.73	0.46
1:A:841:LEU:HD23	1:A:841:LEU:C	2.40	0.46
1:B:676:CYS:SG	1:B:749:SER:HB3	2.56	0.46
1:A:741:TRP:HZ2	1:A:771:ALA:C	2.24	0.46
1:A:860:LEU:CD1	1:A:861:PHE:HB2	2.45	0.46
1:A:862:LYS:O	1:A:864:SER:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:ALA:O	1:B:837:VAL:HG12	2.15	0.46
1:A:794:ARG:O	1:A:801:ASN:ND2	2.49	0.46
1:B:828:TYR:O	1:B:832:VAL:CG2	2.64	0.46
1:A:687:PHE:HE2	1:A:779:THR:CG2	2.29	0.46
1:B:636:PHE:HB3	1:B:639:THR:OG1	2.16	0.46
1:A:828:TYR:O	1:A:832:VAL:HG23	2.16	0.45
1:B:672:GLN:O	1:B:675:THR:N	2.50	0.45
1:B:676:CYS:HB3	1:B:764:CYS:SG	2.56	0.45
1:B:815:ILE:HG13	1:B:816:VAL:H	1.77	0.45
1:A:228:GLU:O	1:A:231:GLU:HG3	2.16	0.45
1:A:633:PHE:HB3	1:A:637:ARG:NE	2.25	0.45
1:A:667:PHE:C	1:A:668:ILE:HD12	2.41	0.45
1:A:672:GLN:O	1:A:675:THR:N	2.49	0.45
1:A:676:CYS:HB3	1:A:764:CYS:SG	2.56	0.45
1:A:821:ILE:CG2	1:A:822:PRO:CD	2.94	0.45
1:B:588:TYR:C	1:B:600:LYS:HG2	2.42	0.45
1:B:617:LEU:CA	1:B:620:VAL:HG12	2.47	0.45
1:B:688:VAL:HA	1:B:691:ILE:HG22	1.98	0.45
1:B:860:LEU:HD12	1:B:860:LEU:C	2.41	0.45
1:A:601:GLN:O	1:A:759:ILE:HG23	2.16	0.45
1:B:341:LYS:O	1:B:341:LYS:CG	2.64	0.45
1:B:753:HIS:CB	1:B:760:ILE:HG12	2.39	0.45
1:A:54:ARG:NH2	1:B:455:GLU:OE2	2.50	0.45
1:A:147:SER:OG	1:A:218:TYR:HB2	2.17	0.45
1:A:860:LEU:HD12	1:A:860:LEU:C	2.41	0.45
1:B:603:GLU:CG	1:B:761:PHE:HD1	2.30	0.45
1:B:821:ILE:CG2	1:B:822:PRO:CD	2.94	0.45
1:A:352:TRP:HE1	1:A:396:GLY:HA2	1.82	0.45
1:A:688:VAL:HA	1:A:691:ILE:HG22	1.98	0.45
1:A:819:SER:O	1:A:822:PRO:HD2	2.17	0.45
1:B:667:PHE:C	1:B:668:ILE:HD12	2.41	0.45
1:B:687:PHE:HE2	1:B:779:THR:CG2	2.29	0.45
1:B:741:TRP:HZ2	1:B:771:ALA:C	2.24	0.45
1:A:785:ILE:HG13	1:A:786:CYS:N	2.32	0.45
1:B:625:LEU:HD23	1:B:625:LEU:C	2.42	0.45
1:B:629:VAL:O	1:B:633:PHE:HD2	2.00	0.45
1:A:629:VAL:O	1:A:633:PHE:HD2	2.00	0.45
1:B:695:LEU:C	1:B:695:LEU:HD23	2.42	0.45
1:B:840:ILE:CG1	1:B:841:LEU:H	2.16	0.45
1:A:99:ASP:OD1	1:A:100:THR:N	2.50	0.45
1:A:811:LEU:HD12	1:A:814:PHE:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:TYR:HE1	1:A:830:LYS:HB3	1.82	0.45
1:A:253:GLN:O	1:A:257:GLU:HG2	2.16	0.45
1:A:695:LEU:C	1:A:695:LEU:HD23	2.42	0.45
1:A:821:ILE:N	1:A:822:PRO:CD	2.80	0.45
1:A:603:GLU:CG	1:A:761:PHE:HD1	2.30	0.44
1:A:632:VAL:O	1:A:635:LYS:HB2	2.17	0.44
1:A:749:SER:HA	1:A:764:CYS:SG	2.57	0.44
1:B:289:THR:HG23	1:B:313:VAL:HA	1.98	0.44
1:B:588:TYR:HA	1:B:599:PRO:HA	2.00	0.44
1:B:665:LEU:HD23	1:B:665:LEU:O	2.17	0.44
1:B:752:ASN:OD1	1:B:753:HIS:N	2.51	0.44
1:B:811:LEU:HD12	1:B:814:PHE:HD2	1.82	0.44
1:A:752:ASN:OD1	1:A:753:HIS:N	2.51	0.44
1:A:756:GLU:OE1	1:A:756:GLU:CA	2.65	0.44
1:B:604:PHE:HB3	1:B:762:ILE:HG12	1.99	0.44
1:B:632:VAL:O	1:B:635:LYS:HB2	2.17	0.44
1:B:741:TRP:HE1	1:B:771:ALA:HB3	1.83	0.44
1:B:749:SER:HA	1:B:764:CYS:SG	2.57	0.44
1:B:821:ILE:N	1:B:822:PRO:CD	2.80	0.44
1:A:292:ILE:HD11	1:A:537:PRO:HG2	2.00	0.44
1:A:588:TYR:HB3	1:A:597:CYS:HB3	2.00	0.44
1:A:790:ALA:HB3	1:A:807:THR:HG23	2.00	0.44
1:B:193:GLN:HE22	1:B:297:GLU:H	1.64	0.44
1:A:806:ILE:O	1:A:810:MET:HG3	2.18	0.44
1:B:396:GLY:O	1:B:397:ASP:OD1	2.35	0.44
1:A:625:LEU:C	1:A:625:LEU:HD23	2.42	0.44
1:A:667:PHE:N	1:A:668:ILE:HD12	2.31	0.44
1:A:817:TRP:O	1:A:818:ILE:C	2.60	0.44
1:A:623:ILE:HD12	1:A:658:LEU:HG	2.00	0.44
1:A:683:PHE:CE1	1:A:687:PHE:CB	3.01	0.44
1:B:140:ALA:HB2	1:B:163:PRO:HG2	1.99	0.44
1:B:785:ILE:HG13	1:B:786:CYS:N	2.32	0.44
1:A:665:LEU:O	1:A:665:LEU:HD23	2.17	0.44
1:A:741:TRP:HE1	1:A:771:ALA:HB3	1.83	0.44
1:A:828:TYR:HE1	1:A:831:PHE:H	1.65	0.44
1:B:218:TYR:OH	1:B:296:SER:OG	2.33	0.44
1:B:683:PHE:CG	7:B:1110:H43:C23	3.00	0.44
1:A:617:LEU:O	1:A:620:VAL:CG1	2.66	0.44
1:A:665:LEU:HD22	1:A:666:PHE:HE1	1.79	0.44
1:A:677:ARG:HG2	1:A:747:PRO:CG	2.45	0.44
1:A:791:PHE:O	1:A:792:LYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:LEU:O	1:A:847:LEU:HD12	2.18	0.44
1:B:338:HIS:CD2	1:B:340:LYS:HB2	2.52	0.44
1:B:649:LEU:HD23	1:B:649:LEU:HA	1.87	0.44
1:B:91:MET:HE3	1:B:91:MET:HA	2.00	0.44
1:B:778:TYR:HE1	1:B:782:LEU:HD11	1.75	0.44
1:B:819:SER:O	1:B:822:PRO:HD2	2.17	0.43
1:A:238:ASP:OD2	1:A:262:SER:HB2	2.19	0.43
1:A:603:GLU:HB3	1:A:761:PHE:HD1	1.83	0.43
1:B:193:GLN:HE22	1:B:297:GLU:N	2.16	0.43
1:B:492:ASN:HD22	1:B:494:HIS:CD2	2.36	0.43
1:B:603:GLU:HB3	1:B:761:PHE:HD1	1.83	0.43
1:B:617:LEU:HA	1:B:620:VAL:CG1	2.46	0.43
1:B:792:LYS:HB2	1:B:792:LYS:HE2	1.84	0.43
1:A:487:ASN:ND2	1:A:511:ASN:OD1	2.51	0.43
1:A:617:LEU:HA	1:A:620:VAL:CG1	2.46	0.43
1:A:781:LEU:HD13	1:A:781:LEU:HA	1.85	0.43
1:B:847:LEU:HD12	1:B:847:LEU:O	2.18	0.43
1:A:857:TYR:O	1:A:860:LEU:HG	2.19	0.43
1:B:847:LEU:HD12	1:B:847:LEU:C	2.43	0.43
1:B:852:PHE:O	1:B:853:PHE:C	2.61	0.43
1:A:162:ILE:O	1:A:182:SER:OG	2.29	0.43
1:A:470:SER:O	1:A:473:GLY:N	2.52	0.43
1:A:721:ASN:O	1:A:722:LEU:C	2.62	0.43
1:A:847:LEU:HD12	1:A:847:LEU:C	2.43	0.43
1:B:793:SER:OG	1:B:796:LEU:HD22	2.19	0.43
1:B:806:ILE:O	1:B:810:MET:HG3	2.18	0.43
1:B:828:TYR:HE1	1:B:830:LYS:HB3	1.82	0.43
1:A:586:GLU:O	1:A:600:LYS:CD	2.66	0.43
1:A:793:SER:OG	1:A:796:LEU:HD22	2.19	0.43
1:B:601:GLN:HG2	1:B:759:ILE:HD13	2.01	0.43
1:B:617:LEU:C	1:B:620:VAL:HG12	2.44	0.43
1:B:623:ILE:HD12	1:B:658:LEU:HG	2.00	0.43
1:B:657:LEU:CD1	1:B:690:CYS:HB3	2.49	0.43
1:B:857:TYR:O	1:B:860:LEU:HG	2.19	0.43
1:A:228:GLU:HG3	1:A:229:GLU:N	2.32	0.43
1:A:617:LEU:C	1:A:620:VAL:HG12	2.44	0.43
1:A:683:PHE:CD1	1:A:683:PHE:C	2.96	0.43
1:A:732:PHE:HA	1:A:735:ILE:HG22	2.01	0.43
1:A:755:LEU:CG	1:A:761:PHE:HE2	2.32	0.43
1:A:793:SER:C	1:A:796:LEU:HD13	2.43	0.43
1:B:587:ASP:O	1:B:600:LYS:N	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:TRP:HZ2	1:B:772:LEU:N	2.17	0.43
1:B:756:GLU:OE1	1:B:756:GLU:CA	2.65	0.43
1:A:284:VAL:HG21	1:A:310:PHE:CD1	2.54	0.43
1:A:604:PHE:HB3	1:A:762:ILE:HG12	1.99	0.43
1:A:657:LEU:CD1	1:A:690:CYS:HB3	2.49	0.43
1:B:617:LEU:O	1:B:620:VAL:CG1	2.66	0.43
1:B:828:TYR:HE1	1:B:831:PHE:H	1.65	0.43
1:B:862:LYS:O	1:B:864:SER:N	2.45	0.43
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.75	0.43
1:A:680:GLN:HB3	1:A:681:PRO:CD	2.48	0.43
1:A:809:SER:CB	1:A:850:CYS:SG	3.06	0.43
1:B:793:SER:C	1:B:796:LEU:HD13	2.43	0.43
1:A:538:PHE:CE1	1:A:540:ASN:HB2	2.54	0.42
1:B:516:LYS:HG2	1:B:519:ARG:NH1	2.34	0.42
1:A:44:VAL:HG13	1:A:60:CYS:SG	2.59	0.42
1:A:143:GLY:HA2	1:A:167:TYR:CE2	2.54	0.42
1:A:802:GLU:OE1	1:A:802:GLU:CA	2.67	0.42
1:A:852:PHE:O	1:A:853:PHE:C	2.61	0.42
1:B:61:ILE:HG13	1:B:62:ARG:H	1.83	0.42
1:B:280:ILE:HG23	1:B:314:ILE:HD11	2.01	0.42
1:B:642:VAL:HB	1:B:859:ILE:CD1	2.49	0.42
1:B:667:PHE:N	1:B:668:ILE:HD12	2.31	0.42
1:B:680:GLN:HB3	1:B:681:PRO:CD	2.48	0.42
1:B:721:ASN:O	1:B:722:LEU:C	2.62	0.42
1:B:732:PHE:HA	1:B:735:ILE:HG22	2.01	0.42
1:A:166:SER:OG	1:A:169:SER:OG	2.30	0.42
1:A:652:LEU:HD23	1:A:693:CYS:SG	2.60	0.42
1:A:732:PHE:O	1:A:733:VAL:C	2.62	0.42
1:B:755:LEU:CG	1:B:761:PHE:HE2	2.32	0.42
1:B:791:PHE:O	1:B:792:LYS:C	2.61	0.42
1:B:207:ASN:ND2	1:B:560:CYS:HB2	2.35	0.42
1:B:858:ILE:O	1:B:862:LYS:N	2.50	0.42
1:A:60:CYS:HB2	1:A:101:CYS:SG	2.59	0.42
1:A:538:PHE:CZ	1:A:540:ASN:HB2	2.55	0.42
1:B:652:LEU:HD23	1:B:693:CYS:SG	2.59	0.42
1:B:732:PHE:O	1:B:733:VAL:C	2.62	0.42
1:A:607:TRP:HA	1:A:668:ILE:CG2	2.50	0.42
1:A:741:TRP:HZ2	1:A:772:LEU:N	2.17	0.42
1:B:689:LEU:HD23	1:B:689:LEU:C	2.45	0.42
1:A:190:ASP:O	1:A:190:ASP:CG	2.62	0.42
1:B:106:LYS:O	1:B:109:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LYS:HA	1:B:177:LYS:HD3	1.87	0.42
1:B:607:TRP:HA	1:B:668:ILE:CG2	2.50	0.42
1:B:618:PHE:CD1	1:B:621:LEU:HD21	2.55	0.42
1:B:653:LEU:HD21	1:B:690:CYS:O	2.19	0.42
1:B:660:CYS:SG	1:B:661:PHE:N	2.92	0.42
1:A:550:ARG:NH2	1:A:551:LYS:O	2.52	0.42
1:A:741:TRP:CH2	1:A:772:LEU:HD23	2.55	0.42
1:B:674:TRP:H	1:B:674:TRP:HD1	1.68	0.42
1:A:108:LEU:HA	1:A:108:LEU:HD23	1.73	0.42
1:A:167:TYR:CD2	1:A:419:VAL:HG22	2.55	0.42
1:A:642:VAL:HB	1:A:859:ILE:CD1	2.49	0.42
1:A:653:LEU:HD21	1:A:690:CYS:O	2.19	0.42
1:A:660:CYS:SG	1:A:661:PHE:N	2.92	0.42
1:A:806:ILE:O	1:A:810:MET:HE2	2.20	0.42
1:A:828:TYR:CE1	1:A:830:LYS:HB3	2.55	0.42
1:B:724:PHE:O	1:B:725:LEU:C	2.61	0.42
1:A:63:TYR:CD1	1:A:354:GLU:HG3	2.55	0.41
1:A:617:LEU:CA	1:A:620:VAL:HG12	2.47	0.41
1:A:724:PHE:O	1:A:725:LEU:C	2.61	0.41
1:A:750:TYR:CD1	1:A:750:TYR:C	2.97	0.41
1:A:840:ILE:CG1	1:A:841:LEU:N	2.69	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.79	0.41
1:B:741:TRP:CH2	1:B:772:LEU:CG	3.04	0.41
1:A:637:ARG:HA	1:A:637:ARG:HD3	1.88	0.41
1:B:275:ASP:OD1	1:B:275:ASP:N	2.53	0.41
1:B:391:ARG:N	1:B:392:PRO:HD2	2.35	0.41
1:B:590:SER:HA	1:B:597:CYS:SG	2.60	0.41
1:B:677:ARG:HG2	1:B:747:PRO:CD	2.50	0.41
1:B:812:ILE:HG23	1:B:813:PHE:N	2.35	0.41
1:A:86:ASN:OD1	1:A:87:LEU:N	2.54	0.41
1:A:107:ALA:O	1:A:111:THR:HG23	2.20	0.41
1:A:618:PHE:CD1	1:A:621:LEU:HD21	2.55	0.41
1:A:741:TRP:CH2	1:A:772:LEU:CG	3.04	0.41
1:A:793:SER:CA	1:A:796:LEU:HD13	2.50	0.41
1:B:238:ASP:OD2	1:B:262:SER:HB2	2.19	0.41
1:B:741:TRP:CH2	1:B:772:LEU:HD23	2.55	0.41
1:B:631:GLY:O	1:B:634:THR:HB	2.21	0.41
1:B:633:PHE:HB3	1:B:637:ARG:NE	2.25	0.41
1:B:750:TYR:CD1	1:B:750:TYR:C	2.97	0.41
1:B:806:ILE:O	1:B:810:MET:HE2	2.20	0.41
1:A:639:THR:C	1:A:641:ILE:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:SER:O	1:A:659:CYS:SG	2.79	0.41
1:B:697:LYS:NZ	1:B:851:ILE:HD11	2.34	0.41
1:A:689:LEU:HD23	1:A:689:LEU:C	2.45	0.41
1:A:740:ILE:HG23	1:A:744:THR:HG21	2.03	0.41
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.93	0.41
1:B:603:GLU:OE1	1:B:603:GLU:HA	2.21	0.41
1:B:656:SER:O	1:B:659:CYS:SG	2.79	0.41
1:A:589:TRP:HB2	1:A:600:LYS:HG2	2.03	0.41
1:A:631:GLY:O	1:A:634:THR:HB	2.20	0.41
1:B:793:SER:CA	1:B:796:LEU:HD13	2.50	0.41
1:A:607:TRP:H	1:A:607:TRP:CD1	2.39	0.41
1:A:607:TRP:CD1	1:A:607:TRP:N	2.89	0.41
1:A:674:TRP:H	1:A:674:TRP:HD1	1.68	0.41
1:A:739:VAL:O	1:A:742:LEU:HB3	2.21	0.41
1:A:788:PHE:CE1	1:A:792:LYS:HD2	2.56	0.41
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.89	0.41
1:B:739:VAL:O	1:B:742:LEU:HB3	2.21	0.41
1:B:741:TRP:HZ2	1:B:771:ALA:CB	2.34	0.41
1:B:788:PHE:CE1	1:B:792:LYS:HD2	2.56	0.41
1:B:809:SER:CB	1:B:850:CYS:SG	3.06	0.41
1:B:828:TYR:CE1	1:B:830:LYS:HB3	2.55	0.41
1:A:677:ARG:HG2	1:A:747:PRO:CD	2.51	0.41
1:A:741:TRP:CZ2	1:A:771:ALA:CB	3.04	0.41
1:A:781:LEU:O	1:A:785:ILE:HG23	2.21	0.41
1:A:808:PHE:O	1:A:812:ILE:HG23	2.20	0.41
1:B:338:HIS:CD2	1:B:340:LYS:H	2.39	0.41
1:B:607:TRP:CD1	1:B:607:TRP:N	2.89	0.41
1:A:29:LYS:HE2	1:A:29:LYS:H	1.86	0.40
1:A:653:LEU:HD11	1:A:694:ILE:N	2.37	0.40
1:A:763:THR:OG1	1:A:764:CYS:N	2.54	0.40
1:B:607:TRP:CD1	1:B:607:TRP:H	2.39	0.40
1:B:741:TRP:CZ2	1:B:771:ALA:CB	3.04	0.40
1:B:763:THR:OG1	1:B:764:CYS:N	2.54	0.40
1:B:803:ALA:O	1:B:807:THR:HG23	2.21	0.40
1:A:750:TYR:HE1	1:A:752:ASN:HB2	1.86	0.40
1:B:639:THR:C	1:B:641:ILE:N	2.78	0.40
1:B:730:CYS:O	1:B:731:THR:C	2.64	0.40
1:B:781:LEU:O	1:B:785:ILE:HG23	2.21	0.40
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.83	0.40
1:B:653:LEU:HD11	1:B:694:ILE:N	2.37	0.40
1:B:683:PHE:CD2	1:B:840:ILE:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:ILE:HG23	1:B:744:THR:HG21	2.03	0.40
1:B:755:LEU:HG	1:B:761:PHE:CE2	2.54	0.40
1:B:769:LEU:HD23	1:B:769:LEU:N	2.33	0.40
1:A:691:ILE:HD11	1:A:783:ALA:CB	2.51	0.40
1:A:800:PHE:O	1:A:801:ASN:C	2.65	0.40
1:A:856:VAL:O	1:A:860:LEU:CG	2.69	0.40
1:B:637:ARG:HD2	1:B:651:TYR:OH	2.22	0.40
1:B:790:ALA:HB3	1:B:807:THR:HG23	2.00	0.40
1:A:53:SER:OG	1:A:54:ARG:N	2.54	0.40
1:A:450:ASP:OD1	1:A:450:ASP:N	2.53	0.40
1:A:637:ARG:HD2	1:A:651:TYR:OH	2.22	0.40
1:A:803:ALA:O	1:A:807:THR:HG23	2.21	0.40
1:B:725:LEU:O	1:B:726:LEU:C	2.65	0.40
1:B:732:PHE:C	1:B:735:ILE:HG22	2.45	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	783/1069 (73%)	720 (92%)	63 (8%)	0	100	100
1	B	784/1069 (73%)	720 (92%)	64 (8%)	0	100	100
All	All	1567/2138 (73%)	1440 (92%)	127 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	671/926 (72%)	670 (100%)	1 (0%)	88	91
1	B	675/926 (73%)	672 (100%)	3 (0%)	84	86
All	All	1346/1852 (73%)	1342 (100%)	4 (0%)	84	88

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

Mol	Chain	Res	Type
1	A	824	TYR
1	B	598	ILE
1	B	600	LYS
1	B	824	TYR

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	24	GLN
1	A	83	ASN
1	A	118	ASN
1	A	193	GLN
1	A	338	HIS
1	A	428	HIS
1	A	509	HIS
1	A	593	ASN
1	A	594	HIS
1	A	734	GLN
1	B	23	ASN
1	B	64	ASN
1	B	72	GLN
1	B	102	ASN
1	B	118	ASN
1	B	193	GLN
1	B	245	GLN
1	B	260	GLN
1	B	338	HIS
1	B	492	ASN
1	B	494	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides 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
2	NAG	C	1	1,2	14,14,15	1.65	4 (28%)	17,19,21	2.28	6 (35%)
2	NAG	C	2	2	14,14,15	1.83	4 (28%)	17,19,21	1.59	6 (35%)
2	NAG	D	1	1,2	14,14,15	1.72	5 (35%)	17,19,21	1.28	2 (11%)
2	NAG	D	2	2	14,14,15	1.83	4 (28%)	17,19,21	1.25	2 (11%)
2	NAG	E	1	1,2	14,14,15	1.86	4 (28%)	17,19,21	1.71	5 (29%)
2	NAG	E	2	2	14,14,15	1.80	4 (28%)	17,19,21	1.22	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.76	5 (35%)	17,19,21	1.22	2 (11%)
2	NAG	F	2	2	14,14,15	1.75	3 (21%)	17,19,21	1.26	2 (11%)

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	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C7-N2	3.52	1.45	1.34
2	C	2	NAG	C7-N2	3.48	1.45	1.34
2	D	2	NAG	C7-N2	3.47	1.45	1.34
2	C	1	NAG	C7-N2	3.45	1.45	1.34
2	E	2	NAG	C7-N2	3.44	1.45	1.34
2	F	2	NAG	C7-N2	3.43	1.45	1.34
2	E	1	NAG	C7-N2	3.42	1.45	1.34
2	D	1	NAG	C7-N2	3.38	1.45	1.34
2	E	1	NAG	O5-C1	3.27	1.49	1.43
2	D	2	NAG	O5-C1	3.12	1.48	1.43
2	E	2	NAG	O5-C1	2.94	1.48	1.43
2	F	1	NAG	O5-C1	2.92	1.48	1.43
2	C	2	NAG	O5-C1	2.91	1.48	1.43
2	D	1	NAG	O5-C1	2.87	1.48	1.43
2	F	2	NAG	O5-C1	2.80	1.48	1.43
2	C	2	NAG	O5-C5	2.65	1.48	1.43
2	E	1	NAG	O5-C5	2.54	1.48	1.43
2	D	2	NAG	O5-C5	2.44	1.48	1.43
2	E	2	NAG	O5-C5	2.44	1.48	1.43
2	F	2	NAG	O5-C5	2.40	1.48	1.43
2	E	1	NAG	C3-C2	-2.31	1.47	1.52
2	C	2	NAG	C3-C2	-2.30	1.47	1.52
2	C	1	NAG	O5-C1	2.29	1.47	1.43
2	C	1	NAG	O5-C5	2.25	1.47	1.43
2	D	2	NAG	C3-C2	-2.21	1.47	1.52
2	D	1	NAG	O5-C5	2.16	1.47	1.43
2	F	1	NAG	O5-C5	2.07	1.47	1.43
2	E	2	NAG	C3-C2	-2.06	1.48	1.52
2	F	1	NAG	C3-C2	-2.05	1.48	1.52
2	F	1	NAG	O7-C7	-2.04	1.18	1.23
2	D	1	NAG	O7-C7	-2.02	1.18	1.23
2	D	1	NAG	C3-C2	-2.01	1.48	1.52
2	C	1	NAG	O7-C7	-2.00	1.18	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C3-C4-C5	5.12	119.52	110.23
2	C	1	NAG	C1-O5-C5	-4.80	105.75	112.19
2	E	1	NAG	C1-O5-C5	3.49	116.86	112.19
2	C	2	NAG	C2-N2-C7	-3.36	118.40	122.90
2	D	2	NAG	C2-N2-C7	-3.30	118.47	122.90
2	C	1	NAG	C4-C3-C2	3.28	115.83	111.02
2	F	2	NAG	C2-N2-C7	-3.09	118.76	122.90
2	D	1	NAG	C2-N2-C7	-2.94	118.96	122.90
2	F	1	NAG	C2-N2-C7	-2.70	119.28	122.90
2	E	2	NAG	C2-N2-C7	-2.68	119.31	122.90
2	F	1	NAG	C8-C7-N2	2.58	120.39	116.12
2	F	2	NAG	C8-C7-N2	2.56	120.36	116.12
2	C	2	NAG	C8-C7-N2	2.48	120.23	116.12
2	D	1	NAG	C8-C7-N2	2.45	120.19	116.12
2	D	2	NAG	C8-C7-N2	2.42	120.14	116.12
2	E	2	NAG	C8-C7-N2	2.38	120.06	116.12
2	C	2	NAG	C6-C5-C4	-2.36	107.23	113.02
2	C	2	NAG	C1-O5-C5	2.36	115.34	112.19
2	C	1	NAG	C8-C7-N2	2.25	119.86	116.12
2	E	1	NAG	C8-C7-N2	2.24	119.84	116.12
2	E	1	NAG	C3-C4-C5	2.20	114.22	110.23
2	E	1	NAG	C1-C2-N2	-2.20	106.97	110.43
2	E	1	NAG	O5-C1-C2	2.12	114.58	111.29
2	C	2	NAG	O5-C5-C4	2.09	115.91	110.83
2	C	2	NAG	C3-C4-C5	2.02	113.90	110.23
2	C	1	NAG	C2-N2-C7	-2.02	120.19	122.90
2	C	1	NAG	O5-C1-C2	-2.01	108.17	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

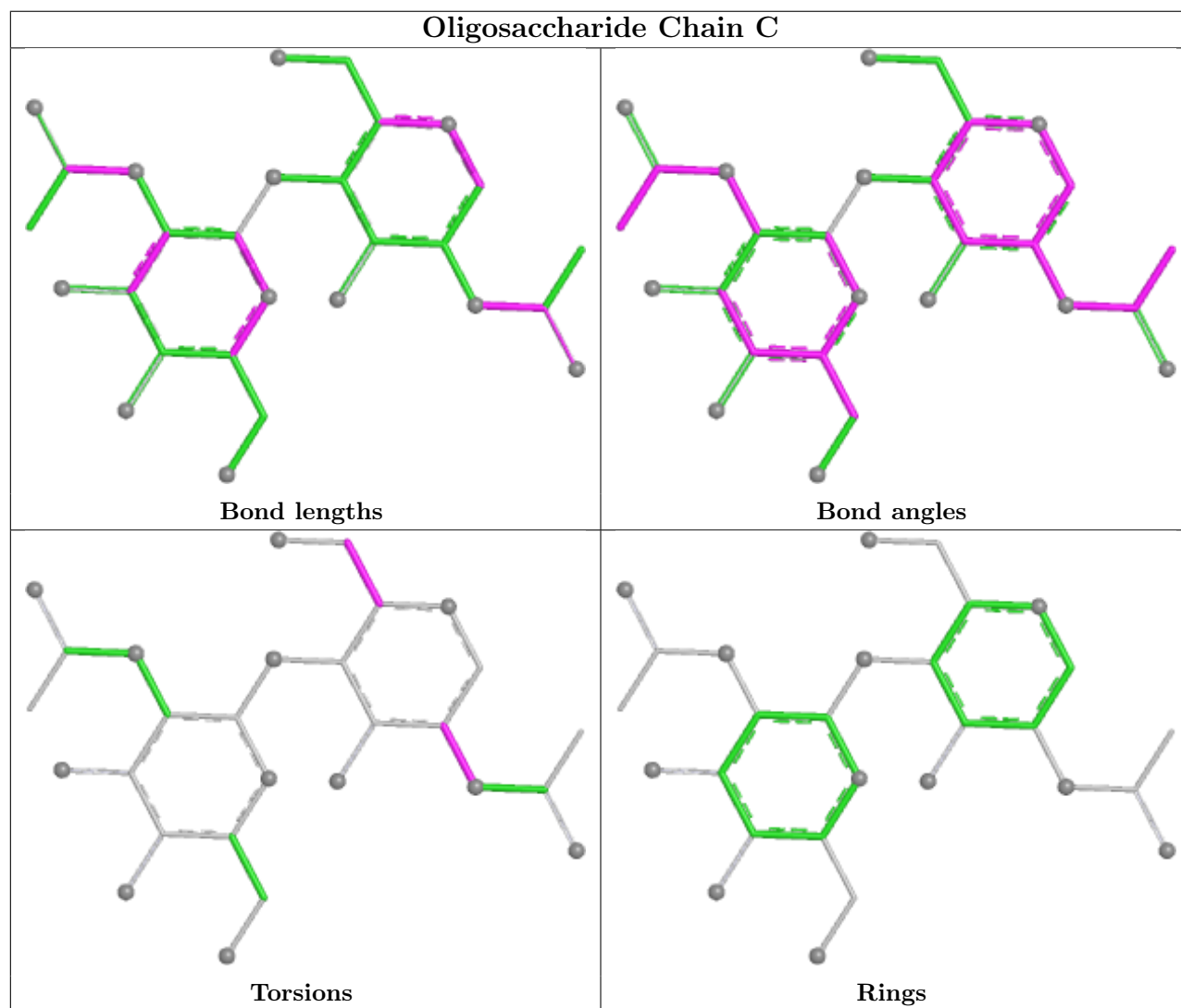
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

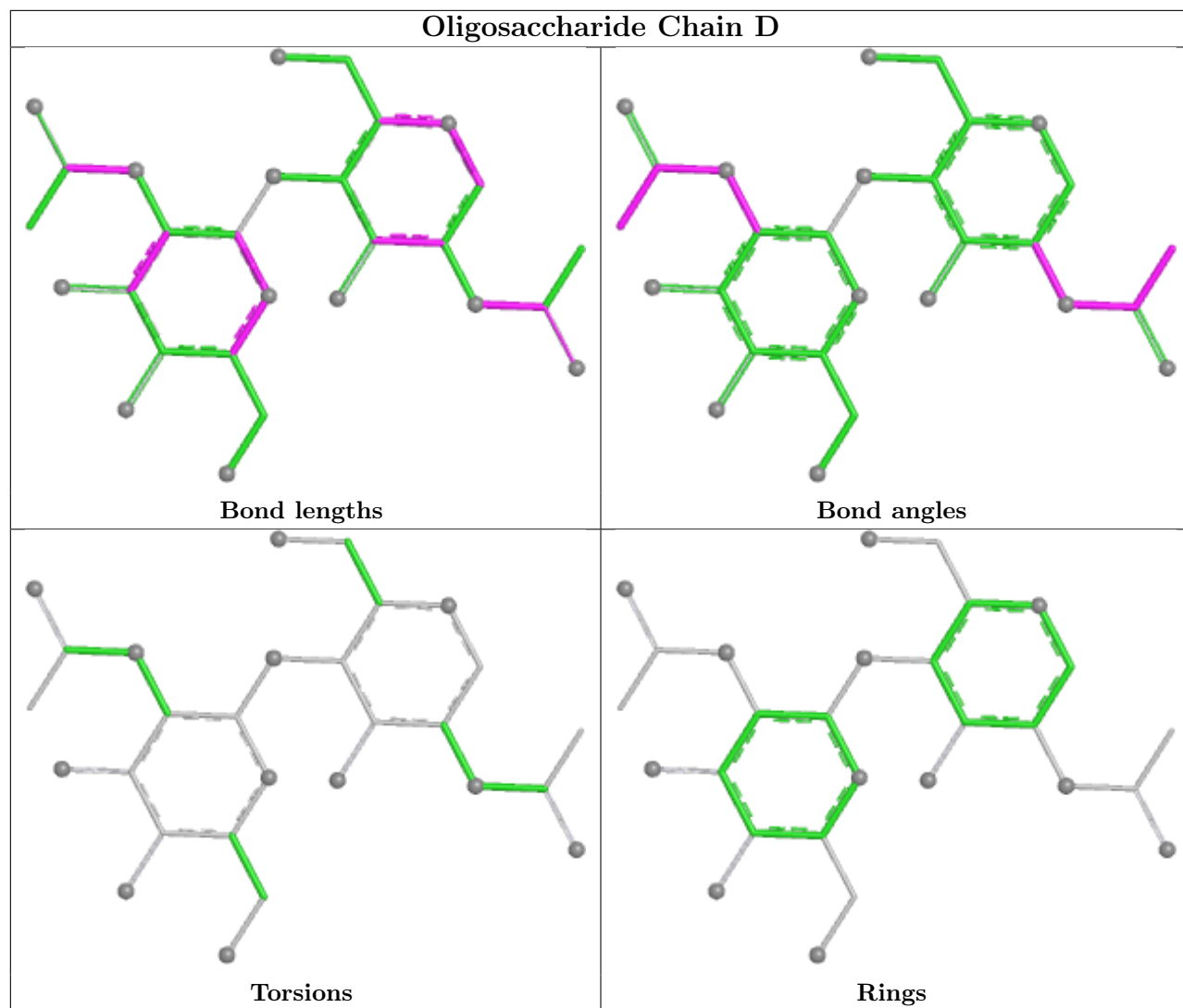
There are no ring outliers.

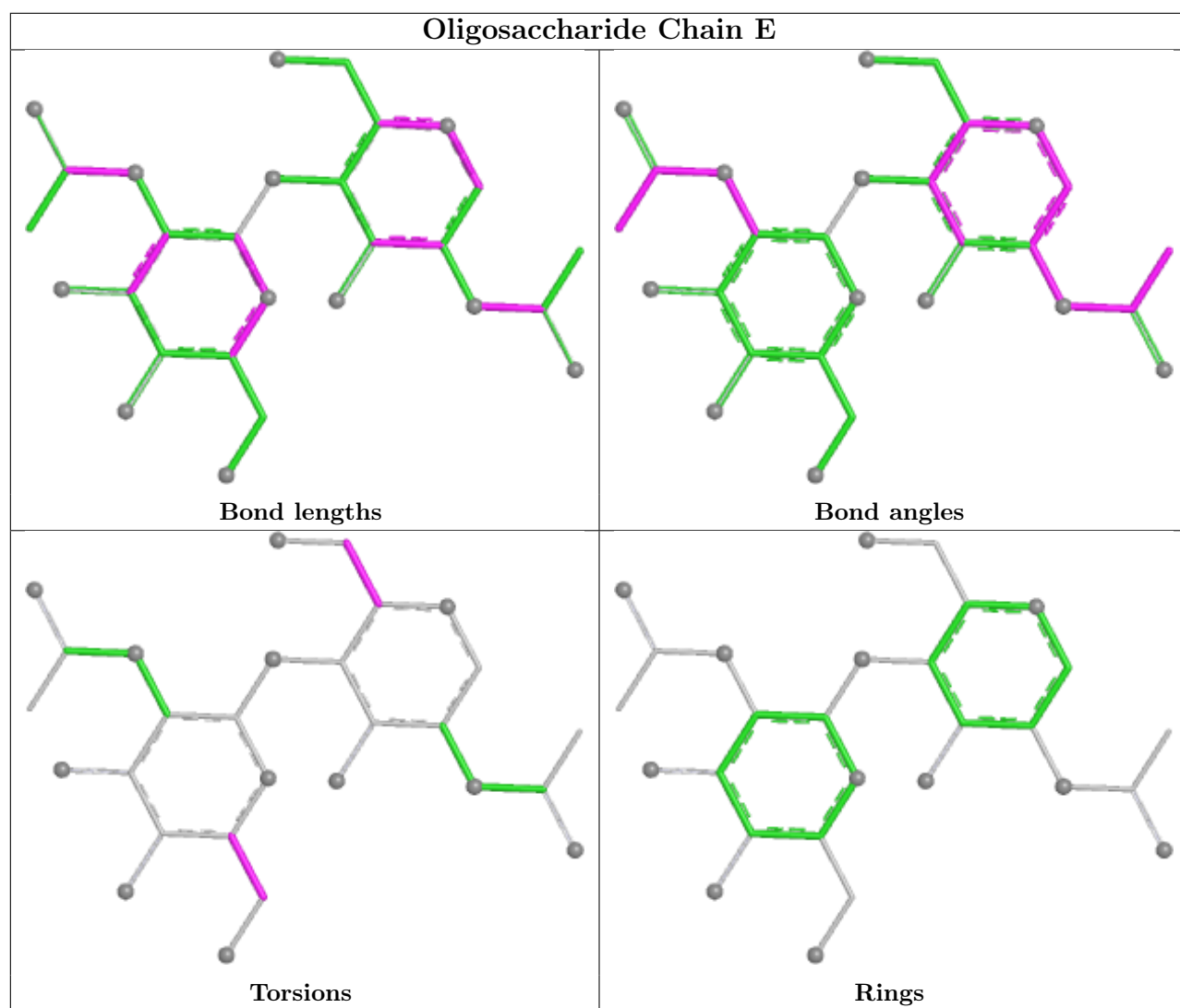
4 monomers are involved in 5 short contacts:

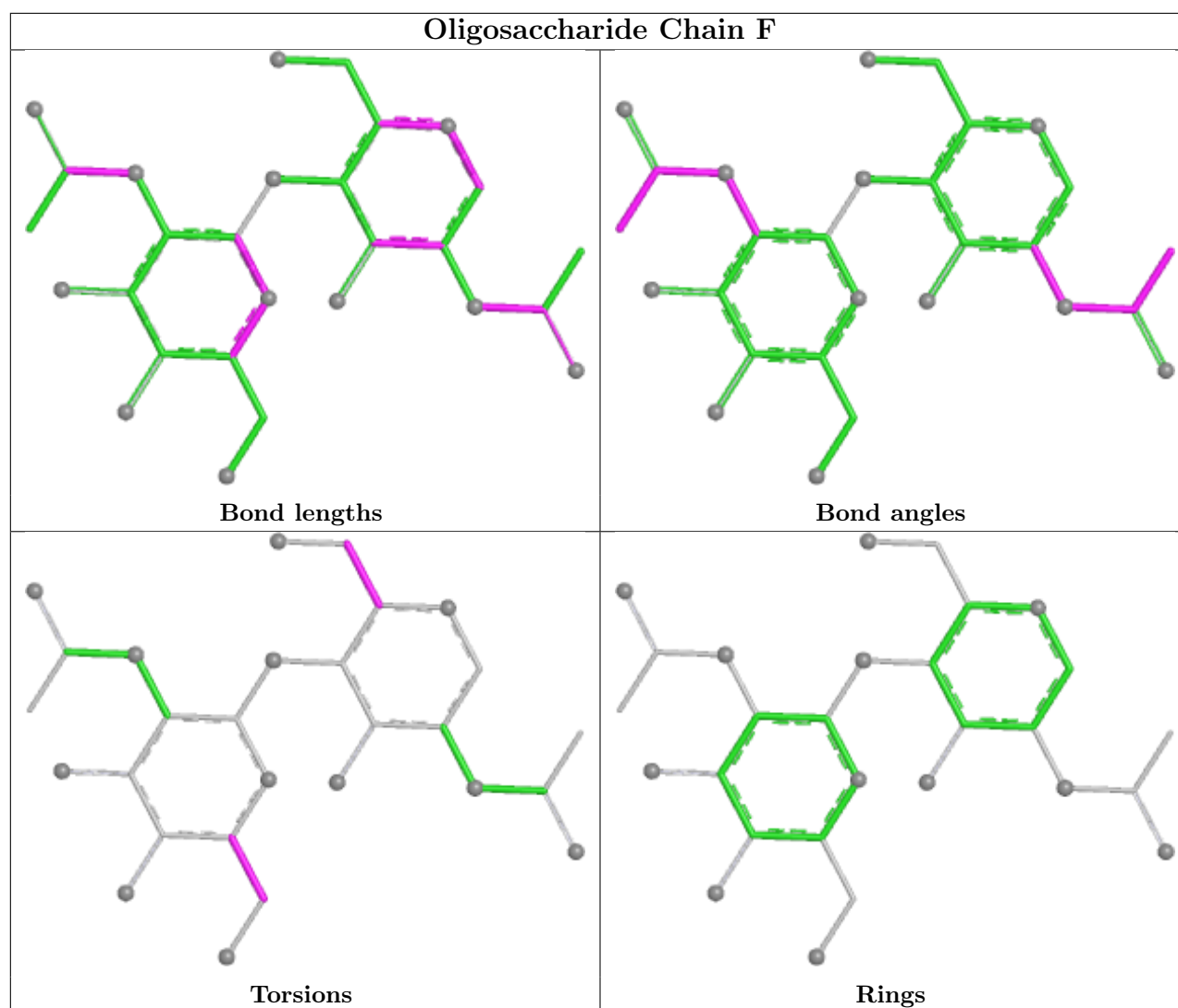
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	F	2	NAG	1	0
2	F	1	NAG	2	0
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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$
5	NAG	A	1105	1	14,14,15	1.87	3 (21%)	17,19,21	1.31	2 (11%)
5	NAG	A	1104	1	14,14,15	1.79	3 (21%)	17,19,21	1.10	2 (11%)
5	NAG	B	1108	1	14,14,15	1.82	5 (35%)	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TRP	A	1107	-	15,16,16	1.55	4 (26%)	18,22,22	1.00	1 (5%)
5	NAG	B	1107	1	14,14,15	1.78	3 (21%)	17,19,21	1.39	4 (23%)
7	H43	B	1110	-	31,31,31	3.67	11 (35%)	37,43,43	2.43	6 (16%)
5	NAG	B	1106	1	14,14,15	1.83	4 (28%)	17,19,21	1.07	1 (5%)
5	NAG	A	1106	1	14,14,15	1.80	3 (21%)	17,19,21	1.04	1 (5%)
6	TRP	B	1109	-	15,16,16	1.54	3 (20%)	18,22,22	1.04	1 (5%)
7	H43	A	1108	-	31,31,31	3.67	11 (35%)	37,43,43	2.43	6 (16%)

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
5	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1104	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1108	1	-	2/6/23/26	0/1/1/1
6	TRP	A	1107	-	-	1/8/8/8	0/2/2/2
5	NAG	B	1107	1	-	3/6/23/26	0/1/1/1
7	H43	B	1110	-	-	8/16/35/35	0/4/4/4
5	NAG	B	1106	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1106	1	-	4/6/23/26	0/1/1/1
6	TRP	B	1109	-	-	2/8/8/8	0/2/2/2
7	H43	A	1108	-	-	8/16/35/35	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1110	H43	C10-C11	-10.73	1.34	1.53
7	A	1108	H43	C10-C11	-10.71	1.34	1.53
7	B	1110	H43	C25-C26	-9.87	1.34	1.52
7	A	1108	H43	C25-C26	-9.87	1.34	1.52
7	A	1108	H43	C26-N9	7.36	1.59	1.46
7	B	1110	H43	C26-N9	7.34	1.59	1.46
7	A	1108	H43	C10-N9	7.32	1.57	1.46
7	B	1110	H43	C10-N9	7.32	1.57	1.46
7	B	1110	H43	C25-C11	4.58	1.64	1.52
7	A	1108	H43	C25-C11	4.57	1.64	1.52
7	A	1108	H43	C15-C20	-4.21	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1110	H43	C15-C20	-4.17	1.35	1.43
7	B	1110	H43	C8-N9	3.90	1.49	1.38
7	A	1108	H43	C8-N9	3.89	1.49	1.38
7	A	1108	H43	C4-C5	3.88	1.57	1.51
7	B	1110	H43	C4-C5	3.85	1.57	1.51
5	A	1106	NAG	C7-N2	3.55	1.45	1.34
5	B	1107	NAG	C7-N2	3.55	1.45	1.34
5	B	1106	NAG	C7-N2	3.54	1.45	1.34
5	B	1108	NAG	C7-N2	3.50	1.45	1.34
5	A	1105	NAG	C7-N2	3.44	1.45	1.34
5	A	1104	NAG	C7-N2	3.42	1.45	1.34
5	A	1105	NAG	O5-C1	3.36	1.49	1.43
5	A	1104	NAG	O5-C1	3.09	1.48	1.43
6	A	1107	TRP	CD1-NE1	-3.04	1.32	1.37
6	B	1109	TRP	CD1-NE1	-3.01	1.32	1.37
5	A	1106	NAG	O5-C1	3.00	1.48	1.43
5	B	1106	NAG	O5-C1	2.93	1.48	1.43
5	B	1108	NAG	O5-C1	2.89	1.48	1.43
6	B	1109	TRP	CD2-CE2	-2.88	1.37	1.41
5	B	1107	NAG	O5-C1	2.86	1.48	1.43
6	A	1107	TRP	CD2-CE2	-2.83	1.37	1.41
7	B	1110	H43	C14-C15	-2.76	1.38	1.43
7	A	1108	H43	C14-C15	-2.74	1.38	1.43
5	B	1108	NAG	O5-C5	2.65	1.48	1.43
5	B	1106	NAG	O5-C5	2.58	1.48	1.43
5	A	1105	NAG	O5-C5	2.54	1.48	1.43
5	B	1107	NAG	O5-C5	2.47	1.48	1.43
5	A	1106	NAG	O5-C5	2.29	1.47	1.43
5	A	1104	NAG	O5-C5	2.27	1.47	1.43
6	B	1109	TRP	CE2-NE1	-2.27	1.34	1.37
6	A	1107	TRP	CE2-NE1	-2.24	1.34	1.37
6	A	1107	TRP	CD2-CG	-2.20	1.40	1.44
7	A	1108	H43	C13-N12	-2.20	1.43	1.47
7	B	1110	H43	C13-N12	-2.19	1.43	1.47
7	B	1110	H43	C4-C2	2.14	1.55	1.51
5	B	1106	NAG	C3-C2	-2.13	1.48	1.52
7	A	1108	H43	C4-C2	2.13	1.55	1.51
5	B	1108	NAG	C3-C2	-2.10	1.48	1.52
5	B	1108	NAG	C2-N2	2.02	1.49	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1110	H43	C10-N9-C8	-10.00	107.77	122.71
7	A	1108	H43	C10-N9-C8	-9.99	107.78	122.71
7	B	1110	H43	C26-N9-C8	-6.38	112.26	123.53
7	A	1108	H43	C26-N9-C8	-6.36	112.29	123.53
7	B	1110	H43	C13-N12-C11	-5.90	107.07	116.30
7	A	1108	H43	C13-N12-C11	-5.90	107.08	116.30
7	A	1108	H43	C16-C15-C14	-3.15	119.54	123.37
5	A	1105	NAG	C2-N2-C7	-3.12	118.72	122.90
7	B	1110	H43	C16-C15-C14	-3.11	119.59	123.37
5	B	1107	NAG	C3-C4-C5	2.78	115.28	110.23
5	A	1105	NAG	C8-C7-N2	2.47	120.21	116.12
6	B	1109	TRP	CZ2-CE2-CD2	-2.41	119.86	122.19
5	A	1104	NAG	C8-C7-N2	2.40	120.09	116.12
5	B	1107	NAG	C8-C7-N2	2.27	119.89	116.12
5	B	1108	NAG	C3-C4-C5	2.21	114.24	110.23
6	A	1107	TRP	CZ2-CE2-CD2	-2.21	120.05	122.19
5	B	1107	NAG	C2-N2-C7	-2.19	119.97	122.90
7	A	1108	H43	C7-C8-N9	-2.18	118.36	121.39
7	B	1110	H43	C7-C8-N9	-2.18	118.37	121.39
5	B	1108	NAG	C6-C5-C4	-2.15	107.74	113.02
5	A	1104	NAG	C2-N2-C7	-2.11	120.08	122.90
7	A	1108	H43	C16-C15-C20	2.10	120.63	117.92
5	B	1106	NAG	C6-C5-C4	-2.09	107.90	113.02
7	B	1110	H43	C16-C15-C20	2.07	120.60	117.92
5	B	1107	NAG	C4-C3-C2	2.02	113.98	111.02
5	A	1106	NAG	C8-C7-N2	2.01	119.46	116.12

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1108	H43	C10-C11-N12-C13
7	A	1108	H43	C25-C11-N12-C13
7	B	1110	H43	C10-C11-N12-C13
7	B	1110	H43	C25-C11-N12-C13
5	A	1106	NAG	O5-C5-C6-O6
5	B	1107	NAG	O5-C5-C6-O6
5	A	1104	NAG	O5-C5-C6-O6
5	A	1106	NAG	C4-C5-C6-O6
7	A	1108	H43	C27-C8-N9-C10
7	B	1110	H43	C27-C8-N9-C10
5	B	1107	NAG	C4-C5-C6-O6
7	A	1108	H43	C7-C8-N9-C10

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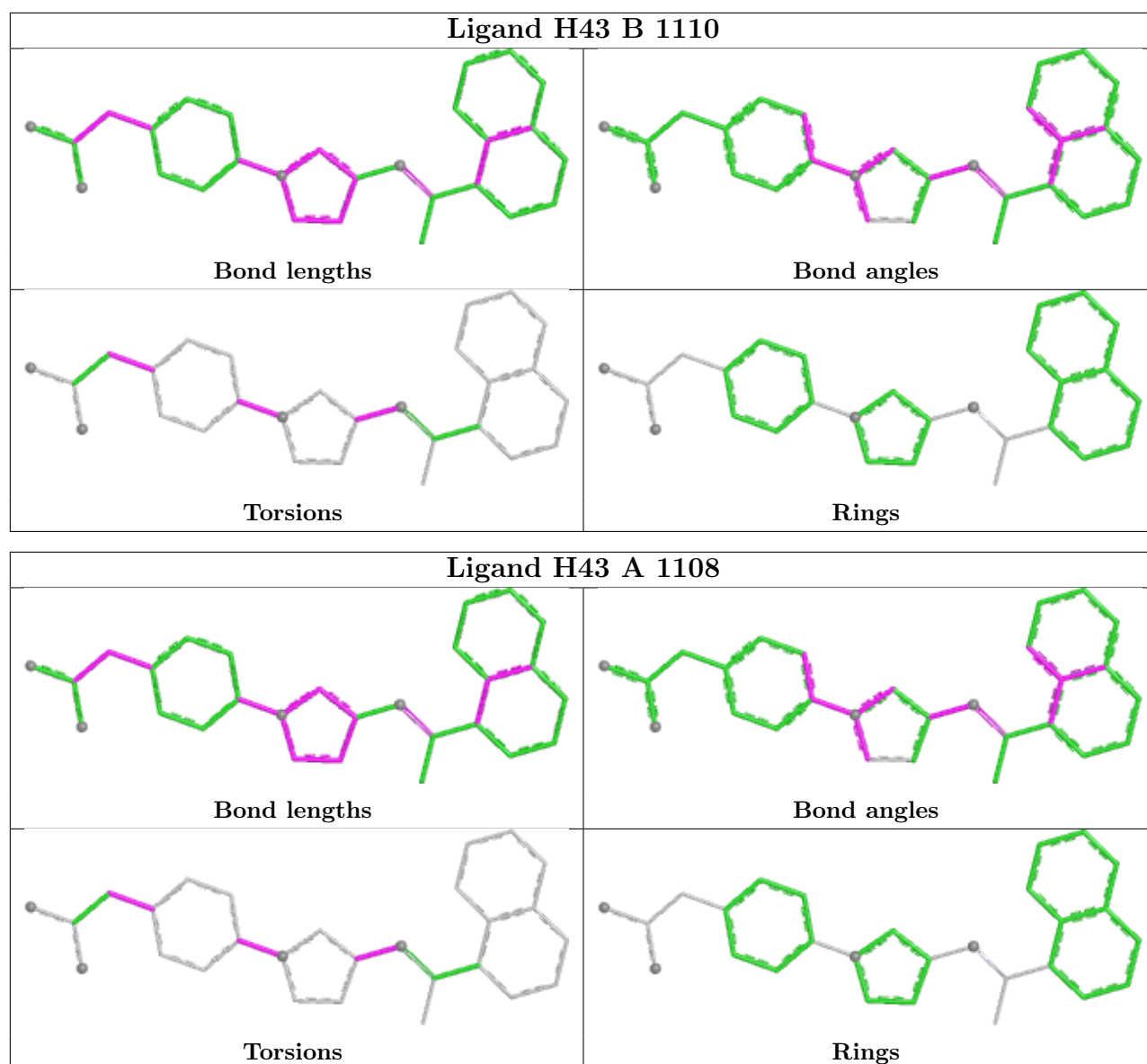
Mol	Chain	Res	Type	Atoms
7	B	1110	H43	C7-C8-N9-C10
7	A	1108	H43	C2-C4-C5-C6
7	B	1110	H43	C2-C4-C5-C6
5	A	1104	NAG	C4-C5-C6-O6
7	A	1108	H43	C2-C4-C5-C28
7	B	1110	H43	C2-C4-C5-C28
7	A	1108	H43	C7-C8-N9-C26
7	B	1110	H43	C7-C8-N9-C26
7	A	1108	H43	C27-C8-N9-C26
7	B	1110	H43	C27-C8-N9-C26
5	A	1106	NAG	C1-C2-N2-C7
5	B	1106	NAG	C1-C2-N2-C7
5	B	1108	NAG	C1-C2-N2-C7
6	B	1109	TRP	CA-CB-CG-CD1
6	A	1107	TRP	N-CA-CB-CG
6	B	1109	TRP	CA-CB-CG-CD2
5	A	1106	NAG	C3-C2-N2-C7
5	B	1106	NAG	C3-C2-N2-C7
5	B	1107	NAG	C3-C2-N2-C7
5	B	1108	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1107	TRP	2	0
7	B	1110	H43	12	0
6	B	1109	TRP	1	0
7	A	1108	H43	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

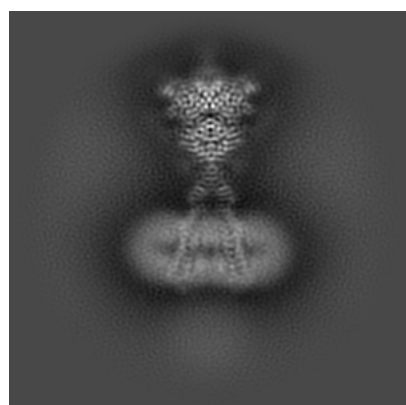
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30647. These allow visual inspection of the internal detail of the map and identification of artifacts.

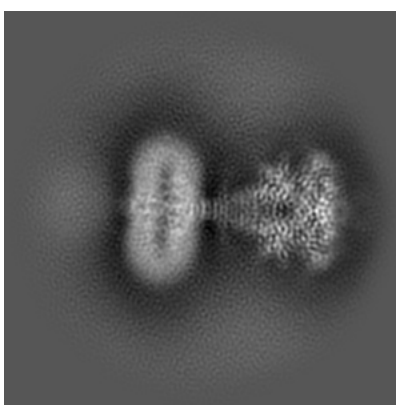
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

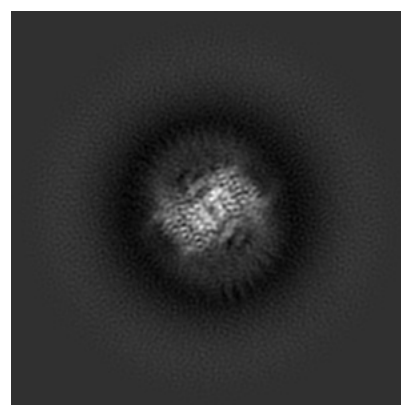
6.1.1 Primary map



X



Y

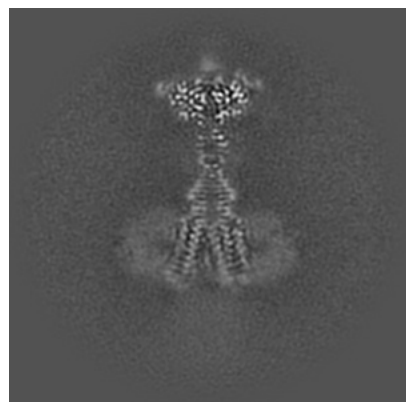


Z

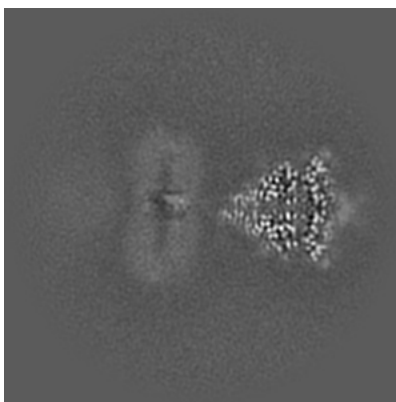
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

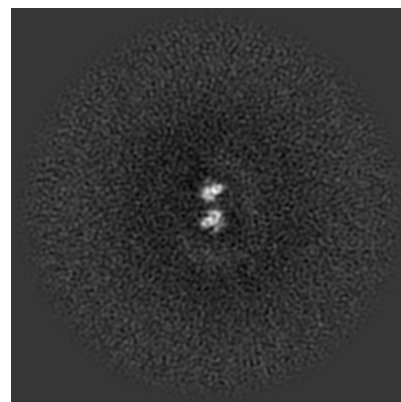
6.2.1 Primary map



X Index: 150



Y Index: 150

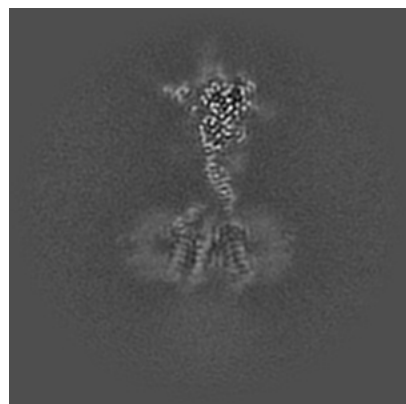


Z Index: 150

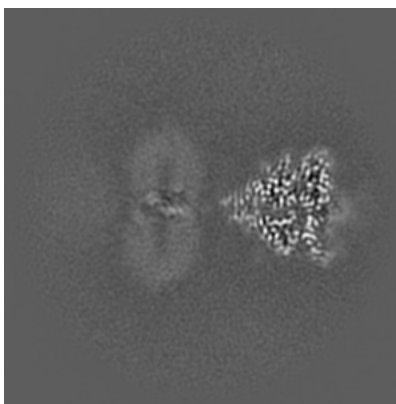
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

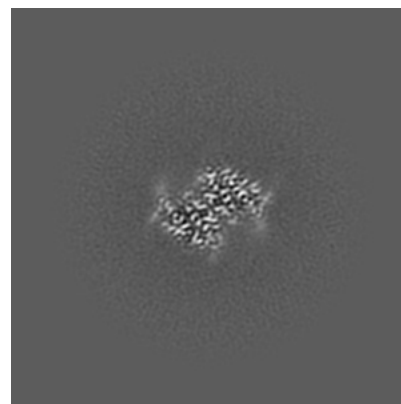
6.3.1 Primary map



X Index: 157



Y Index: 153

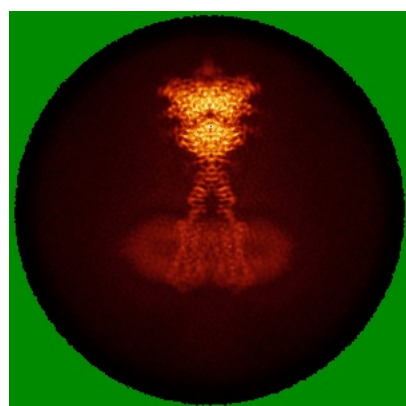


Z Index: 234

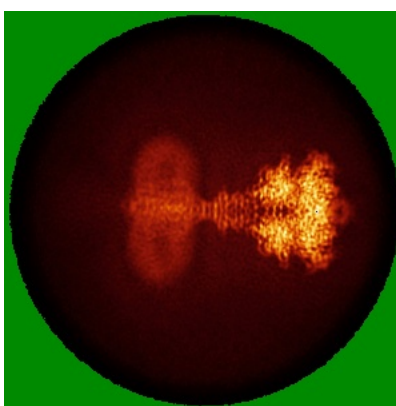
The images above show the largest variance slices of the map in three orthogonal directions.

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

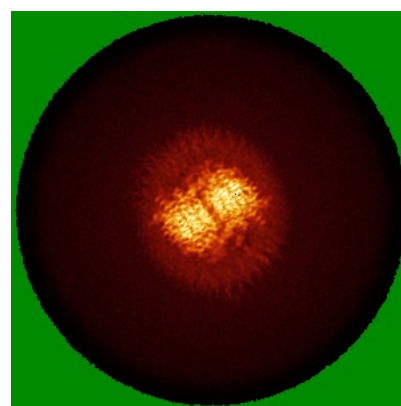
6.4.1 Primary map



X



Y

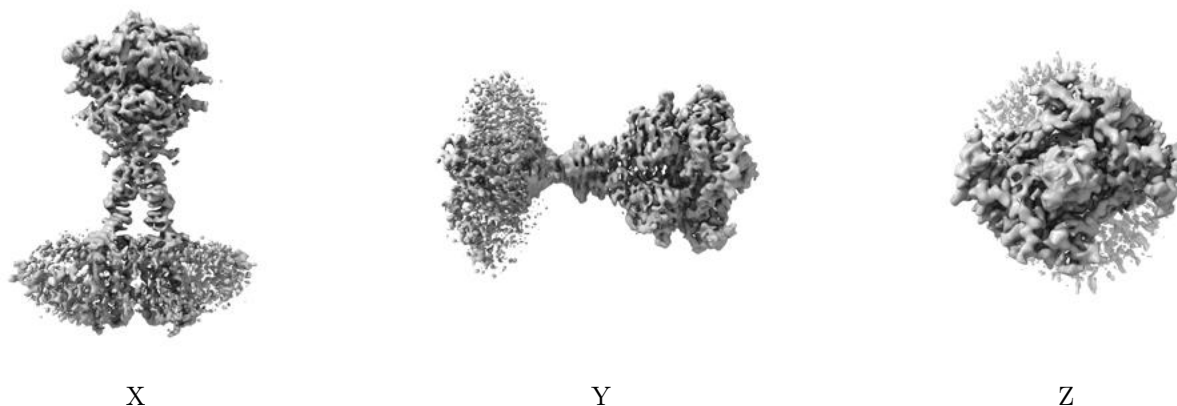


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

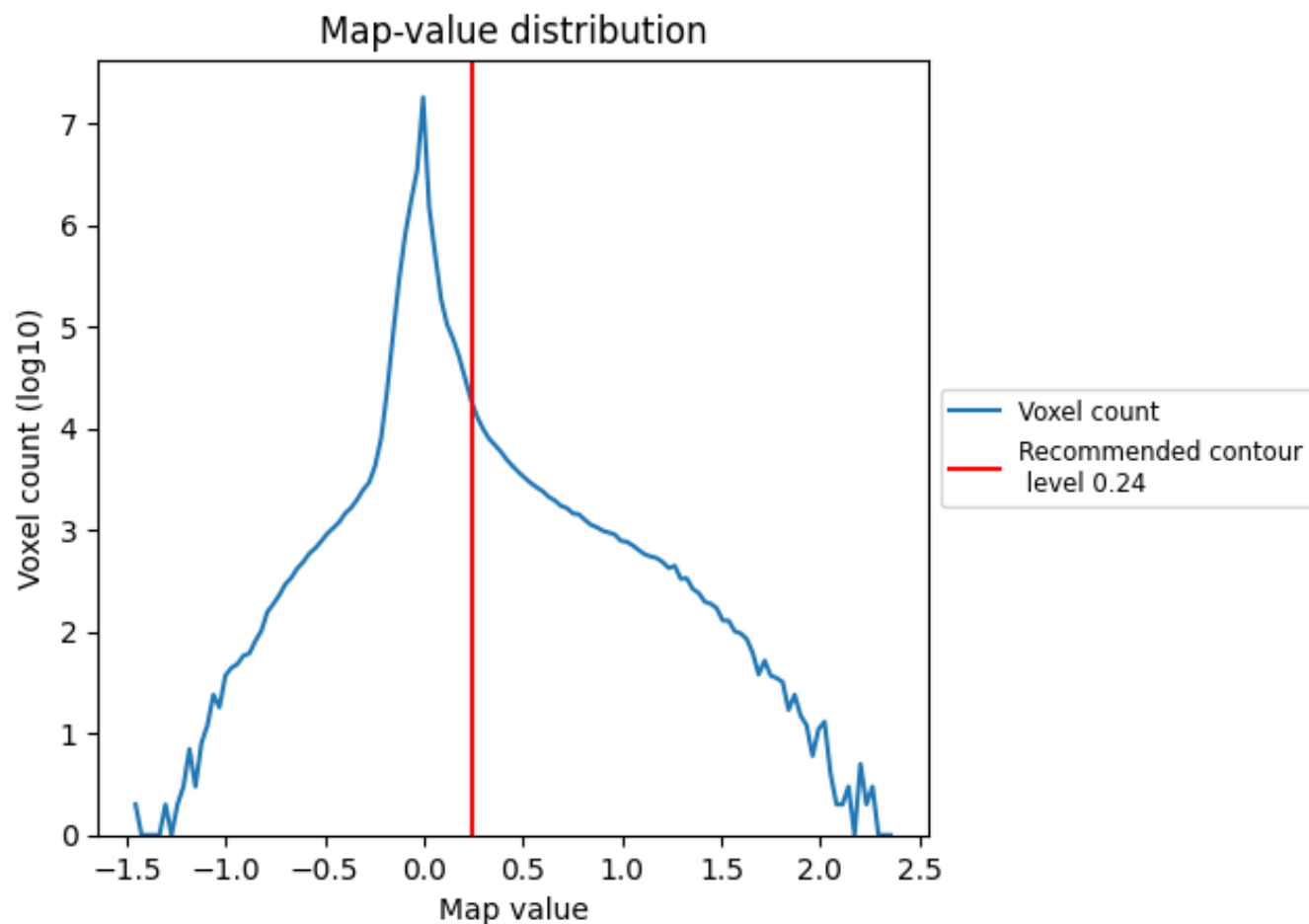
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

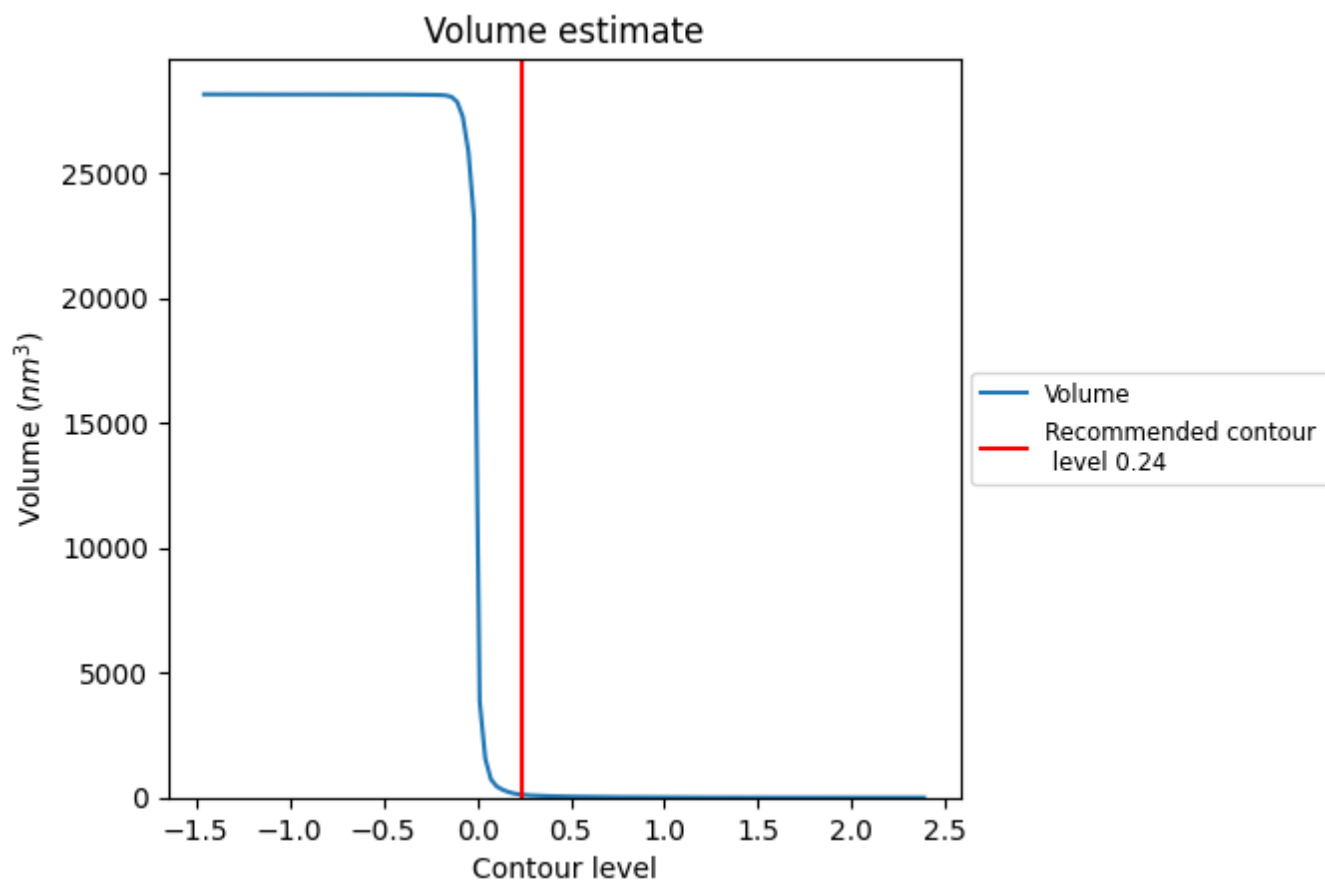
This section contains the results of statistical analysis of the map.

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.

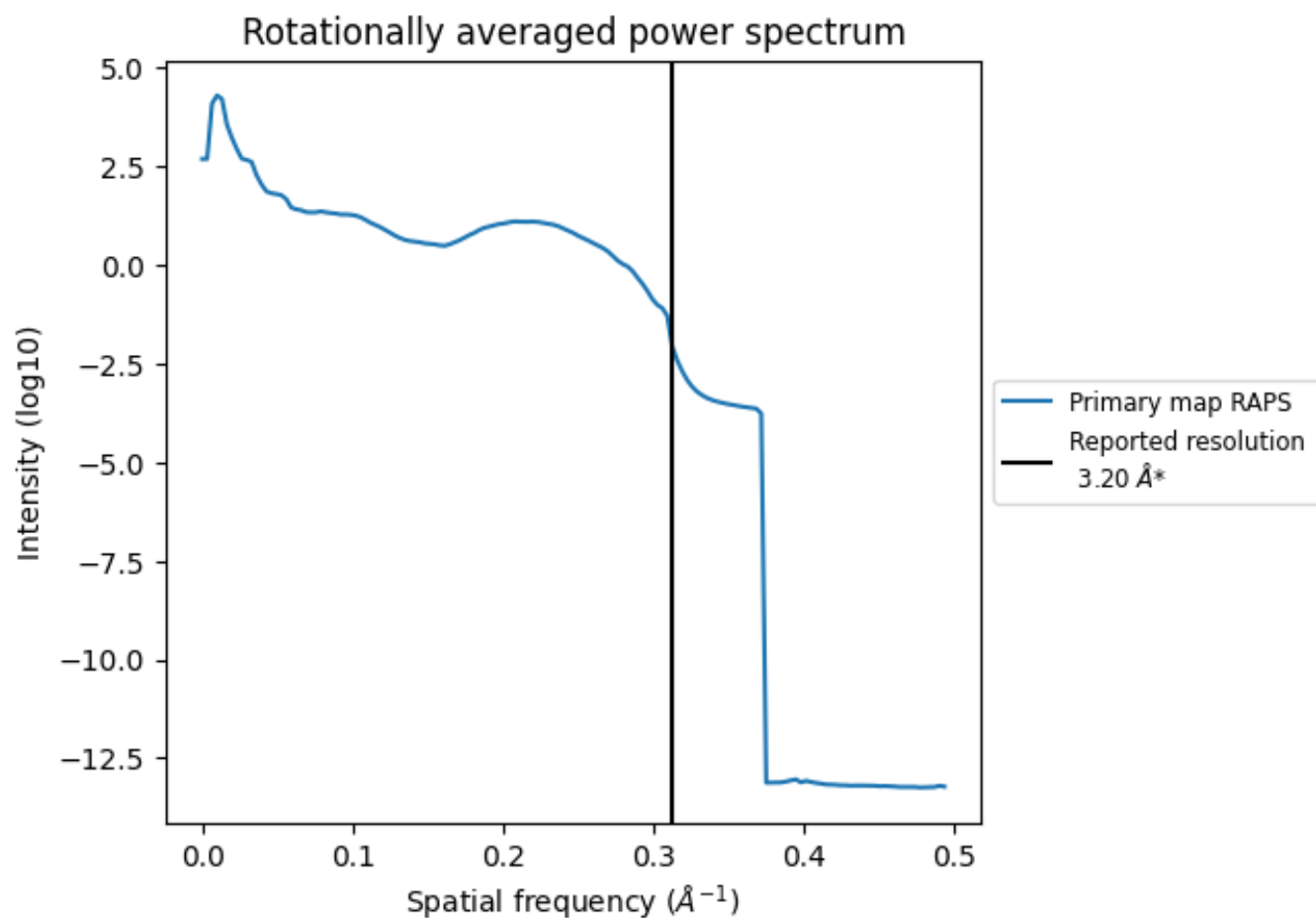
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm^3 ; this corresponds to an approximate mass of 104 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

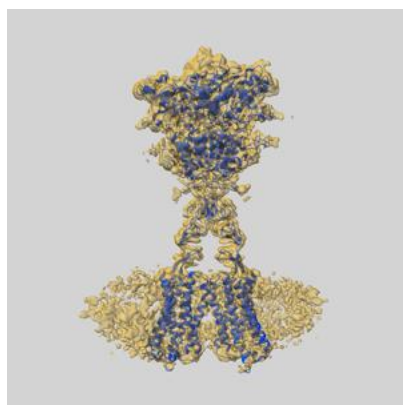
8 Fourier-Shell correlation ⓘ

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

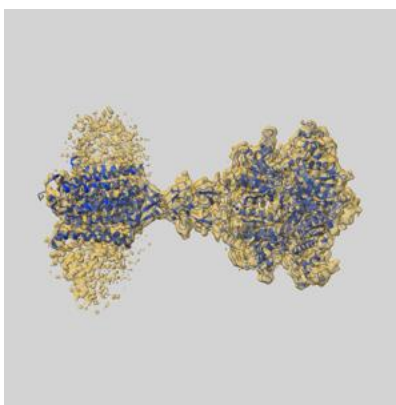
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30647 and PDB model 7DD7. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

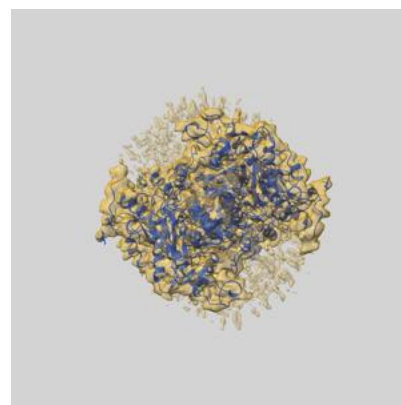
9.1 Map-model overlay [i](#)



X



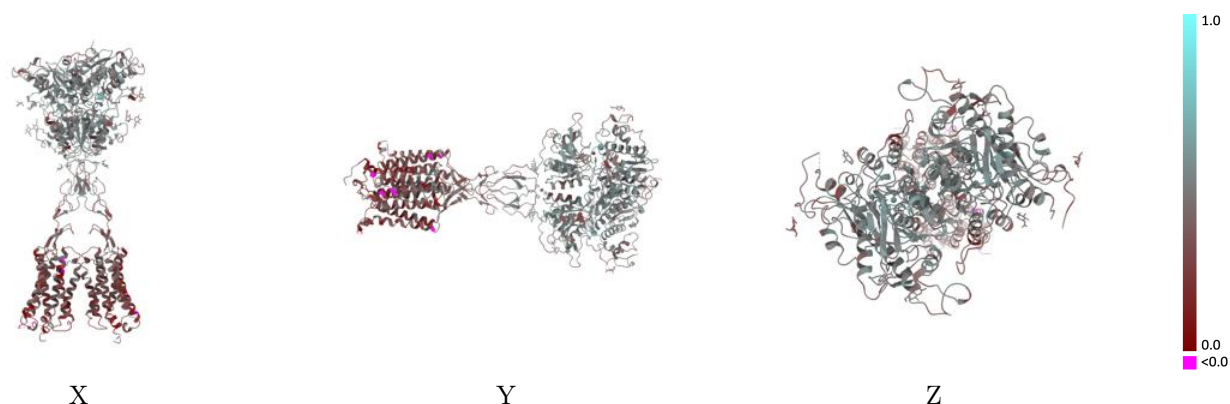
Y



Z

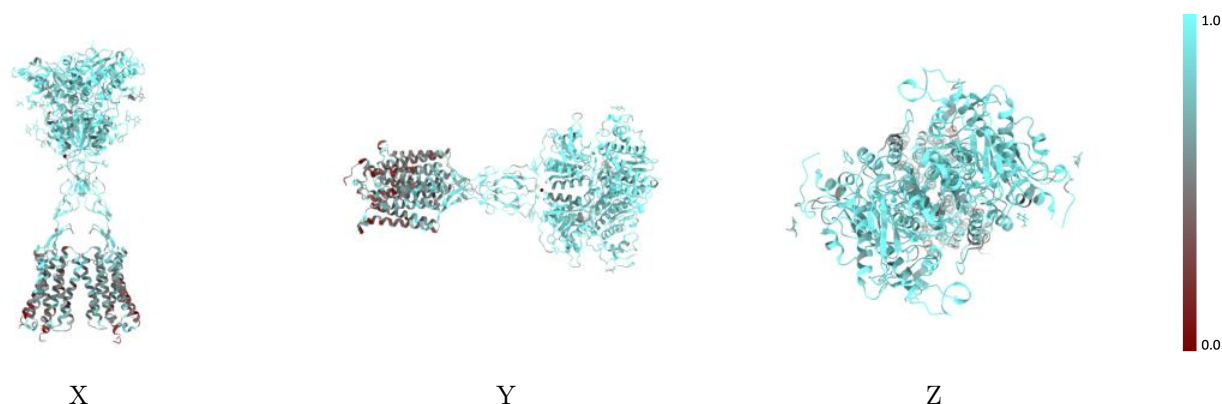
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



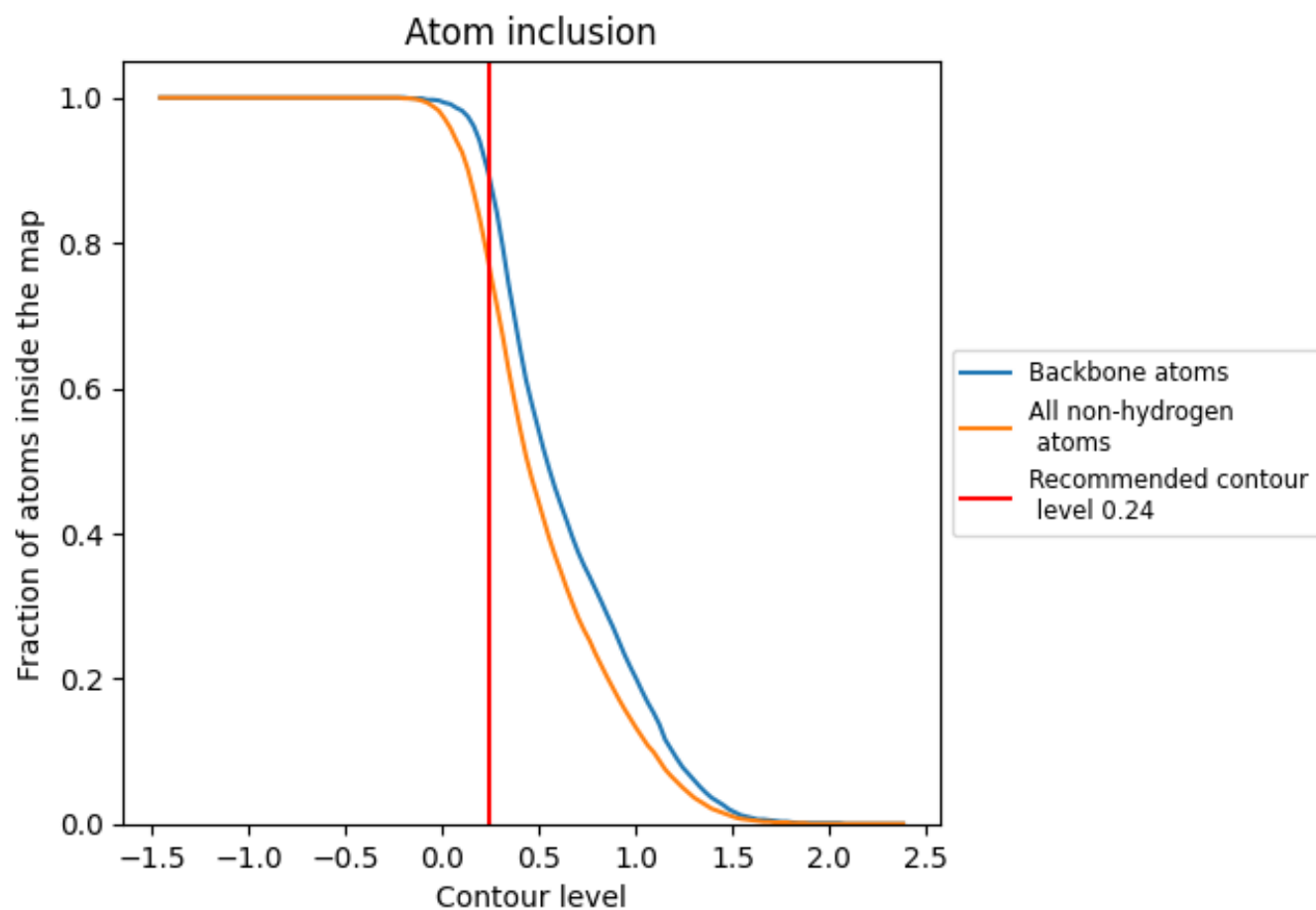
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.4140
A	0.7720	0.4090
B	0.7740	0.4190
C	0.8210	0.3580
D	0.9290	0.5030
E	0.8570	0.4710
F	0.8570	0.4890

1.0

0.0

<0.0