Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:20 pm GMT

PDB ID	:	5MKE
EMDB ID	:	EMD-3523
Title	:	cryoEM Structure of Polycystin-2 in complex with cations and lipids
Authors	:	Wilkes, M.; Madej, M.G.; Ziegler, C.
Deposited on	:	2016-12-04
Resolution	:	4.30 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:

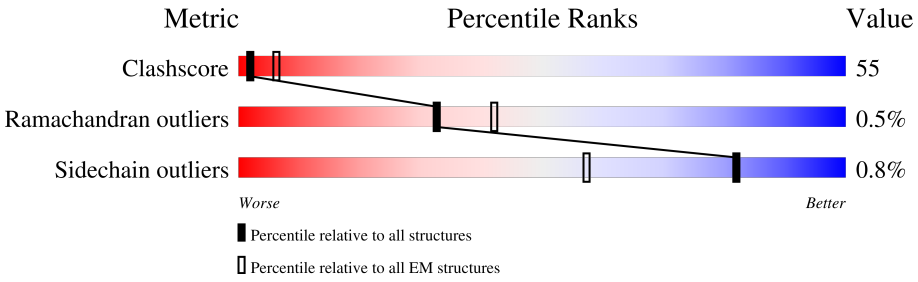
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	968	28% 14% 35% · 51%
1	B	968	28% 13% 34% · 51%
1	C	968	27% 14% 35% · 51%
1	D	968	27% 14% 34% · 51%
2	E	2	100% 50% 50%
2	F	2	100% 50% 50%
2	G	2	100% 50% 50%

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	NAG	A	1002	-	-	X	-
3	NAG	B	1002	-	-	X	-
3	NAG	C	1002	-	-	X	-
3	NAG	D	1002	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16426 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.

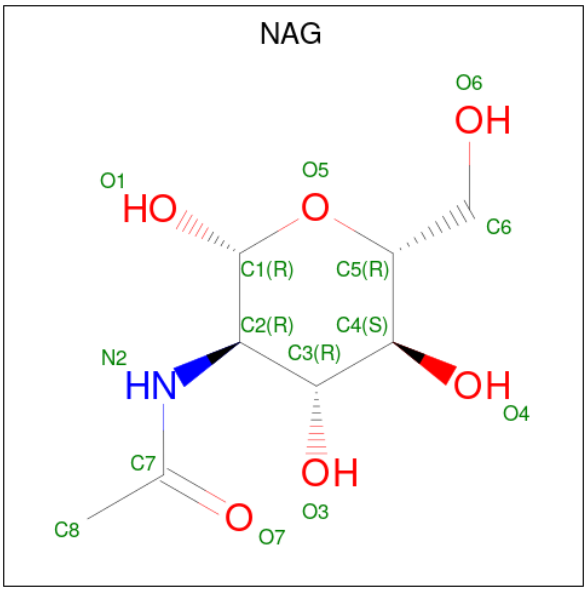
- Molecule 1 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	B	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	C	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	D	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		

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

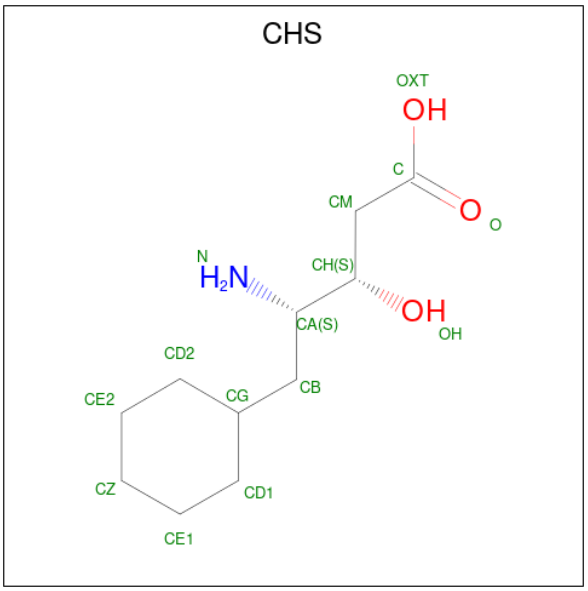
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



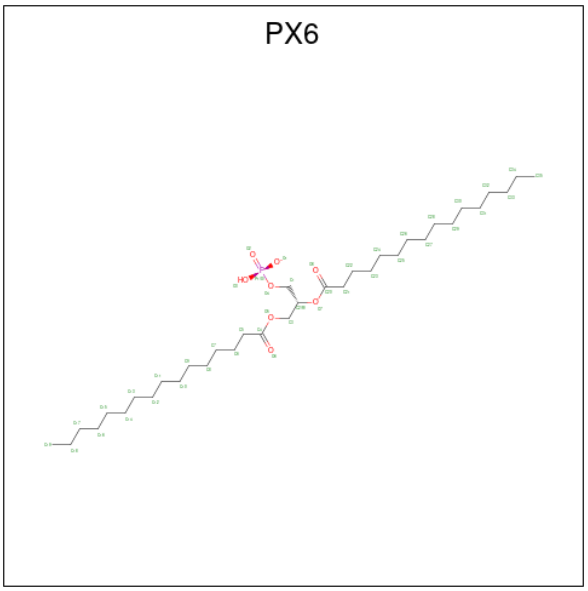
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	B	1	Total	C	N	O	0
			28	16	2	10	
3	B	1	Total	C	N	O	0
			28	16	2	10	
3	C	1	Total	C	N	O	0
			28	16	2	10	
3	C	1	Total	C	N	O	0
			28	16	2	10	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: $C_{11}H_{21}NO_3$).



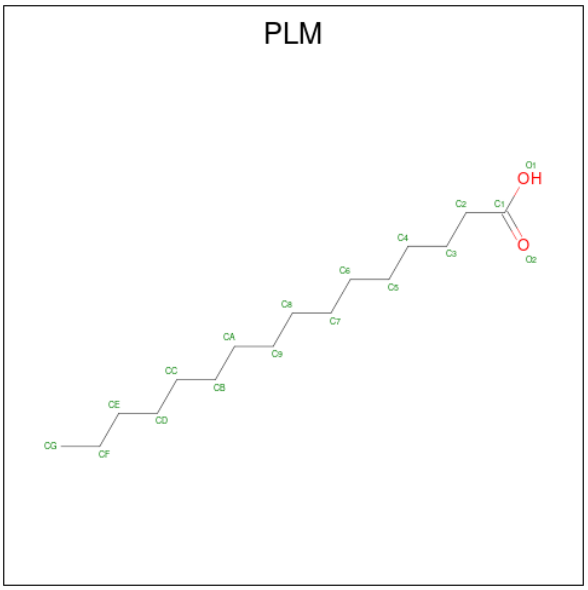
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			30	22	2	6	
4	A	1	Total	C	N	O	0
			30	22	2	6	
4	B	1	Total	C	N	O	0
			30	22	2	6	
4	B	1	Total	C	N	O	0
			30	22	2	6	
4	C	1	Total	C	N	O	0
			30	22	2	6	
4	C	1	Total	C	N	O	0
			30	22	2	6	
4	D	1	Total	C	N	O	0
			30	22	2	6	
4	D	1	Total	C	N	O	0
			30	22	2	6	

- Molecule 5 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: $C_{35}H_{68}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			40	31	8	1	
5	B	1	Total	C	O	P	0
			40	31	8	1	
5	C	1	Total	C	O	P	0
			40	31	8	1	
5	D	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			54	48	6	
6	A	1	Total	C	O	0
			54	48	6	
6	A	1	Total	C	O	0
			54	48	6	
6	B	1	Total	C	O	0
			54	48	6	
6	B	1	Total	C	O	0
			54	48	6	
6	B	1	Total	C	O	0
			54	48	6	
6	C	1	Total	C	O	0
			54	48	6	
6	C	1	Total	C	O	0
			54	48	6	
6	C	1	Total	C	O	0
			54	48	6	
6	D	1	Total	C	O	0
			54	48	6	
6	D	1	Total	C	O	0
			54	48	6	
6	D	1	Total	C	O	0
			54	48	6	

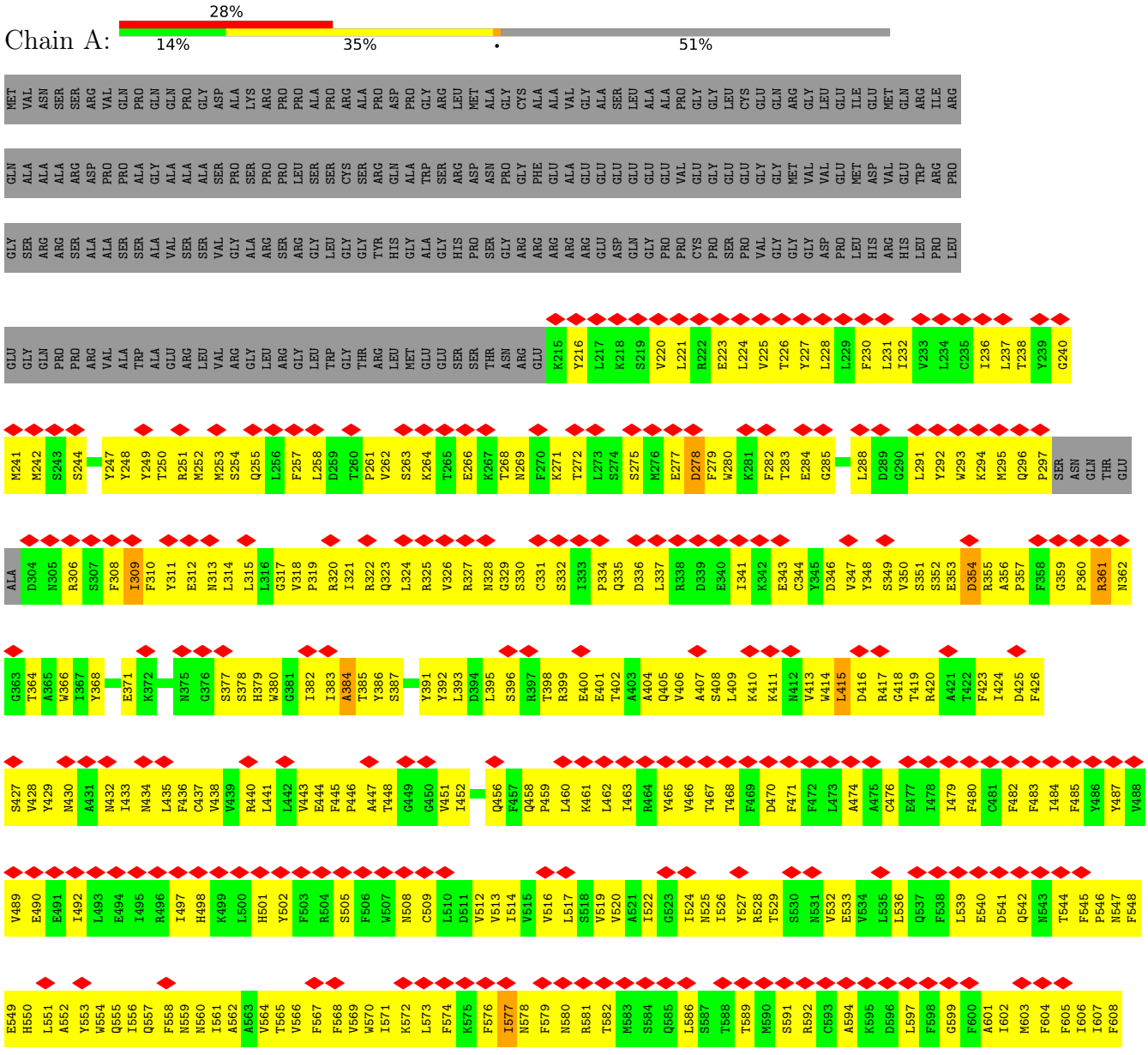
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

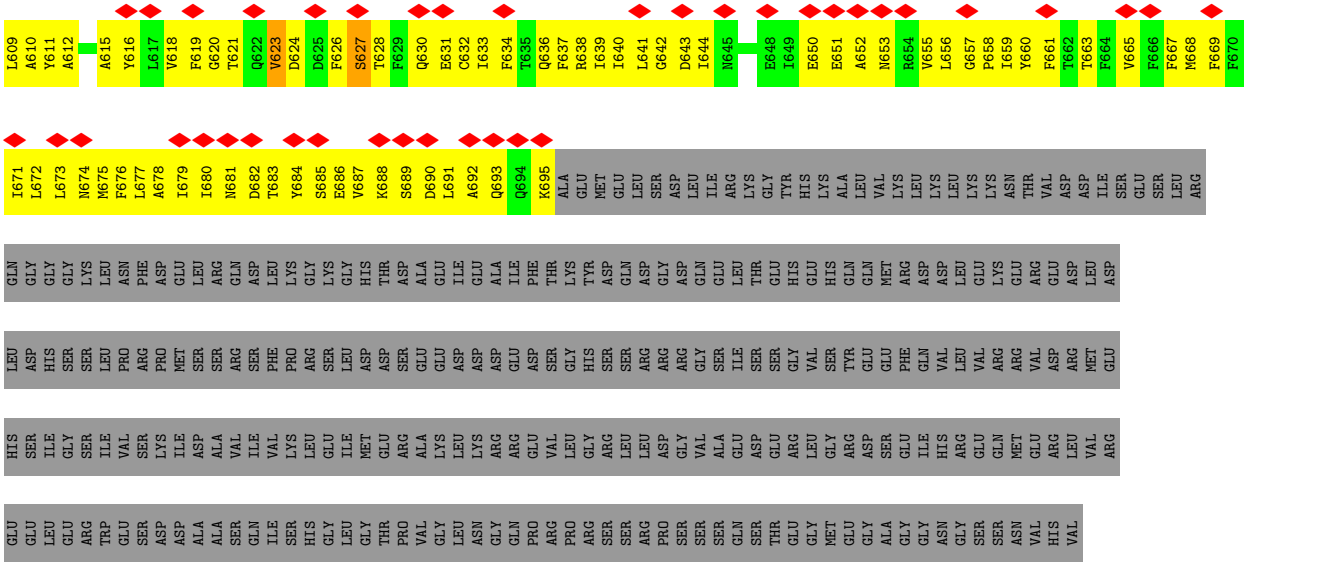
Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Ca	0
			2	2	

3 Residue-property plots (i)

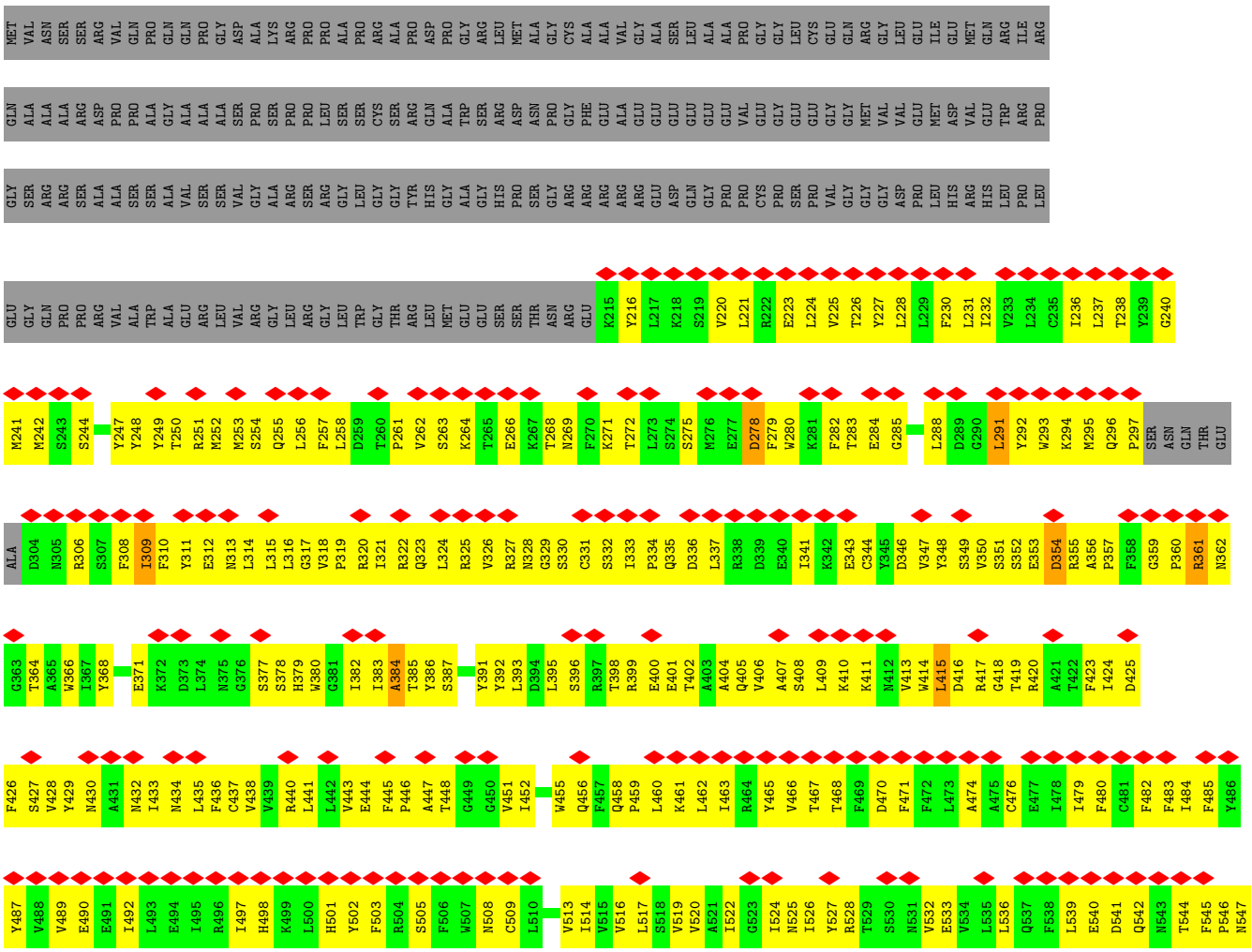
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

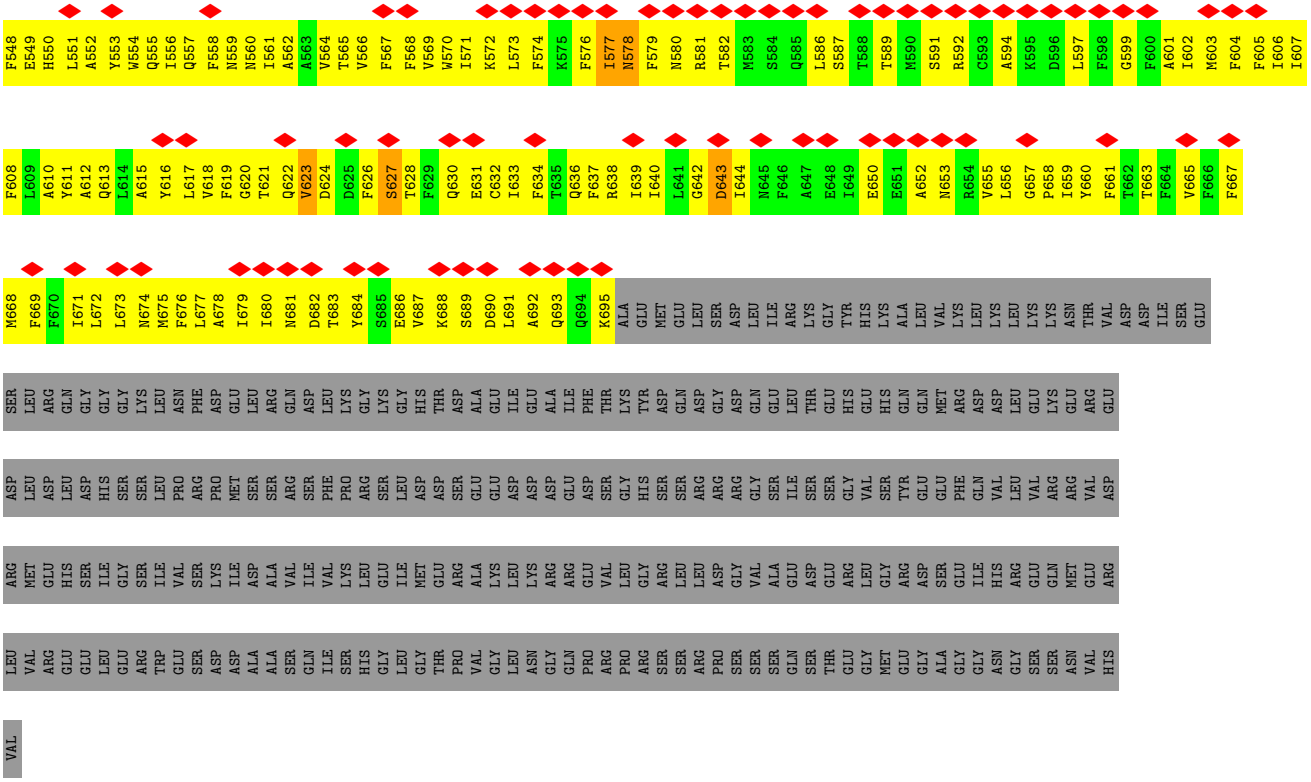
- Molecule 1: Polycystin-2





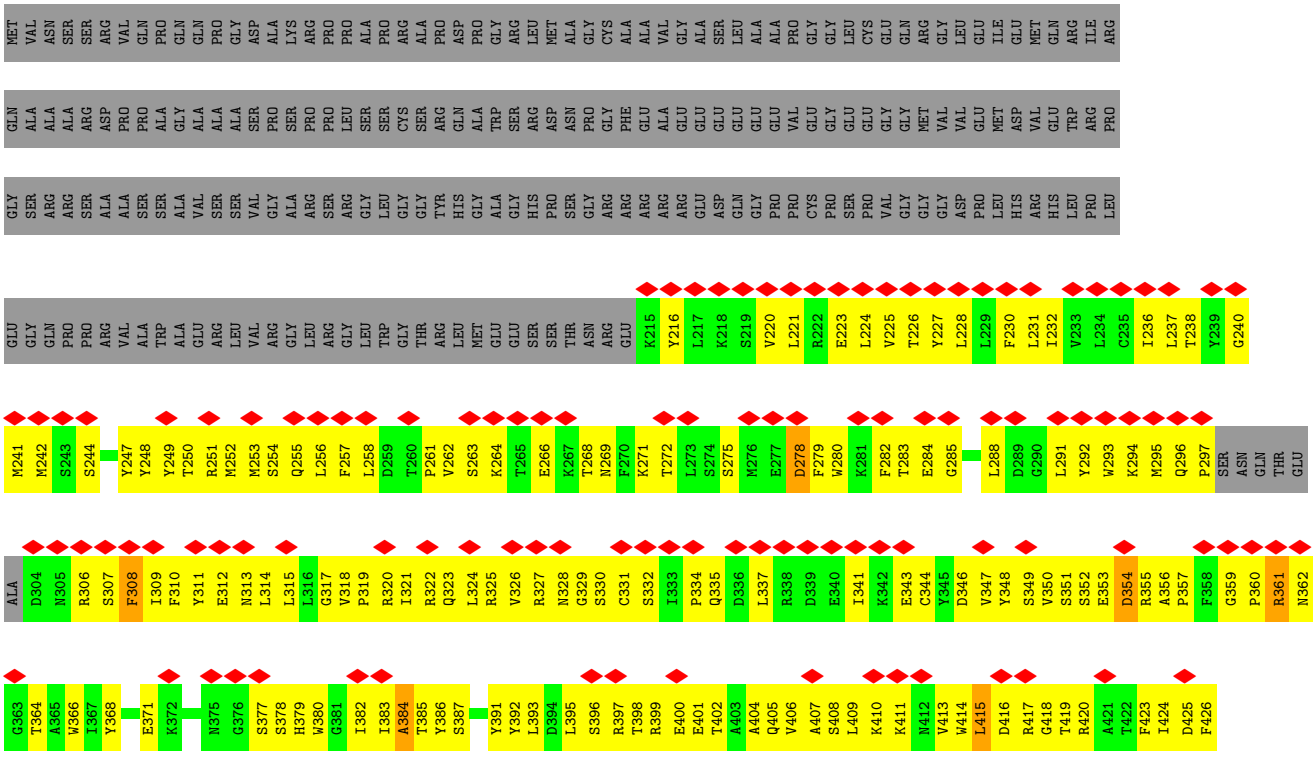
- Molecule 1: Polycystin-2

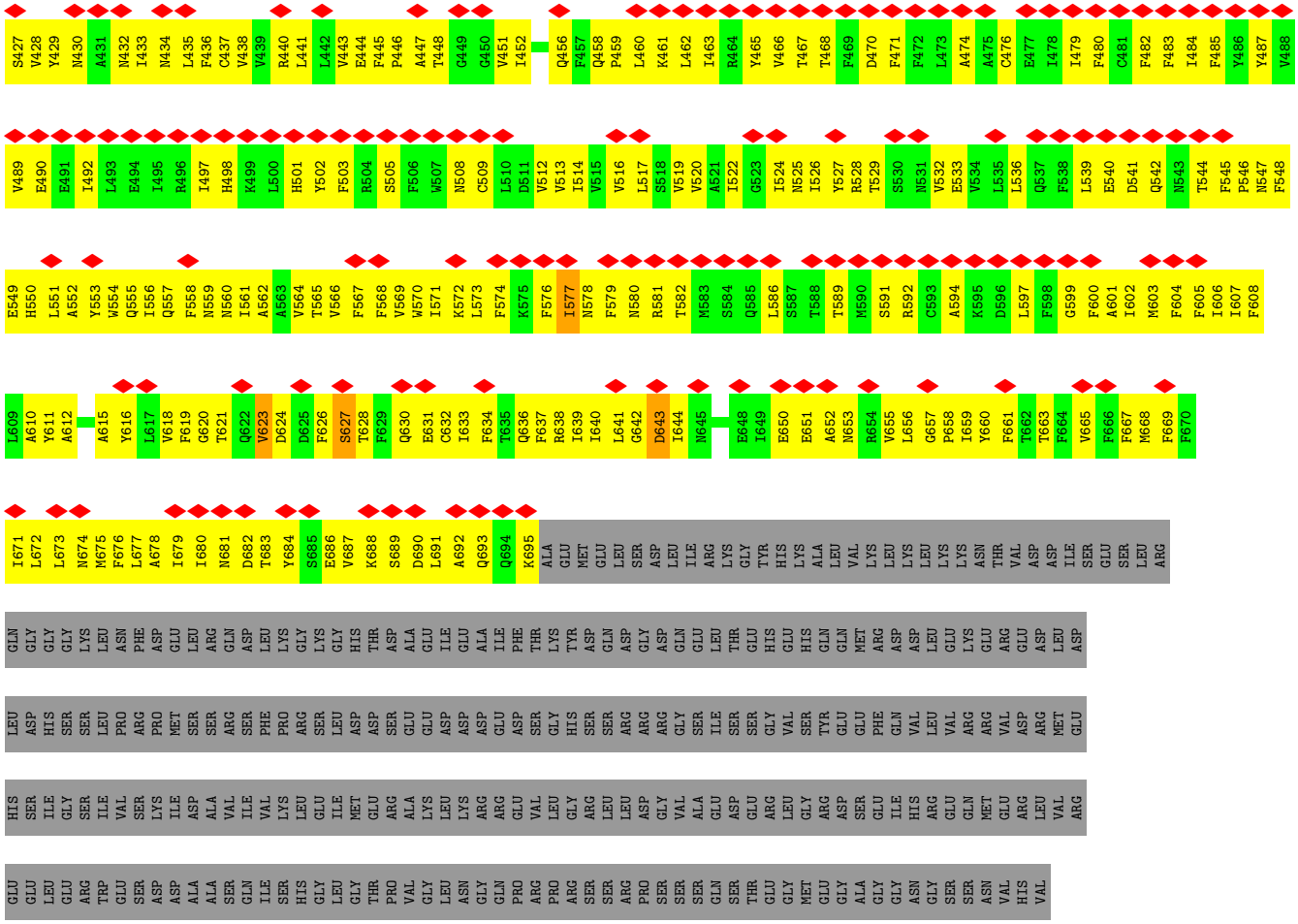




• Molecule 1: Polycystin-2

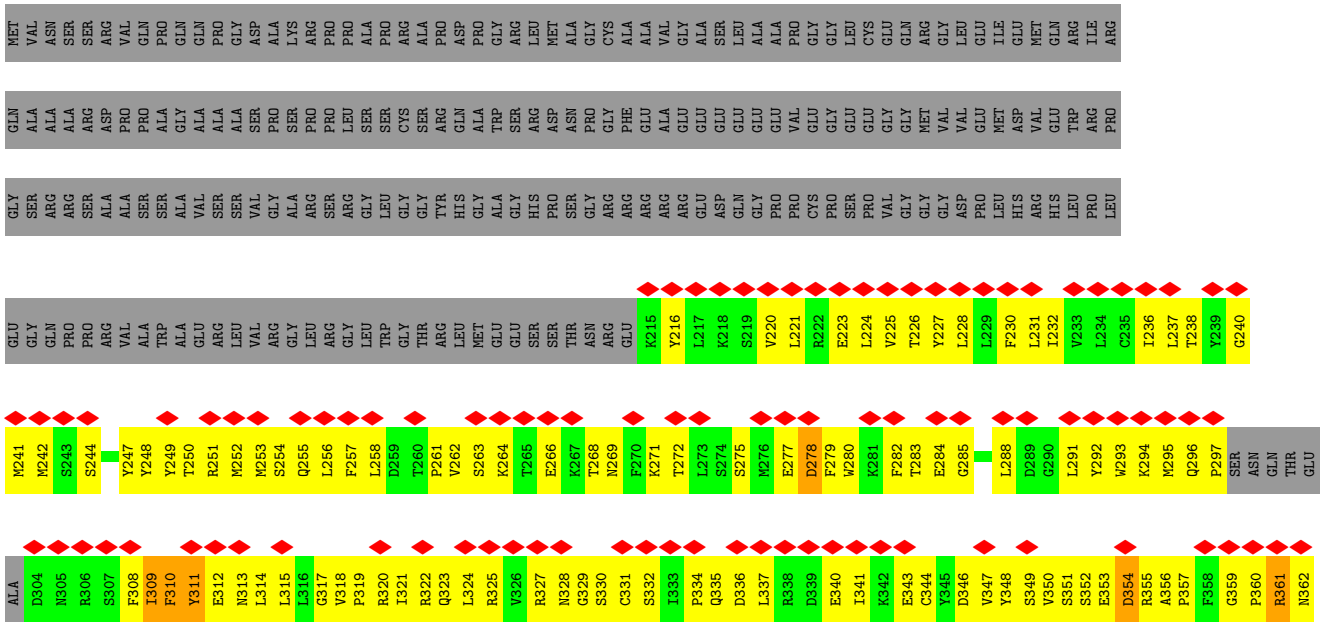
Chain C:

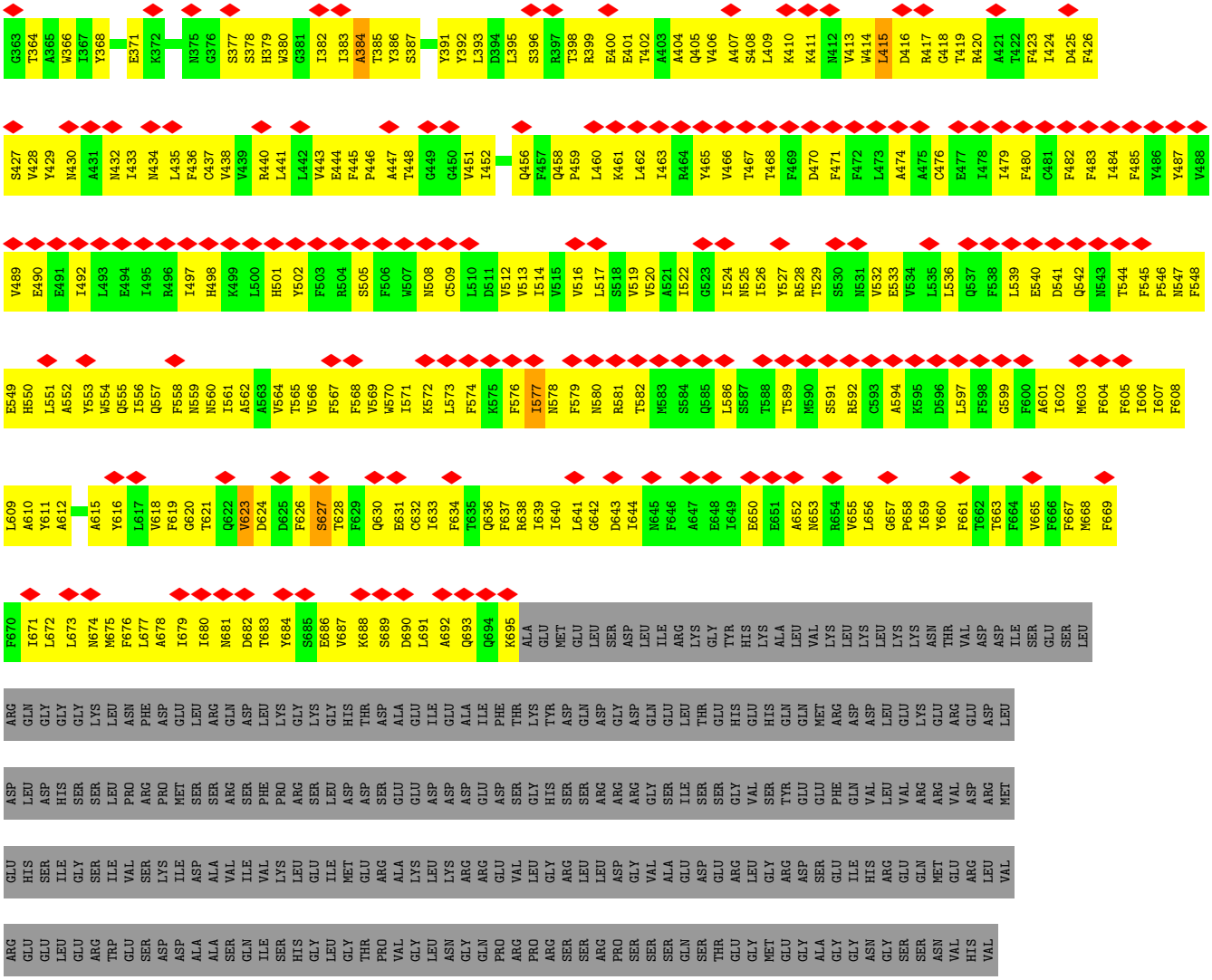




• Molecule 1: Polycystin-2

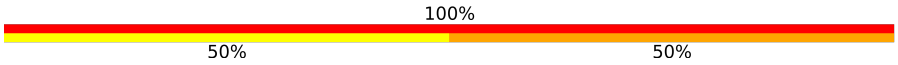
Chain D:





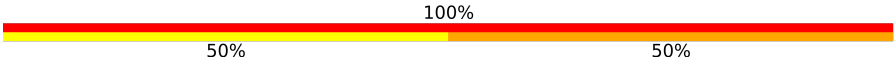
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



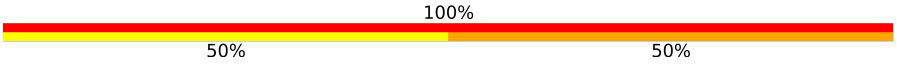
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	42268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.8	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	0.098	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0345	Depositor
Map size (Å)	191.52, 191.52, 191.52	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHS, PX6, CA, NAG, PLM

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	0.49	0/4031	0.62	2/5469 (0.0%)
1	B	0.49	0/4031	0.62	3/5469 (0.1%)
1	C	0.49	0/4031	0.62	3/5469 (0.1%)
1	D	0.49	0/4031	0.63	2/5469 (0.0%)
All	All	0.49	0/16124	0.62	10/21876 (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	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	278	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	278	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	278	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	384	ALA	C-N-CA	5.16	134.60	121.70
1	C	384	ALA	C-N-CA	5.14	134.55	121.70
1	B	384	ALA	C-N-CA	5.13	134.53	121.70
1	D	384	ALA	C-N-CA	5.12	134.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	643	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	643	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	LEU	Peptide
1	A	354	ASP	Peptide
1	A	361	ARG	Peptide
1	A	578	ASN	Peptide
1	A	627	SER	Peptide
1	B	291	LEU	Peptide
1	B	354	ASP	Peptide
1	B	361	ARG	Peptide
1	B	578	ASN	Peptide
1	B	627	SER	Peptide
1	C	291	LEU	Peptide
1	C	354	ASP	Peptide
1	C	361	ARG	Peptide
1	C	578	ASN	Peptide
1	C	627	SER	Peptide
1	D	291	LEU	Peptide
1	D	354	ASP	Peptide
1	D	361	ARG	Peptide
1	D	578	ASN	Peptide
1	D	627	SER	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	3926	0	3880	489	0
1	B	3926	0	3880	496	0
1	C	3926	0	3880	476	0
1	D	3926	0	3880	490	0
2	E	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	2	0
2	G	28	0	25	2	0
3	A	28	0	26	8	0
3	B	28	0	26	8	0
3	C	28	0	26	8	0
3	D	56	0	51	16	0
4	A	30	0	40	3	0
4	B	30	0	40	4	0
4	C	30	0	40	5	0
4	D	30	0	40	4	0
5	A	40	0	56	3	0
5	B	40	0	56	6	0
5	C	40	0	56	4	0
5	D	40	0	56	4	0
6	A	54	0	93	9	0
6	B	54	0	93	8	0
6	C	54	0	93	9	0
6	D	54	0	93	6	0
7	A	2	0	0	0	0
All	All	16426	0	16480	1816	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 55.

All (1816) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ILE:CD1	1:D:573:LEU:HD11	1.21	1.66
1:A:606:ILE:HD11	1:D:573:LEU:CD1	1.26	1.63
1:A:573:LEU:CD1	1:B:606:ILE:HD11	1.17	1.62
1:C:573:LEU:HD11	1:D:606:ILE:CD1	1.18	1.58
1:B:573:LEU:CD1	1:C:606:ILE:HD11	1.15	1.57
1:A:573:LEU:HD11	1:B:606:ILE:CD1	1.16	1.56
1:B:573:LEU:HD11	1:C:606:ILE:CD1	1.13	1.55
1:C:573:LEU:CD1	1:D:606:ILE:HD11	1.22	1.53
1:B:573:LEU:CD1	1:C:606:ILE:CD1	1.81	1.34
1:C:573:LEU:CD1	1:D:606:ILE:CD1	1.87	1.34
1:A:573:LEU:CD1	1:B:606:ILE:CD1	1.83	1.28
1:A:606:ILE:CD1	1:D:573:LEU:CD1	1.91	1.23
1:A:309:ILE:HD11	1:A:315:LEU:N	1.52	1.22
1:B:309:ILE:HD11	1:B:315:LEU:N	1.54	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:HG12	1:B:313:ASN:O	1.42	1.18
1:A:294:LYS:HE2	1:A:310:PHE:H	1.10	1.14
1:A:309:ILE:HG12	1:A:313:ASN:O	1.46	1.13
1:B:361:ARG:O	3:B:1002:NAG:H82	1.50	1.12
1:C:361:ARG:O	3:C:1002:NAG:H82	1.50	1.11
1:A:361:ARG:O	3:A:1002:NAG:H82	1.50	1.11
1:D:361:ARG:O	3:D:1002:NAG:H82	1.50	1.10
1:B:294:LYS:HE2	1:B:310:PHE:H	1.08	1.10
1:A:309:ILE:HD11	1:A:315:LEU:H	0.92	1.08
1:D:309:ILE:HD11	1:D:314:LEU:C	1.75	1.07
1:C:294:LYS:HE2	1:C:310:PHE:H	1.08	1.07
1:D:309:ILE:HD11	1:D:314:LEU:CA	1.83	1.06
1:D:294:LYS:HE2	1:D:310:PHE:H	1.19	1.06
1:B:309:ILE:HG13	1:B:314:LEU:N	1.71	1.05
1:B:309:ILE:HD11	1:B:315:LEU:H	0.90	1.04
1:B:309:ILE:HG13	1:B:313:ASN:C	1.78	1.04
1:D:309:ILE:CD1	1:D:314:LEU:CA	2.36	1.03
1:B:309:ILE:CG1	1:B:313:ASN:O	2.07	1.02
1:D:309:ILE:HD11	1:D:315:LEU:N	1.72	1.02
1:D:309:ILE:HD12	1:D:313:ASN:C	1.80	1.01
1:A:309:ILE:HG13	1:A:314:LEU:N	1.76	1.01
1:B:309:ILE:CG1	1:B:313:ASN:C	2.30	0.98
1:C:361:ARG:O	3:C:1002:NAG:C8	2.11	0.98
1:A:361:ARG:O	3:A:1002:NAG:C8	2.11	0.98
1:D:309:ILE:CD1	1:D:314:LEU:N	2.27	0.98
1:D:309:ILE:HD12	1:D:313:ASN:O	1.63	0.98
1:A:306:ARG:HG2	1:A:308:PHE:CE1	1.98	0.98
1:B:361:ARG:O	3:B:1002:NAG:C8	2.11	0.97
1:D:361:ARG:O	3:D:1002:NAG:C8	2.11	0.97
1:A:309:ILE:CG1	1:A:313:ASN:C	2.35	0.95
1:D:310:PHE:O	1:D:312:GLU:OE1	1.85	0.95
1:A:314:LEU:HB3	1:A:429:TYR:HD2	1.34	0.93
1:D:294:LYS:NZ	1:D:309:ILE:HA	1.84	0.93
1:A:384:ALA:HA	1:A:385:THR:HG22	1.50	0.92
1:C:384:ALA:HA	1:C:385:THR:HG22	1.50	0.92
1:D:314:LEU:HB3	1:D:429:TYR:HD2	1.34	0.92
1:D:384:ALA:HA	1:D:385:THR:HG22	1.50	0.92
1:B:384:ALA:HA	1:B:385:THR:HG22	1.50	0.92
1:C:314:LEU:HB3	1:C:429:TYR:HD2	1.34	0.91
1:A:309:ILE:CG1	1:A:313:ASN:O	2.18	0.90
1:B:314:LEU:HB3	1:B:429:TYR:HD2	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:HG13	1:A:313:ASN:C	1.90	0.89
1:B:309:ILE:CD1	1:B:315:LEU:H	1.84	0.89
1:D:310:PHE:O	1:D:312:GLU:CD	2.11	0.88
1:B:306:ARG:HG2	1:B:308:PHE:CE1	2.09	0.88
1:B:309:ILE:CD1	1:B:315:LEU:N	2.35	0.88
1:A:241:MET:HG3	1:A:242:MET:HG2	1.56	0.87
1:A:309:ILE:CD1	1:A:315:LEU:N	2.36	0.87
1:D:241:MET:HG3	1:D:242:MET:HG2	1.56	0.86
1:A:466:VAL:H	1:A:470:ASP:HB2	1.40	0.86
1:A:573:LEU:CD1	1:B:606:ILE:HD13	2.02	0.86
1:B:577:ILE:CD1	1:C:602:ILE:HD11	2.06	0.86
1:B:466:VAL:H	1:B:470:ASP:HB2	1.40	0.86
1:A:573:LEU:HD13	1:B:606:ILE:HD11	1.56	0.85
1:C:466:VAL:H	1:C:470:ASP:HB2	1.40	0.85
1:A:573:LEU:HD13	1:B:606:ILE:CD1	2.06	0.85
1:B:241:MET:HG3	1:B:242:MET:HG2	1.56	0.84
1:C:241:MET:HG3	1:C:242:MET:HG2	1.56	0.84
1:D:294:LYS:HE2	1:D:310:PHE:N	1.91	0.84
1:D:309:ILE:CD1	1:D:313:ASN:C	2.46	0.84
1:D:398:THR:HB	3:D:1001:NAG:C6	2.08	0.84
1:B:573:LEU:HD12	1:C:606:ILE:CD1	2.05	0.84
1:C:396:SER:HB2	1:C:398:THR:HG22	1.60	0.83
1:D:309:ILE:HD11	1:D:314:LEU:HA	1.60	0.83
1:D:398:THR:HB	3:D:1001:NAG:H61	1.61	0.83
1:B:573:LEU:CD1	1:C:606:ILE:HD12	2.07	0.83
1:D:466:VAL:H	1:D:470:ASP:HB2	1.40	0.83
1:C:294:LYS:HE2	1:C:310:PHE:N	1.93	0.83
1:D:396:SER:HB2	1:D:398:THR:HG22	1.60	0.83
1:B:606:ILE:CG2	1:B:607:ILE:N	2.42	0.82
1:A:606:ILE:CG2	1:A:607:ILE:N	2.42	0.82
1:A:306:ARG:HG2	1:A:308:PHE:CZ	2.14	0.82
1:A:525:ASN:OD1	1:A:526:ILE:N	2.13	0.82
1:B:611:TYR:O	1:B:615:ALA:N	2.13	0.82
1:B:573:LEU:CD1	1:C:606:ILE:HD13	2.04	0.82
1:A:396:SER:HB2	1:A:398:THR:HG22	1.60	0.82
1:B:396:SER:HB2	1:B:398:THR:HG22	1.60	0.81
1:D:525:ASN:OD1	1:D:526:ILE:N	2.13	0.81
1:A:294:LYS:HE2	1:A:310:PHE:N	1.93	0.81
1:A:611:TYR:O	1:A:615:ALA:N	2.13	0.81
1:A:247:TYR:OH	1:B:624:ASP:HA	1.81	0.81
1:B:650:GLU:HA	1:B:658:PRO:HG3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ASN:OD1	1:B:526:ILE:N	2.13	0.81
1:D:323:GLN:NE2	1:D:416:ASP:OD1	2.14	0.81
1:B:294:LYS:HE2	1:B:310:PHE:N	1.93	0.81
1:A:323:GLN:NE2	1:A:416:ASP:OD1	2.14	0.80
1:B:577:ILE:HD13	1:C:602:ILE:HD11	1.63	0.80
1:C:323:GLN:NE2	1:C:416:ASP:OD1	2.14	0.80
1:C:606:ILE:CG2	1:C:607:ILE:N	2.42	0.80
1:D:606:ILE:CG2	1:D:607:ILE:N	2.42	0.80
1:C:525:ASN:OD1	1:C:526:ILE:N	2.13	0.80
1:B:573:LEU:HD13	1:C:606:ILE:CD1	2.08	0.80
1:A:577:ILE:CD1	1:B:602:ILE:HD11	2.11	0.80
1:B:306:ARG:HG2	1:B:308:PHE:CZ	2.16	0.80
1:A:573:LEU:HD12	1:B:606:ILE:CD1	2.09	0.80
1:A:650:GLU:HA	1:A:658:PRO:HG3	1.62	0.80
1:C:573:LEU:CD1	1:D:606:ILE:HD13	2.06	0.80
1:A:406:VAL:HG13	1:A:414:TRP:HE1	1.47	0.79
1:B:323:GLN:NE2	1:B:416:ASP:OD1	2.14	0.79
1:D:436:PHE:O	1:D:460:LEU:N	2.15	0.79
1:B:269:ASN:OD1	1:B:272:THR:N	2.16	0.79
1:D:611:TYR:O	1:D:615:ALA:N	2.13	0.79
1:B:406:VAL:HG13	1:B:414:TRP:HE1	1.47	0.79
1:B:436:PHE:O	1:B:460:LEU:N	2.15	0.79
1:D:650:GLU:HA	1:D:658:PRO:HG3	1.62	0.79
1:C:650:GLU:HA	1:C:658:PRO:HG3	1.62	0.79
1:C:611:TYR:O	1:C:615:ALA:N	2.13	0.78
1:A:247:TYR:HH	1:B:624:ASP:HA	1.48	0.78
1:A:269:ASN:OD1	1:A:272:THR:N	2.15	0.78
1:D:406:VAL:HG13	1:D:414:TRP:HE1	1.47	0.78
1:C:418:GLY:O	1:C:420:ARG:NH2	2.17	0.78
1:D:418:GLY:O	1:D:420:ARG:NH2	2.17	0.78
1:A:418:GLY:O	1:A:420:ARG:NH2	2.17	0.78
1:C:406:VAL:HG13	1:C:414:TRP:HE1	1.47	0.78
1:C:436:PHE:O	1:C:460:LEU:N	2.15	0.78
1:B:380:TRP:O	1:B:385:THR:N	2.17	0.77
1:A:436:PHE:O	1:A:460:LEU:N	2.15	0.77
1:A:677:LEU:HD23	1:A:680:ILE:HD12	1.67	0.77
1:B:327:ARG:HG3	1:B:330:SER:HB2	1.65	0.77
1:B:418:GLY:O	1:B:420:ARG:NH2	2.17	0.77
1:D:380:TRP:O	1:D:385:THR:N	2.17	0.77
1:B:247:TYR:OH	1:C:624:ASP:HA	1.85	0.77
1:B:606:ILE:HG22	1:B:607:ILE:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:PHE:O	1:A:636:GLN:NE2	2.18	0.77
1:C:327:ARG:HG3	1:C:330:SER:HB2	1.65	0.77
1:D:677:LEU:HD23	1:D:680:ILE:HD12	1.67	0.77
1:A:327:ARG:HG3	1:A:330:SER:HB2	1.64	0.77
1:A:554:TRP:O	1:A:558:PHE:N	2.14	0.77
1:C:606:ILE:HG22	1:C:607:ILE:H	1.50	0.77
1:C:573:LEU:HD13	1:D:606:ILE:CD1	2.11	0.77
1:C:554:TRP:O	1:C:558:PHE:N	2.14	0.77
1:C:577:ILE:CD1	1:D:602:ILE:HD11	2.15	0.77
1:D:327:ARG:HG3	1:D:330:SER:HB2	1.65	0.77
1:B:577:ILE:CD1	1:C:602:ILE:CD1	2.62	0.76
1:B:608:PHE:O	1:B:636:GLN:NE2	2.18	0.76
1:A:606:ILE:HG22	1:A:607:ILE:H	1.50	0.76
1:A:606:ILE:HD13	1:D:573:LEU:CD1	2.10	0.76
1:B:677:LEU:HD23	1:B:680:ILE:HD12	1.67	0.76
1:C:247:TYR:OH	1:D:624:ASP:HA	1.85	0.76
1:A:573:LEU:CD1	1:B:606:ILE:HD12	2.13	0.76
1:C:677:LEU:HD23	1:C:680:ILE:HD12	1.67	0.76
1:A:236:ILE:O	1:A:240:GLY:N	2.18	0.76
1:D:606:ILE:HG22	1:D:607:ILE:H	1.50	0.76
1:C:653:ASN:HB2	1:C:656:LEU:HB3	1.69	0.75
1:C:236:ILE:O	1:C:240:GLY:N	2.17	0.75
1:B:681:ASN:HB2	1:C:674:ASN:HD21	1.51	0.75
1:D:236:ILE:O	1:D:240:GLY:N	2.18	0.75
1:B:653:ASN:HB2	1:B:656:LEU:HB3	1.69	0.75
1:A:498:HIS:HB3	1:A:501:HIS:HB3	1.69	0.75
1:D:653:ASN:HB2	1:D:656:LEU:HB3	1.69	0.75
1:A:653:ASN:HB2	1:A:656:LEU:HB3	1.68	0.75
1:A:380:TRP:O	1:A:385:THR:N	2.17	0.75
1:A:602:ILE:HD11	1:D:577:ILE:CD1	2.17	0.75
1:C:356:ALA:O	1:C:391:TYR:OH	2.04	0.75
1:D:309:ILE:CD1	1:D:314:LEU:HA	2.13	0.75
1:D:440:ARG:HB3	1:D:456:GLN:HB3	1.69	0.75
1:D:498:HIS:HB3	1:D:501:HIS:HB3	1.69	0.75
1:B:554:TRP:O	1:B:558:PHE:N	2.14	0.75
1:B:665:VAL:O	1:B:669:PHE:HB3	1.87	0.75
1:B:356:ALA:O	1:B:391:TYR:OH	2.04	0.74
1:A:573:LEU:HD11	1:B:606:ILE:HD13	1.55	0.74
1:A:440:ARG:HB3	1:A:456:GLN:HB3	1.69	0.74
1:B:309:ILE:HG13	1:B:314:LEU:CA	2.17	0.74
1:C:425:ASP:OD1	1:C:441:LEU:N	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HA	1:B:224:LEU:HB2	1.69	0.74
1:C:380:TRP:O	1:C:385:THR:N	2.17	0.74
1:C:573:LEU:HD11	1:D:606:ILE:HD13	1.56	0.74
1:D:221:LEU:HA	1:D:224:LEU:HB2	1.69	0.74
1:A:356:ALA:O	1:A:391:TYR:OH	2.04	0.74
1:D:269:ASN:OD1	1:D:272:THR:N	2.15	0.74
1:D:356:ALA:O	1:D:391:TYR:OH	2.04	0.74
1:D:409:LEU:HB3	1:D:414:TRP:CD1	2.22	0.74
1:C:409:LEU:HB3	1:C:414:TRP:CD1	2.22	0.74
1:C:608:PHE:O	1:C:636:GLN:NE2	2.18	0.74
1:C:498:HIS:HB3	1:C:501:HIS:HB3	1.69	0.74
1:B:409:LEU:HB3	1:B:414:TRP:CD1	2.22	0.74
1:C:405:GLN:O	1:C:409:LEU:N	2.21	0.74
1:C:665:VAL:O	1:C:669:PHE:HB3	1.87	0.74
1:A:550:HIS:CE1	1:A:554:TRP:HE1	2.06	0.73
1:B:568:PHE:HA	1:B:571:ILE:HG12	1.70	0.73
1:C:269:ASN:OD1	1:C:272:THR:N	2.15	0.73
1:A:409:LEU:HB3	1:A:414:TRP:CD1	2.22	0.73
1:B:405:GLN:O	1:B:409:LEU:N	2.21	0.73
1:A:306:ARG:CG	1:A:308:PHE:CE1	2.70	0.73
1:B:498:HIS:HB3	1:B:501:HIS:HB3	1.69	0.73
1:A:624:ASP:HA	1:D:247:TYR:OH	1.88	0.73
1:A:577:ILE:HD13	1:B:602:ILE:HD11	1.70	0.73
1:A:665:VAL:O	1:A:669:PHE:HB3	1.87	0.73
1:B:425:ASP:OD1	1:B:441:LEU:N	2.15	0.73
1:B:440:ARG:HB3	1:B:456:GLN:HB3	1.69	0.73
1:C:409:LEU:O	1:C:414:TRP:N	2.19	0.73
1:D:608:PHE:O	1:D:636:GLN:NE2	2.18	0.73
1:A:405:GLN:O	1:A:409:LEU:N	2.21	0.73
1:D:554:TRP:O	1:D:558:PHE:N	2.14	0.73
1:A:444:GLU:HB2	1:A:452:ILE:HG23	1.71	0.73
1:C:550:HIS:CE1	1:C:554:TRP:HE1	2.07	0.73
1:D:550:HIS:CE1	1:D:554:TRP:HE1	2.07	0.73
1:A:221:LEU:HA	1:A:224:LEU:HB2	1.69	0.73
1:A:568:PHE:HA	1:A:571:ILE:HG12	1.70	0.73
1:B:248:TYR:O	1:B:252:MET:HG2	1.89	0.73
1:C:221:LEU:HA	1:C:224:LEU:HB2	1.69	0.73
1:C:440:ARG:HB3	1:C:456:GLN:HB3	1.69	0.73
1:D:360:PRO:O	1:D:366:TRP:NE1	2.22	0.73
1:A:248:TYR:O	1:A:252:MET:HG2	1.89	0.72
1:A:687:VAL:O	1:A:691:LEU:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:PRO:O	1:C:366:TRP:NE1	2.21	0.72
1:A:502:TYR:O	1:A:508:ASN:ND2	2.22	0.72
1:D:405:GLN:O	1:D:409:LEU:N	2.21	0.72
1:D:409:LEU:O	1:D:414:TRP:N	2.19	0.72
1:D:665:VAL:O	1:D:669:PHE:HB3	1.87	0.72
1:B:502:TYR:O	1:B:508:ASN:ND2	2.22	0.72
1:C:430:ASN:HD21	1:C:435:LEU:HB3	1.55	0.72
1:D:568:PHE:HA	1:D:571:ILE:HG12	1.71	0.72
1:C:444:GLU:HB2	1:C:452:ILE:HG23	1.71	0.72
1:D:348:TYR:HB2	1:D:420:ARG:HG3	1.71	0.72
1:D:444:GLU:HB2	1:D:452:ILE:HG23	1.71	0.72
1:A:657:GLY:O	1:A:660:TYR:N	2.23	0.72
1:D:687:VAL:O	1:D:691:LEU:N	2.22	0.72
1:B:236:ILE:O	1:B:240:GLY:N	2.18	0.72
1:B:430:ASN:HD21	1:B:435:LEU:HB3	1.55	0.72
1:C:606:ILE:O	1:C:610:ALA:N	2.21	0.72
1:D:502:TYR:O	1:D:508:ASN:ND2	2.22	0.72
1:B:550:HIS:CE1	1:B:554:TRP:HE1	2.07	0.72
1:B:657:GLY:O	1:B:660:TYR:N	2.23	0.72
1:C:348:TYR:HB2	1:C:420:ARG:HG3	1.71	0.72
1:C:573:LEU:HD12	1:D:606:ILE:CD1	2.14	0.72
1:C:687:VAL:O	1:C:691:LEU:N	2.22	0.72
1:C:502:TYR:O	1:C:508:ASN:ND2	2.22	0.71
1:C:573:LEU:CD1	1:D:606:ILE:HD12	2.15	0.71
1:D:604:PHE:O	1:D:608:PHE:N	2.19	0.71
1:C:687:VAL:HA	1:C:690:ASP:HB3	1.72	0.71
1:B:444:GLU:HB2	1:B:452:ILE:HG23	1.71	0.71
1:D:248:TYR:O	1:D:252:MET:HG2	1.89	0.71
1:D:309:ILE:HD13	1:D:314:LEU:N	2.05	0.71
1:C:248:TYR:O	1:C:252:MET:HG2	1.89	0.71
1:C:577:ILE:HD13	1:D:602:ILE:HD11	1.72	0.71
1:D:309:ILE:CD1	1:D:314:LEU:C	2.53	0.71
1:D:310:PHE:HB2	1:D:312:GLU:OE1	1.90	0.71
1:A:360:PRO:O	1:A:366:TRP:NE1	2.22	0.71
1:A:348:TYR:HB2	1:A:420:ARG:HG3	1.71	0.71
1:A:606:ILE:HD12	1:D:573:LEU:CD1	2.17	0.71
1:C:309:ILE:HD11	1:C:315:LEU:N	2.05	0.71
1:C:657:GLY:O	1:C:660:TYR:N	2.23	0.71
1:A:430:ASN:HD21	1:A:435:LEU:HB3	1.55	0.71
1:B:687:VAL:O	1:B:691:LEU:N	2.22	0.71
1:C:604:PHE:O	1:C:608:PHE:N	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:O	1:A:414:TRP:N	2.19	0.71
1:A:606:ILE:CD1	1:D:573:LEU:HD13	2.16	0.71
1:B:348:TYR:HB2	1:B:420:ARG:HG3	1.71	0.71
1:B:577:ILE:HD11	1:C:602:ILE:CD1	2.21	0.71
1:C:306:ARG:HG2	1:C:308:PHE:CE1	2.26	0.71
1:A:566:VAL:O	1:A:570:TRP:N	2.22	0.70
1:D:294:LYS:HZ3	1:D:309:ILE:HA	1.54	0.70
1:C:568:PHE:HA	1:C:571:ILE:HG12	1.71	0.70
1:D:687:VAL:HA	1:D:690:ASP:HB3	1.72	0.70
1:C:566:VAL:O	1:C:570:TRP:N	2.22	0.70
1:D:309:ILE:HD11	1:D:315:LEU:H	1.56	0.70
1:A:309:ILE:CD1	1:A:315:LEU:H	1.87	0.70
1:D:430:ASN:HD21	1:D:435:LEU:HB3	1.55	0.70
1:D:606:ILE:O	1:D:610:ALA:N	2.21	0.70
1:D:657:GLY:O	1:D:660:TYR:N	2.23	0.70
1:A:577:ILE:CD1	1:B:602:ILE:CD1	2.70	0.70
1:A:606:ILE:O	1:A:610:ALA:N	2.21	0.70
1:B:360:PRO:O	1:B:366:TRP:NE1	2.22	0.70
1:B:606:ILE:O	1:B:610:ALA:N	2.21	0.70
1:B:687:VAL:HA	1:B:690:ASP:HB3	1.72	0.70
1:C:232:ILE:HG22	1:C:236:ILE:HG13	1.74	0.70
1:A:606:ILE:CD1	1:D:573:LEU:HD12	2.16	0.70
1:A:357:PRO:O	1:A:361:ARG:NE	2.25	0.69
1:A:406:VAL:HA	1:A:409:LEU:HB2	1.74	0.69
1:A:681:ASN:HB2	1:B:674:ASN:HD21	1.55	0.69
1:A:328:ASN:OD1	1:A:329:GLY:N	2.26	0.69
1:A:562:ALA:O	1:A:565:THR:OG1	2.10	0.69
1:A:602:ILE:HD11	1:D:577:ILE:HD13	1.74	0.69
1:A:687:VAL:HA	1:A:690:ASP:HB3	1.72	0.69
1:D:404:ALA:O	1:D:408:SER:N	2.20	0.69
1:B:409:LEU:O	1:B:414:TRP:N	2.19	0.69
1:D:232:ILE:HG22	1:D:236:ILE:HG13	1.74	0.69
1:A:353:GLU:O	1:A:355:ARG:NH1	2.26	0.69
1:B:406:VAL:HA	1:B:409:LEU:HB2	1.74	0.69
1:D:328:ASN:OD1	1:D:329:GLY:N	2.26	0.69
1:B:357:PRO:O	1:B:361:ARG:NE	2.25	0.69
1:B:562:ALA:O	1:B:565:THR:OG1	2.10	0.69
1:A:309:ILE:CG1	1:A:314:LEU:N	2.54	0.69
1:C:353:GLU:O	1:C:355:ARG:NH1	2.26	0.69
1:D:353:GLU:O	1:D:355:ARG:NH1	2.26	0.69
1:A:448:THR:OG1	1:D:252:MET:SD	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASN:OD1	1:B:329:GLY:N	2.26	0.69
1:C:324:LEU:HD11	1:C:386:TYR:CE1	2.28	0.69
1:C:681:ASN:HB2	1:D:674:ASN:HD21	1.57	0.69
1:B:322:ARG:HG2	1:B:323:GLN:H	1.58	0.68
1:B:690:ASP:OD1	1:B:693:GLN:NE2	2.27	0.68
1:C:406:VAL:HA	1:C:409:LEU:HB2	1.74	0.68
1:B:232:ILE:HG22	1:B:236:ILE:HG13	1.74	0.68
1:B:566:VAL:O	1:B:570:TRP:N	2.22	0.68
1:B:353:GLU:O	1:B:355:ARG:NH1	2.26	0.68
1:C:328:ASN:OD1	1:C:329:GLY:N	2.26	0.68
1:C:690:ASP:OD1	1:C:693:GLN:NE2	2.27	0.68
1:B:324:LEU:HD11	1:B:386:TYR:CE1	2.28	0.68
1:B:580:ASN:OD1	1:B:581:ARG:N	2.27	0.68
1:C:357:PRO:O	1:C:361:ARG:NE	2.25	0.68
1:D:357:PRO:O	1:D:361:ARG:NE	2.25	0.68
1:A:580:ASN:OD1	1:A:581:ARG:N	2.27	0.68
1:A:663:THR:HG21	6:D:1008:PLM:HG3	1.76	0.68
1:C:322:ARG:HG2	1:C:323:GLN:H	1.59	0.68
1:D:325:ARG:HH21	1:D:355:ARG:HA	1.59	0.68
1:D:562:ALA:O	1:D:565:THR:OG1	2.10	0.68
1:A:232:ILE:HG22	1:A:236:ILE:HG13	1.74	0.68
1:A:318:VAL:HG22	1:A:395:LEU:HB3	1.76	0.68
1:A:324:LEU:HD11	1:A:386:TYR:CE1	2.28	0.68
1:C:318:VAL:HG22	1:C:395:LEU:HB3	1.76	0.68
1:C:562:ALA:O	1:C:565:THR:OG1	2.11	0.68
1:A:349:SER:H	1:A:352:SER:HB3	1.59	0.68
1:B:604:PHE:O	1:B:608:PHE:N	2.18	0.68
1:D:324:LEU:HD11	1:D:386:TYR:CE1	2.28	0.68
1:D:406:VAL:HA	1:D:409:LEU:HB2	1.74	0.68
1:A:627:SER:N	1:A:632:CYS:SG	2.61	0.68
1:C:349:SER:H	1:C:352:SER:HB3	1.59	0.68
1:A:682:ASP:OD1	1:A:683:THR:N	2.25	0.68
1:B:309:ILE:CG1	1:B:314:LEU:CA	2.71	0.68
1:A:294:LYS:HD3	1:A:308:PHE:O	1.94	0.67
1:B:325:ARG:HH21	1:B:355:ARG:HA	1.59	0.67
4:C:1005:CHS:HZ2	4:C:1006:CHS:HE22	1.76	0.67
1:D:627:SER:N	1:D:632:CYS:SG	2.61	0.67
1:A:292:TYR:HD2	1:A:294:LYS:HE3	1.60	0.67
1:C:626:PHE:HD1	1:C:632:CYS:HG	1.41	0.67
1:D:690:ASP:OD1	1:D:693:GLN:NE2	2.26	0.67
1:B:223:GLU:O	1:B:226:THR:OG1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ASN:O	1:D:656:LEU:N	2.28	0.67
1:B:292:TYR:HD2	1:B:294:LYS:HE3	1.59	0.67
1:D:318:VAL:HG22	1:D:395:LEU:HB3	1.76	0.67
1:A:309:ILE:HG13	1:A:314:LEU:CA	2.24	0.67
1:B:404:ALA:O	1:B:408:SER:N	2.20	0.67
6:B:1008:PLM:HG3	1:C:663:THR:HG21	1.77	0.67
1:D:398:THR:HA	3:D:1001:NAG:O6	1.95	0.67
1:A:674:ASN:HD21	1:D:681:ASN:HB2	1.58	0.67
1:C:325:ARG:HH21	1:C:355:ARG:HA	1.59	0.67
1:D:349:SER:H	1:D:352:SER:HB3	1.59	0.67
1:D:580:ASN:OD1	1:D:581:ARG:N	2.27	0.67
1:A:577:ILE:HD11	1:B:602:ILE:CD1	2.25	0.67
1:B:237:LEU:O	1:B:241:MET:N	2.21	0.67
1:B:309:ILE:CG1	1:B:314:LEU:HA	2.24	0.67
1:B:318:VAL:HG22	1:B:395:LEU:HB3	1.76	0.67
1:A:322:ARG:HG2	1:A:323:GLN:H	1.59	0.67
1:A:417:ARG:NH1	1:D:311:TYR:O	2.28	0.67
1:C:577:ILE:CD1	1:D:602:ILE:CD1	2.72	0.67
1:C:580:ASN:OD1	1:C:581:ARG:N	2.27	0.67
1:A:626:PHE:HD1	1:A:632:CYS:HG	1.40	0.67
1:B:349:SER:H	1:B:352:SER:HB3	1.59	0.67
1:B:682:ASP:OD1	1:B:683:THR:N	2.26	0.66
4:B:1005:CHS:HZ2	4:B:1006:CHS:HE22	1.77	0.66
1:C:682:ASP:OD1	1:C:683:THR:N	2.26	0.66
1:A:690:ASP:OD1	1:A:693:GLN:NE2	2.27	0.66
1:D:292:TYR:HD2	1:D:294:LYS:HE3	1.59	0.66
1:D:427:SER:OG	1:D:437:CYS:O	2.10	0.66
1:A:604:PHE:O	1:A:608:PHE:N	2.19	0.66
1:C:223:GLU:O	1:C:226:THR:OG1	2.08	0.66
1:B:653:ASN:O	1:B:656:LEU:N	2.28	0.66
1:C:292:TYR:HD2	1:C:294:LYS:HE3	1.60	0.66
1:C:653:ASN:O	1:C:656:LEU:N	2.28	0.66
1:A:325:ARG:HH21	1:A:355:ARG:HA	1.59	0.66
1:D:223:GLU:O	1:D:226:THR:OG1	2.08	0.66
1:D:322:ARG:HG2	1:D:323:GLN:H	1.58	0.66
1:C:237:LEU:O	1:C:241:MET:N	2.21	0.66
1:A:653:ASN:O	1:A:656:LEU:N	2.28	0.66
1:A:425:ASP:OD1	1:A:441:LEU:N	2.15	0.66
1:B:427:SER:OG	1:B:437:CYS:O	2.10	0.66
1:C:252:MET:SD	1:D:448:THR:OG1	2.49	0.66
4:A:1005:CHS:HZ2	4:A:1006:CHS:HE22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:SER:OG	1:A:437:CYS:O	2.10	0.65
1:C:247:TYR:HH	1:D:624:ASP:HA	1.59	0.65
1:B:398:THR:HG23	1:B:398:THR:O	1.96	0.65
1:A:602:ILE:CD1	1:D:577:ILE:CD1	2.74	0.65
1:B:306:ARG:CG	1:B:308:PHE:CE1	2.78	0.65
1:A:404:ALA:O	1:A:408:SER:N	2.20	0.65
1:B:309:ILE:CG1	1:B:314:LEU:N	2.54	0.65
1:A:309:ILE:CG1	1:A:314:LEU:CA	2.74	0.65
1:C:398:THR:HG23	1:C:398:THR:O	1.96	0.65
1:C:547:ASN:OD1	1:C:549:GLU:N	2.29	0.65
1:D:425:ASP:OD1	1:D:441:LEU:N	2.15	0.65
1:A:682:ASP:O	1:A:686:GLU:N	2.30	0.65
1:B:362:ASN:OD1	3:B:1002:NAG:C7	2.44	0.65
1:C:362:ASN:OD1	3:C:1002:NAG:C7	2.44	0.65
1:C:404:ALA:O	1:C:408:SER:N	2.20	0.65
1:D:606:ILE:HG23	1:D:607:ILE:N	2.12	0.65
1:B:547:ASN:OD1	1:B:549:GLU:N	2.29	0.65
1:D:682:ASP:OD1	1:D:683:THR:N	2.26	0.65
1:A:362:ASN:OD1	3:A:1002:NAG:C7	2.44	0.65
1:A:547:ASN:OD1	1:A:549:GLU:N	2.29	0.64
1:D:547:ASN:OD1	1:D:549:GLU:N	2.29	0.64
1:A:398:THR:O	1:A:398:THR:HG23	1.96	0.64
1:C:606:ILE:HG23	1:C:607:ILE:N	2.12	0.64
1:C:682:ASP:O	1:C:686:GLU:N	2.30	0.64
1:A:502:TYR:HD1	1:A:508:ASN:HD22	1.46	0.64
1:B:502:TYR:HD1	1:B:508:ASN:HD22	1.46	0.64
1:D:502:TYR:HD1	1:D:508:ASN:HD22	1.46	0.64
1:A:232:ILE:O	1:A:236:ILE:N	2.24	0.64
1:D:362:ASN:OD1	3:D:1002:NAG:C7	2.44	0.64
1:C:241:MET:HB2	1:C:461:LYS:HD3	1.80	0.64
1:A:606:ILE:HG23	1:A:607:ILE:N	2.12	0.64
1:C:436:PHE:N	1:C:460:LEU:O	2.29	0.64
1:C:502:TYR:HD1	1:C:508:ASN:HD22	1.46	0.64
1:D:398:THR:HG23	1:D:398:THR:O	1.96	0.64
1:A:467:THR:OG1	1:B:335:GLN:OE1	2.15	0.64
1:C:427:SER:OG	1:C:437:CYS:O	2.10	0.64
1:A:223:GLU:O	1:A:226:THR:OG1	2.08	0.63
4:D:1005:CHS:HZ2	4:D:1006:CHS:HE22	1.79	0.63
1:A:384:ALA:HA	1:A:385:THR:CG2	2.27	0.63
1:B:458:GLN:NE2	1:B:459:PRO:HD2	2.14	0.63
1:B:241:MET:HB2	1:B:461:LYS:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:PHE:O	1:B:665:VAL:HG12	1.99	0.63
1:C:577:ILE:HD11	1:D:602:ILE:CD1	2.28	0.63
1:C:661:PHE:O	1:C:665:VAL:HG12	1.98	0.63
1:D:241:MET:HB2	1:D:461:LYS:HD3	1.80	0.63
1:A:458:GLN:NE2	1:A:459:PRO:HD2	2.14	0.63
1:B:606:ILE:HG23	1:B:607:ILE:N	2.12	0.63
1:C:555:GLN:O	1:C:559:ASN:N	2.24	0.63
1:D:458:GLN:NE2	1:D:459:PRO:HD2	2.14	0.63
1:D:540:GLU:HA	1:D:546:PRO:HD3	1.80	0.63
1:A:540:GLU:HA	1:A:546:PRO:HD3	1.80	0.63
1:B:677:LEU:HD21	1:C:673:LEU:HD12	1.80	0.63
1:A:555:GLN:O	1:A:559:ASN:N	2.24	0.63
1:D:661:PHE:O	1:D:665:VAL:HG12	1.99	0.63
1:C:309:ILE:O	1:C:312:GLU:N	2.29	0.63
1:C:311:TYR:O	1:D:417:ARG:NH1	2.31	0.63
1:B:502:TYR:HB2	1:B:508:ASN:HB3	1.81	0.63
1:C:540:GLU:HA	1:C:546:PRO:HD3	1.80	0.62
1:A:361:ARG:O	3:A:1002:NAG:H81	1.99	0.62
1:B:311:TYR:O	1:C:417:ARG:NH1	2.32	0.62
1:A:241:MET:HB2	1:A:461:LYS:HD3	1.80	0.62
1:A:655:VAL:HG11	5:D:1007:PX6:H41	1.82	0.62
1:C:458:GLN:NE2	1:C:459:PRO:HD2	2.14	0.62
1:D:384:ALA:HA	1:D:385:THR:CG2	2.27	0.62
1:D:502:TYR:HB2	1:D:508:ASN:HB3	1.82	0.62
1:B:232:ILE:O	1:B:236:ILE:N	2.24	0.62
1:B:476:CYS:HA	1:B:479:ILE:HD12	1.82	0.62
1:D:566:VAL:O	1:D:570:TRP:N	2.22	0.62
1:A:502:TYR:HB2	1:A:508:ASN:HB3	1.81	0.62
1:B:509:CYS:O	1:B:513:VAL:N	2.33	0.62
1:B:540:GLU:HA	1:B:546:PRO:HD3	1.80	0.62
1:C:323:GLN:HG2	1:C:324:LEU:N	2.15	0.62
1:D:294:LYS:CE	1:D:310:PHE:H	2.03	0.62
1:D:436:PHE:N	1:D:460:LEU:O	2.29	0.62
1:A:683:THR:HA	1:A:686:GLU:HB3	1.82	0.62
1:B:361:ARG:O	3:B:1002:NAG:H81	1.99	0.62
1:B:681:ASN:HB2	1:C:674:ASN:ND2	2.12	0.62
1:C:398:THR:OG1	1:C:400:GLU:OE1	2.16	0.62
1:C:502:TYR:HB2	1:C:508:ASN:HB3	1.82	0.62
1:D:323:GLN:HG2	1:D:324:LEU:N	2.15	0.62
1:D:509:CYS:O	1:D:513:VAL:N	2.33	0.62
1:A:466:VAL:HG12	1:A:468:THR:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:PHE:O	1:A:665:VAL:HG12	1.99	0.62
1:B:683:THR:HA	1:B:686:GLU:HB3	1.82	0.62
1:C:683:THR:HA	1:C:686:GLU:HB3	1.82	0.62
1:D:361:ARG:O	3:D:1002:NAG:H81	1.99	0.62
1:D:396:SER:CB	1:D:398:THR:HG22	2.30	0.62
1:B:317:GLY:HA3	1:B:545:PHE:HD1	1.65	0.62
1:D:223:GLU:CD	1:D:227:TYR:HE2	2.03	0.62
1:D:683:THR:HA	1:D:686:GLU:HB3	1.82	0.62
1:A:317:GLY:HA3	1:A:545:PHE:HD1	1.65	0.61
1:B:223:GLU:CD	1:B:227:TYR:HE2	2.04	0.61
1:C:476:CYS:HA	1:C:479:ILE:HD12	1.82	0.61
1:C:570:TRP:HE1	1:D:606:ILE:HG12	1.65	0.61
1:A:404:ALA:HA	1:A:407:ALA:HB3	1.83	0.61
1:B:682:ASP:O	1:B:686:GLU:N	2.30	0.61
1:A:223:GLU:CD	1:A:227:TYR:HE2	2.03	0.61
1:A:237:LEU:O	1:A:241:MET:N	2.21	0.61
1:A:476:CYS:HA	1:A:479:ILE:HD12	1.82	0.61
1:B:247:TYR:HH	1:C:624:ASP:HA	1.63	0.61
1:B:323:GLN:HG2	1:B:324:LEU:N	2.15	0.61
1:C:317:GLY:HA3	1:C:545:PHE:HD1	1.65	0.61
1:C:404:ALA:HA	1:C:407:ALA:HB3	1.83	0.61
1:A:509:CYS:O	1:A:513:VAL:N	2.33	0.61
1:B:404:ALA:HA	1:B:407:ALA:HB3	1.83	0.61
1:C:254:SER:OG	1:C:255:GLN:N	2.33	0.61
6:A:1008:PLM:HG3	1:B:663:THR:HG21	1.83	0.61
1:B:384:ALA:HA	1:B:385:THR:CG2	2.27	0.61
1:B:555:GLN:O	1:B:559:ASN:N	2.24	0.61
1:D:682:ASP:O	1:D:686:GLU:N	2.30	0.61
1:A:323:GLN:HG2	1:A:324:LEU:N	2.15	0.61
1:B:352:SER:N	1:B:353:GLU:OE1	2.34	0.61
1:B:577:ILE:HG12	1:C:602:ILE:HD13	1.83	0.61
1:B:268:THR:OG1	1:B:272:THR:O	2.19	0.61
1:B:466:VAL:HG12	1:B:468:THR:H	1.65	0.61
1:C:466:VAL:HG12	1:C:468:THR:H	1.65	0.61
1:A:268:THR:OG1	1:A:272:THR:O	2.19	0.61
1:B:254:SER:OG	1:B:255:GLN:N	2.33	0.61
1:C:361:ARG:O	3:C:1002:NAG:H81	1.99	0.61
1:C:684:TYR:O	1:C:687:VAL:HG22	2.01	0.61
6:C:1008:PLM:HG3	1:D:663:THR:HG21	1.83	0.61
1:D:404:ALA:HA	1:D:407:ALA:HB3	1.83	0.61
1:B:573:LEU:HD11	1:C:606:ILE:HD13	1.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:GLU:CD	1:C:227:TYR:HE2	2.04	0.61
1:C:352:SER:N	1:C:353:GLU:OE1	2.34	0.61
1:C:509:CYS:O	1:C:513:VAL:N	2.33	0.60
1:C:517:LEU:HB3	1:C:565:THR:HG22	1.83	0.60
1:D:466:VAL:HG12	1:D:468:THR:H	1.65	0.60
1:A:602:ILE:CD1	1:D:577:ILE:HD11	2.31	0.60
1:A:684:TYR:O	1:A:687:VAL:HG22	2.01	0.60
1:B:589:THR:HA	1:B:592:ARG:HB3	1.83	0.60
1:D:352:SER:N	1:D:353:GLU:OE1	2.34	0.60
1:A:589:THR:HA	1:A:592:ARG:HB3	1.83	0.60
1:C:384:ALA:HA	1:C:385:THR:CG2	2.27	0.60
1:C:502:TYR:HB2	1:C:508:ASN:CB	2.32	0.60
1:A:254:SER:OG	1:A:255:GLN:N	2.33	0.60
1:A:570:TRP:HE1	1:B:606:ILE:HG12	1.65	0.60
1:D:268:THR:OG1	1:D:272:THR:O	2.19	0.60
1:D:476:CYS:HA	1:D:479:ILE:HD12	1.82	0.60
1:D:502:TYR:HB2	1:D:508:ASN:CB	2.31	0.60
1:D:684:TYR:O	1:D:687:VAL:HG22	2.01	0.60
1:A:262:VAL:N	1:A:268:THR:O	2.33	0.60
1:A:417:ARG:NH1	1:D:311:TYR:HB3	2.16	0.60
1:D:317:GLY:HA3	1:D:545:PHE:HD1	1.65	0.60
1:A:314:LEU:HB3	1:A:429:TYR:CD2	2.26	0.60
1:B:466:VAL:HB	1:B:470:ASP:N	2.17	0.60
1:C:466:VAL:HB	1:C:470:ASP:N	2.17	0.60
1:D:237:LEU:O	1:D:241:MET:N	2.21	0.60
1:D:517:LEU:HB3	1:D:565:THR:HG22	1.83	0.60
1:D:555:GLN:O	1:D:559:ASN:N	2.24	0.60
1:A:502:TYR:HB2	1:A:508:ASN:CB	2.31	0.60
1:B:221:LEU:O	1:B:225:VAL:N	2.29	0.60
1:B:684:TYR:O	1:B:687:VAL:HG22	2.01	0.60
1:A:396:SER:CB	1:A:398:THR:HG22	2.30	0.60
1:A:466:VAL:HB	1:A:470:ASP:N	2.17	0.60
1:A:352:SER:N	1:A:353:GLU:OE1	2.34	0.60
1:B:396:SER:CB	1:B:398:THR:HG22	2.30	0.60
1:D:466:VAL:HB	1:D:470:ASP:N	2.17	0.60
1:A:309:ILE:CG1	1:A:314:LEU:HA	2.31	0.60
1:B:502:TYR:HB2	1:B:508:ASN:CB	2.31	0.60
1:B:570:TRP:HE1	1:C:606:ILE:HG12	1.67	0.60
1:C:268:THR:OG1	1:C:272:THR:O	2.19	0.60
1:A:681:ASN:HB2	1:B:674:ASN:ND2	2.17	0.59
1:B:310:PHE:HB2	1:B:312:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:LYS:HG3	1:B:576:PHE:CE2	2.37	0.59
1:C:310:PHE:HB2	1:C:312:GLU:OE1	2.02	0.59
1:C:589:THR:HA	1:C:592:ARG:HB3	1.83	0.59
1:C:570:TRP:HE1	1:D:606:ILE:CG1	2.15	0.59
1:B:517:LEU:HB3	1:B:565:THR:HG22	1.83	0.59
5:B:1007:PX6:H41	1:C:655:VAL:HG11	1.85	0.59
1:A:221:LEU:O	1:A:225:VAL:N	2.29	0.59
1:A:463:ILE:HD12	1:A:465:TYR:HB2	1.84	0.59
1:C:572:LYS:HG3	1:C:576:PHE:CE2	2.37	0.59
1:C:627:SER:N	1:C:632:CYS:SG	2.61	0.59
1:D:589:THR:HA	1:D:592:ARG:HB3	1.83	0.59
1:B:570:TRP:HE1	1:C:606:ILE:CG1	2.15	0.59
1:B:627:SER:N	1:B:632:CYS:SG	2.61	0.59
1:C:262:VAL:N	1:C:268:THR:O	2.33	0.59
1:D:254:SER:OG	1:D:255:GLN:N	2.33	0.59
1:C:615:ALA:HA	1:C:619:PHE:HD2	1.68	0.59
1:A:572:LYS:HG3	1:A:576:PHE:CE2	2.37	0.59
1:B:314:LEU:HB3	1:B:429:TYR:CD2	2.26	0.59
1:B:436:PHE:N	1:B:460:LEU:O	2.29	0.59
1:B:674:ASN:O	1:B:677:LEU:N	2.36	0.59
1:C:309:ILE:HG13	1:C:314:LEU:CA	2.33	0.59
1:D:262:VAL:N	1:D:268:THR:O	2.33	0.59
1:D:466:VAL:N	1:D:470:ASP:HB2	2.16	0.59
1:D:572:LYS:HG3	1:D:576:PHE:CE2	2.37	0.59
1:A:436:PHE:N	1:A:460:LEU:O	2.29	0.59
1:A:674:ASN:O	1:A:677:LEU:N	2.36	0.59
1:B:463:ILE:HD12	1:B:465:TYR:HB2	1.84	0.59
1:D:615:ALA:HA	1:D:619:PHE:HD2	1.68	0.59
1:A:466:VAL:N	1:A:470:ASP:HB2	2.16	0.59
1:A:517:LEU:HB3	1:A:565:THR:HG22	1.83	0.59
1:C:307:SER:HB3	1:C:397:ARG:NH2	2.17	0.59
1:C:674:ASN:O	1:C:677:LEU:N	2.36	0.59
1:B:615:ALA:HA	1:B:619:PHE:HD2	1.68	0.59
1:C:681:ASN:HB2	1:D:674:ASN:ND2	2.18	0.59
1:A:310:PHE:HB2	1:A:312:GLU:OE1	2.02	0.58
1:A:606:ILE:HG12	1:D:570:TRP:HE1	1.68	0.58
1:A:674:ASN:ND2	1:D:681:ASN:HB2	2.18	0.58
1:C:396:SER:CB	1:C:398:THR:HG22	2.30	0.58
1:C:573:LEU:HD13	1:D:606:ILE:HD11	1.62	0.58
1:A:606:ILE:CG1	1:D:570:TRP:HE1	2.16	0.58
1:A:653:ASN:ND2	1:D:456:GLN:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ASP:O	1:B:474:ALA:N	2.22	0.58
1:D:463:ILE:HD12	1:D:465:TYR:HB2	1.84	0.58
1:D:221:LEU:O	1:D:225:VAL:N	2.29	0.58
1:D:604:PHE:HA	1:D:607:ILE:HG22	1.85	0.58
1:A:615:ALA:HA	1:A:619:PHE:HD2	1.68	0.58
1:C:463:ILE:HD12	1:C:465:TYR:HB2	1.84	0.58
1:C:539:LEU:HD11	2:G:2:NAG:O6	2.03	0.58
1:D:294:LYS:CE	1:D:309:ILE:HA	2.34	0.58
1:D:674:ASN:O	1:D:677:LEU:N	2.36	0.58
1:A:624:ASP:HA	1:D:247:TYR:HH	1.65	0.58
1:C:624:ASP:O	1:C:626:PHE:N	2.37	0.58
1:D:325:ARG:HH21	1:D:356:ALA:H	1.51	0.58
1:A:677:LEU:HD22	1:B:674:ASN:HB2	1.86	0.58
1:C:677:LEU:HD21	1:D:673:LEU:HD12	1.86	0.58
1:D:566:VAL:HA	1:D:569:VAL:HB	1.86	0.58
1:D:677:LEU:O	1:D:681:ASN:N	2.24	0.58
1:D:470:ASP:O	1:D:474:ALA:N	2.22	0.58
1:A:624:ASP:O	1:A:626:PHE:N	2.37	0.58
1:A:673:LEU:HD12	1:D:677:LEU:HD21	1.86	0.58
1:B:604:PHE:HA	1:B:607:ILE:HG22	1.85	0.58
1:D:539:LEU:HD11	3:D:1004:NAG:O6	2.03	0.58
1:A:263:SER:OG	1:A:285:GLY:O	2.22	0.58
1:B:573:LEU:HD13	1:C:606:ILE:HD11	1.60	0.58
1:B:624:ASP:O	1:B:626:PHE:N	2.37	0.58
1:C:232:ILE:O	1:C:236:ILE:N	2.24	0.58
1:A:306:ARG:CG	1:A:308:PHE:HE1	2.16	0.58
1:A:456:GLN:OE1	1:B:653:ASN:ND2	2.35	0.58
1:A:570:TRP:HE1	1:B:606:ILE:CG1	2.17	0.58
1:A:604:PHE:HA	1:A:607:ILE:HG22	1.85	0.58
1:B:263:SER:OG	1:B:285:GLY:O	2.22	0.58
1:C:325:ARG:HH21	1:C:356:ALA:H	1.51	0.58
1:A:224:LEU:HA	1:A:227:TYR:HD2	1.69	0.57
1:C:263:SER:OG	1:C:285:GLY:O	2.22	0.57
1:C:306:ARG:HG2	1:C:308:PHE:CZ	2.39	0.57
1:C:406:VAL:HA	1:C:409:LEU:HD12	1.86	0.57
1:D:224:LEU:HA	1:D:227:TYR:HD2	1.69	0.57
1:C:309:ILE:HG13	1:C:314:LEU:HA	1.86	0.57
1:D:263:SER:OG	1:D:285:GLY:O	2.22	0.57
1:A:674:ASN:HB2	1:D:677:LEU:HD22	1.86	0.57
1:A:322:ARG:HB3	1:A:423:PHE:HB2	1.87	0.57
1:A:566:VAL:HA	1:A:569:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HA	1:C:227:TYR:HD2	1.69	0.57
1:A:539:LEU:HD11	2:E:2:NAG:O6	2.03	0.57
1:B:539:LEU:HD11	2:F:2:NAG:O6	2.03	0.57
1:C:604:PHE:HA	1:C:607:ILE:HG22	1.85	0.57
1:D:624:ASP:O	1:D:626:PHE:N	2.37	0.57
1:A:325:ARG:HH21	1:A:356:ALA:H	1.51	0.57
1:A:432:ASN:ND2	1:B:447:ALA:O	2.37	0.57
1:C:221:LEU:O	1:C:225:VAL:N	2.29	0.57
1:C:677:LEU:HD22	1:D:674:ASN:HB2	1.87	0.57
1:A:311:TYR:O	1:B:417:ARG:NH1	2.38	0.57
1:B:406:VAL:HA	1:B:409:LEU:HD12	1.87	0.57
1:C:677:LEU:O	1:C:681:ASN:N	2.24	0.57
1:A:382:ILE:HG23	1:A:383:ILE:H	1.70	0.57
1:B:224:LEU:HA	1:B:227:TYR:HD2	1.69	0.57
1:A:677:LEU:HD21	1:B:673:LEU:HD12	1.87	0.57
1:B:382:ILE:HG23	1:B:383:ILE:H	1.70	0.57
1:B:533:GLU:HA	1:B:536:LEU:HD22	1.87	0.57
1:B:566:VAL:HA	1:B:569:VAL:HB	1.86	0.57
1:B:677:LEU:O	1:B:681:ASN:N	2.24	0.57
1:C:533:GLU:HA	1:C:536:LEU:HD22	1.87	0.57
1:B:640:ILE:HD12	1:B:672:LEU:HD21	1.87	0.56
1:C:466:VAL:N	1:C:470:ASP:HB2	2.16	0.56
1:C:566:VAL:HA	1:C:569:VAL:HB	1.86	0.56
1:A:395:LEU:HG	1:A:396:SER:H	1.70	0.56
1:D:322:ARG:HB3	1:D:423:PHE:HB2	1.87	0.56
1:D:406:VAL:HA	1:D:409:LEU:HD12	1.87	0.56
1:A:323:GLN:HG2	1:A:324:LEU:H	1.70	0.56
1:A:489:VAL:HA	1:A:492:ILE:HD12	1.87	0.56
1:B:489:VAL:HA	1:B:492:ILE:HD12	1.87	0.56
1:C:323:GLN:HG2	1:C:324:LEU:H	1.70	0.56
1:C:489:VAL:HA	1:C:492:ILE:HD12	1.87	0.56
1:C:640:ILE:HD12	1:C:672:LEU:HD21	1.87	0.56
1:D:398:THR:OG1	1:D:400:GLU:OE1	2.16	0.56
1:D:640:ILE:HD12	1:D:672:LEU:HD21	1.87	0.56
1:D:232:ILE:O	1:D:236:ILE:N	2.24	0.56
1:A:470:ASP:O	1:A:474:ALA:N	2.22	0.56
1:B:325:ARG:HH21	1:B:356:ALA:H	1.51	0.56
1:D:395:LEU:HG	1:D:396:SER:H	1.70	0.56
1:B:322:ARG:HB3	1:B:423:PHE:HB2	1.87	0.56
1:D:398:THR:CA	3:D:1001:NAG:O6	2.54	0.56
1:A:509:CYS:O	1:A:513:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LEU:HG	1:C:396:SER:H	1.70	0.56
1:C:456:GLN:OE1	1:D:653:ASN:ND2	2.36	0.56
1:A:324:LEU:HD11	1:A:386:TYR:CZ	2.41	0.56
1:C:314:LEU:HB3	1:C:429:TYR:CD2	2.26	0.56
1:C:509:CYS:O	1:C:513:VAL:HG23	2.06	0.56
1:D:226:THR:HB	1:D:483:PHE:HZ	1.71	0.56
1:A:398:THR:OG1	1:A:400:GLU:OE1	2.16	0.56
1:A:401:GLU:O	1:A:405:GLN:N	2.27	0.56
1:B:323:GLN:HG2	1:B:324:LEU:H	1.70	0.56
1:C:226:THR:HB	1:C:483:PHE:HZ	1.71	0.56
1:D:323:GLN:HG2	1:D:324:LEU:H	1.70	0.56
1:A:406:VAL:HA	1:A:409:LEU:HD12	1.87	0.56
1:A:533:GLU:HA	1:A:536:LEU:HD22	1.87	0.56
4:A:1006:CHS:O	4:A:1006:CHS:OH	2.23	0.56
1:C:322:ARG:HB3	1:C:423:PHE:HB2	1.87	0.56
1:B:458:GLN:HG2	1:B:556:ILE:HG12	1.87	0.55
1:B:509:CYS:O	1:B:513:VAL:HG23	2.06	0.55
1:D:458:GLN:HG2	1:D:556:ILE:HG12	1.87	0.55
1:D:533:GLU:HA	1:D:536:LEU:HD22	1.87	0.55
1:C:382:ILE:HG23	1:C:383:ILE:H	1.70	0.55
1:D:489:VAL:HA	1:D:492:ILE:HD12	1.87	0.55
1:D:509:CYS:O	1:D:513:VAL:HG23	2.06	0.55
1:D:591:SER:HA	1:D:594:ALA:HB3	1.89	0.55
1:A:306:ARG:CG	1:A:308:PHE:CZ	2.88	0.55
1:B:226:THR:HB	1:B:483:PHE:HZ	1.71	0.55
1:B:262:VAL:N	1:B:268:THR:O	2.33	0.55
1:B:250:THR:OG1	1:B:251:ARG:N	2.40	0.55
1:D:382:ILE:HG23	1:D:383:ILE:H	1.70	0.55
1:A:640:ILE:HD12	1:A:672:LEU:HD21	1.87	0.55
1:C:432:ASN:ND2	1:D:447:ALA:O	2.38	0.55
1:A:528:ARG:HH22	1:A:550:HIS:HE1	1.55	0.55
1:A:677:LEU:O	1:A:681:ASN:N	2.24	0.55
1:A:688:LYS:O	1:A:692:ALA:N	2.39	0.55
1:C:324:LEU:HD11	1:C:386:TYR:CZ	2.41	0.55
1:D:324:LEU:HD11	1:D:386:TYR:CZ	2.41	0.55
1:A:250:THR:OG1	1:A:251:ARG:N	2.40	0.55
1:A:623:VAL:HG22	1:A:624:ASP:O	2.07	0.55
1:A:677:LEU:O	1:B:674:ASN:ND2	2.39	0.55
1:C:250:THR:OG1	1:C:251:ARG:N	2.40	0.55
1:A:458:GLN:HG2	1:A:556:ILE:HG12	1.87	0.55
1:C:528:ARG:HH22	1:C:550:HIS:HE1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:MET:HA	1:C:671:ILE:HG22	1.89	0.55
1:C:688:LYS:O	1:C:692:ALA:N	2.39	0.55
1:A:641:LEU:HD21	1:B:642:GLY:HA2	1.89	0.55
1:C:591:SER:HA	1:C:594:ALA:HB3	1.89	0.55
1:A:591:SER:HA	1:A:594:ALA:HB3	1.89	0.55
1:B:362:ASN:OD1	3:B:1002:NAG:N2	2.40	0.55
1:C:362:ASN:OD1	3:C:1002:NAG:N2	2.40	0.55
1:C:638:ARG:HE	1:C:643:ASP:CG	2.10	0.55
1:D:250:THR:OG1	1:D:251:ARG:N	2.40	0.55
1:A:362:ASN:OD1	3:A:1002:NAG:N2	2.40	0.54
1:B:528:ARG:HH22	1:B:550:HIS:HE1	1.55	0.54
1:C:307:SER:O	1:D:340:GLU:OE2	2.25	0.54
1:C:458:GLN:HG2	1:C:556:ILE:HG12	1.87	0.54
1:D:362:ASN:OD1	3:D:1002:NAG:N2	2.40	0.54
1:D:401:GLU:O	1:D:405:GLN:N	2.27	0.54
1:D:497:ILE:HG22	1:D:498:HIS:CD2	2.42	0.54
1:D:528:ARG:HH22	1:D:550:HIS:HE1	1.55	0.54
1:B:306:ARG:HD3	1:B:308:PHE:HZ	1.72	0.54
1:B:324:LEU:HD11	1:B:386:TYR:CZ	2.41	0.54
1:C:279:PHE:CZ	1:C:443:VAL:HG21	2.42	0.54
1:D:310:PHE:O	1:D:312:GLU:N	2.40	0.54
1:D:623:VAL:HG22	1:D:624:ASP:O	2.07	0.54
1:A:553:TYR:HA	1:A:556:ILE:HD12	1.90	0.54
1:A:580:ASN:O	1:A:581:ARG:NH1	2.40	0.54
1:D:321:ILE:HG12	1:D:424:ILE:HG12	1.89	0.54
1:D:638:ARG:HE	1:D:643:ASP:CG	2.10	0.54
1:D:639:ILE:HG12	1:D:644:ILE:CG2	2.38	0.54
1:D:688:LYS:O	1:D:692:ALA:N	2.39	0.54
1:A:462:LEU:HD12	1:A:463:ILE:HG23	1.89	0.54
1:A:497:ILE:HG22	1:A:498:HIS:CD2	2.42	0.54
1:A:562:ALA:O	1:A:566:VAL:HG23	2.08	0.54
1:B:280:TRP:HA	1:B:283:THR:HG23	1.90	0.54
1:B:395:LEU:HG	1:B:396:SER:H	1.70	0.54
1:B:456:GLN:OE1	1:C:653:ASN:ND2	2.39	0.54
1:B:553:TYR:HA	1:B:556:ILE:HD12	1.90	0.54
1:C:576:PHE:HA	1:C:579:PHE:CE2	2.43	0.54
4:C:1006:CHS:O	4:C:1006:CHS:OH	2.23	0.54
1:D:224:LEU:O	1:D:228:LEU:N	2.38	0.54
1:A:576:PHE:HA	1:A:579:PHE:CE2	2.43	0.54
1:B:576:PHE:HA	1:B:579:PHE:CE2	2.43	0.54
1:C:435:LEU:HG	1:C:460:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ILE:HG22	1:C:498:HIS:CD2	2.42	0.54
1:C:639:ILE:HG12	1:C:644:ILE:CG2	2.37	0.54
1:D:553:TYR:HA	1:D:556:ILE:HD12	1.90	0.54
1:D:663:THR:O	1:D:667:PHE:N	2.28	0.54
1:A:226:THR:HB	1:A:483:PHE:HZ	1.71	0.54
1:A:668:MET:HA	1:A:671:ILE:HG22	1.89	0.54
1:B:321:ILE:HG12	1:B:424:ILE:HG12	1.89	0.54
1:C:280:TRP:HA	1:C:283:THR:HG23	1.90	0.54
1:B:497:ILE:HG22	1:B:498:HIS:CD2	2.42	0.54
1:B:668:MET:HA	1:B:671:ILE:HG22	1.89	0.54
1:C:311:TYR:HB3	1:D:417:ARG:NH1	2.22	0.54
1:C:347:VAL:HG12	1:C:348:TYR:H	1.73	0.54
1:C:361:ARG:C	3:C:1002:NAG:H81	2.28	0.54
1:D:279:PHE:CZ	1:D:443:VAL:HG21	2.42	0.54
1:A:306:ARG:HD3	1:A:308:PHE:HZ	1.73	0.54
1:A:321:ILE:HG12	1:A:424:ILE:HG12	1.89	0.54
1:A:347:VAL:HG12	1:A:348:TYR:H	1.73	0.54
1:A:639:ILE:HG12	1:A:644:ILE:CG2	2.38	0.54
1:B:319:PRO:HD2	1:B:395:LEU:HD23	1.89	0.54
1:B:435:LEU:HG	1:B:460:LEU:O	2.07	0.54
1:B:562:ALA:O	1:B:566:VAL:HG23	2.08	0.54
1:B:623:VAL:HG22	1:B:624:ASP:O	2.07	0.54
1:C:321:ILE:HG12	1:C:424:ILE:HG12	1.89	0.54
1:D:435:LEU:HG	1:D:460:LEU:O	2.07	0.54
1:A:280:TRP:HA	1:A:283:THR:HG23	1.90	0.54
1:A:678:ALA:O	1:A:682:ASP:N	2.33	0.54
1:B:347:VAL:HG12	1:B:348:TYR:H	1.73	0.54
1:B:361:ARG:C	3:B:1002:NAG:H81	2.28	0.54
1:B:462:LEU:HD12	1:B:463:ILE:HG23	1.89	0.54
1:D:280:TRP:HA	1:D:283:THR:HG23	1.90	0.54
1:D:309:ILE:HD12	1:D:314:LEU:CA	2.36	0.54
1:A:279:PHE:CZ	1:A:443:VAL:HG21	2.42	0.54
1:B:279:PHE:CZ	1:B:443:VAL:HG21	2.42	0.54
1:D:292:TYR:C	1:D:294:LYS:HZ2	2.11	0.54
1:A:361:ARG:C	3:A:1002:NAG:H81	2.28	0.53
1:A:638:ARG:HE	1:A:643:ASP:CG	2.10	0.53
1:B:252:MET:SD	1:C:448:THR:OG1	2.52	0.53
1:C:553:TYR:HA	1:C:556:ILE:HD12	1.90	0.53
1:D:462:LEU:HD12	1:D:463:ILE:HG23	1.89	0.53
1:A:435:LEU:HG	1:A:460:LEU:O	2.08	0.53
1:B:398:THR:OG1	1:B:400:GLU:OE1	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:SER:HA	1:B:594:ALA:HB3	1.89	0.53
1:B:401:GLU:O	1:B:405:GLN:N	2.27	0.53
1:B:638:ARG:HE	1:B:643:ASP:CG	2.11	0.53
1:C:378:SER:CB	1:C:387:SER:HA	2.39	0.53
1:D:347:VAL:HG12	1:D:348:TYR:H	1.73	0.53
1:C:319:PRO:HD2	1:C:395:LEU:HD23	1.89	0.53
1:C:470:ASP:O	1:C:474:ALA:N	2.22	0.53
1:D:319:PRO:HD2	1:D:395:LEU:HD23	1.89	0.53
1:D:361:ARG:C	3:D:1002:NAG:H81	2.28	0.53
1:A:378:SER:CB	1:A:387:SER:HA	2.39	0.53
1:D:576:PHE:HA	1:D:579:PHE:CE2	2.43	0.53
1:D:668:MET:HA	1:D:671:ILE:HG22	1.89	0.53
1:A:224:LEU:O	1:A:228:LEU:N	2.38	0.53
1:A:539:LEU:CD1	2:E:2:NAG:O6	2.56	0.53
1:B:293:TRP:CH2	1:B:399:ARG:HG2	2.44	0.53
1:B:539:LEU:CD1	2:F:2:NAG:O6	2.56	0.53
1:B:688:LYS:O	1:B:692:ALA:N	2.39	0.53
1:D:562:ALA:O	1:D:566:VAL:HG23	2.08	0.53
1:A:319:PRO:HD2	1:A:395:LEU:HD23	1.89	0.53
1:B:616:TYR:O	1:B:620:GLY:N	2.42	0.53
1:D:674:ASN:OD1	1:D:678:ALA:N	2.42	0.53
1:C:539:LEU:CD1	2:G:2:NAG:O6	2.56	0.53
1:C:623:VAL:HG22	1:C:624:ASP:O	2.07	0.53
1:D:378:SER:CB	1:D:387:SER:HA	2.39	0.53
6:A:1010:PLM:O2	4:D:1005:CHS:N	2.42	0.53
1:C:428:VAL:O	1:C:437:CYS:N	2.36	0.53
1:C:462:LEU:HD12	1:C:463:ILE:HG23	1.89	0.53
1:A:428:VAL:O	1:A:437:CYS:N	2.36	0.53
1:A:674:ASN:OD1	1:A:678:ALA:N	2.42	0.53
1:C:562:ALA:O	1:C:566:VAL:HG23	2.08	0.53
1:C:674:ASN:OD1	1:C:678:ALA:N	2.42	0.53
1:D:519:VAL:HA	1:D:522:ILE:HB	1.91	0.53
1:D:624:ASP:C	1:D:626:PHE:H	2.12	0.53
1:A:293:TRP:CH2	1:A:399:ARG:HG2	2.44	0.52
1:B:378:SER:CB	1:B:387:SER:HA	2.39	0.52
1:B:445:PHE:CE1	1:B:451:VAL:HG22	2.44	0.52
1:B:466:VAL:N	1:B:470:ASP:HB2	2.16	0.52
1:B:639:ILE:HG12	1:B:644:ILE:CG2	2.37	0.52
1:C:519:VAL:HA	1:C:522:ILE:HB	1.91	0.52
1:D:616:TYR:O	1:D:620:GLY:N	2.42	0.52
1:C:293:TRP:CH2	1:C:399:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:PHE:CE1	1:C:451:VAL:HG22	2.44	0.52
1:D:294:LYS:HE2	1:D:309:ILE:CA	2.38	0.52
1:D:678:ALA:O	1:D:682:ASP:N	2.33	0.52
1:C:467:THR:OG1	1:D:335:GLN:OE1	2.27	0.52
1:D:539:LEU:CD1	3:D:1004:NAG:O6	2.56	0.52
1:A:519:VAL:HA	1:A:522:ILE:HB	1.91	0.52
1:B:249:TYR:HE1	1:B:313:ASN:HD21	1.58	0.52
1:C:616:TYR:O	1:C:620:GLY:N	2.42	0.52
5:C:1007:PX6:H41	1:D:655:VAL:HG11	1.92	0.52
1:D:445:PHE:CE1	1:D:451:VAL:HG22	2.44	0.52
1:A:362:ASN:CG	3:A:1002:NAG:C7	2.78	0.52
1:B:678:ALA:O	1:B:682:ASP:N	2.32	0.52
1:C:624:ASP:C	1:C:626:PHE:H	2.12	0.52
1:D:657:GLY:O	1:D:659:ILE:N	2.43	0.52
1:A:361:ARG:HD3	1:A:366:TRP:CD1	2.45	0.52
1:B:362:ASN:CG	3:B:1002:NAG:C7	2.78	0.52
1:B:692:ALA:HA	1:B:695:LYS:HG2	1.92	0.52
1:C:362:ASN:CG	3:C:1002:NAG:C7	2.78	0.52
1:D:528:ARG:HH12	1:D:550:HIS:CE1	2.28	0.52
1:A:528:ARG:HH12	1:A:550:HIS:CE1	2.28	0.52
1:A:659:ILE:O	1:A:663:THR:HG23	2.10	0.52
1:B:306:ARG:CG	1:B:308:PHE:CZ	2.89	0.52
1:C:261:PRO:HA	1:C:269:ASN:HA	1.92	0.52
1:C:663:THR:O	1:C:667:PHE:N	2.28	0.52
1:A:398:THR:O	1:A:398:THR:CG2	2.58	0.52
1:A:657:GLY:O	1:A:659:ILE:N	2.43	0.52
1:B:361:ARG:HD3	1:B:366:TRP:CD1	2.45	0.52
1:B:519:VAL:HA	1:B:522:ILE:HB	1.91	0.52
1:B:624:ASP:C	1:B:626:PHE:H	2.12	0.52
1:D:261:PRO:HA	1:D:269:ASN:HA	1.92	0.52
1:D:359:GLY:HA2	1:D:366:TRP:CD1	2.45	0.52
1:D:398:THR:O	1:D:398:THR:CG2	2.58	0.52
1:D:580:ASN:O	1:D:581:ARG:NH1	2.40	0.52
1:A:683:THR:O	1:A:687:VAL:N	2.43	0.52
1:B:683:THR:O	1:B:687:VAL:N	2.43	0.52
1:D:362:ASN:CG	3:D:1002:NAG:C7	2.78	0.52
1:D:692:ALA:HA	1:D:695:LYS:HG2	1.92	0.52
1:A:445:PHE:CE1	1:A:451:VAL:HG22	2.44	0.52
1:B:674:ASN:OD1	1:B:678:ALA:N	2.42	0.52
1:C:659:ILE:O	1:C:663:THR:HG23	2.10	0.52
1:B:379:HIS:HB3	1:B:423:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ARG:HD3	1:C:366:TRP:CD1	2.45	0.51
1:D:275:SER:HB2	1:D:278:ASP:CG	2.31	0.51
1:D:327:ARG:HD3	1:D:354:ASP:OD2	2.10	0.51
1:D:361:ARG:HD3	1:D:366:TRP:CD1	2.45	0.51
1:D:683:THR:O	1:D:687:VAL:N	2.43	0.51
1:A:249:TYR:HE1	1:A:313:ASN:HD21	1.58	0.51
1:A:616:TYR:O	1:A:620:GLY:N	2.42	0.51
1:A:624:ASP:C	1:A:626:PHE:H	2.12	0.51
1:B:261:PRO:HA	1:B:269:ASN:HA	1.92	0.51
1:B:657:GLY:O	1:B:659:ILE:N	2.43	0.51
1:C:364:THR:HG23	1:C:392:TYR:CZ	2.46	0.51
1:C:379:HIS:HB3	1:C:423:PHE:CZ	2.45	0.51
1:C:516:VAL:O	1:C:520:VAL:HG23	2.11	0.51
1:C:528:ARG:HH12	1:C:550:HIS:CE1	2.28	0.51
1:D:293:TRP:CH2	1:D:399:ARG:HG2	2.44	0.51
1:B:327:ARG:HD3	1:B:354:ASP:OD2	2.10	0.51
1:B:364:THR:HG23	1:B:392:TYR:CZ	2.46	0.51
1:B:428:VAL:O	1:B:437:CYS:N	2.36	0.51
1:B:634:PHE:O	1:B:637:PHE:N	2.44	0.51
1:C:275:SER:HB2	1:C:278:ASP:CG	2.31	0.51
1:C:657:GLY:O	1:C:659:ILE:N	2.43	0.51
1:D:309:ILE:HD12	1:D:314:LEU:N	2.08	0.51
1:A:275:SER:HB2	1:A:278:ASP:CG	2.31	0.51
1:A:573:LEU:O	1:A:577:ILE:N	2.33	0.51
1:B:311:TYR:HB3	1:C:417:ARG:NH1	2.24	0.51
1:B:659:ILE:O	1:B:663:THR:HG23	2.10	0.51
1:B:684:TYR:HA	1:B:687:VAL:HG13	1.93	0.51
1:C:359:GLY:HA2	1:C:366:TRP:CD1	2.45	0.51
1:C:480:PHE:O	1:C:484:ILE:HD12	2.11	0.51
1:A:400:GLU:OE1	1:A:400:GLU:N	2.36	0.51
1:B:275:SER:HB2	1:B:278:ASP:CG	2.30	0.51
1:B:398:THR:O	1:B:398:THR:CG2	2.58	0.51
1:B:528:ARG:HH12	1:B:550:HIS:CE1	2.28	0.51
1:B:570:TRP:O	1:B:573:LEU:HG	2.11	0.51
1:C:249:TYR:HE1	1:C:313:ASN:HD21	1.58	0.51
1:C:570:TRP:O	1:C:573:LEU:HG	2.11	0.51
1:D:364:THR:HG23	1:D:392:TYR:CZ	2.46	0.51
1:D:430:ASN:OD1	1:D:435:LEU:N	2.43	0.51
1:D:516:VAL:O	1:D:520:VAL:HG23	2.11	0.51
4:D:1006:CHS:O	4:D:1006:CHS:OH	2.24	0.51
1:A:364:THR:HG23	1:A:392:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASN:OD1	1:A:435:LEU:N	2.43	0.51
1:A:541:ASP:OD1	1:A:542:GLN:N	2.44	0.51
1:B:430:ASN:OD1	1:B:435:LEU:N	2.43	0.51
1:C:224:LEU:O	1:C:228:LEU:N	2.38	0.51
1:C:279:PHE:O	1:C:282:PHE:HB3	2.11	0.51
1:C:430:ASN:OD1	1:C:435:LEU:N	2.43	0.51
1:C:683:THR:O	1:C:687:VAL:N	2.43	0.51
1:D:294:LYS:HD3	1:D:308:PHE:O	2.10	0.51
1:A:261:PRO:HA	1:A:269:ASN:HA	1.92	0.51
1:A:359:GLY:HA2	1:A:366:TRP:CD1	2.45	0.51
1:A:606:ILE:HD13	1:D:573:LEU:HD11	1.60	0.51
1:A:639:ILE:HG12	1:A:644:ILE:HG21	1.93	0.51
1:C:514:ILE:HA	1:C:517:LEU:HD12	1.92	0.51
1:A:675:MET:O	1:A:679:ILE:HD12	2.11	0.51
4:A:1005:CHS:N	6:B:1010:PLM:O2	2.44	0.51
1:B:514:ILE:HA	1:B:517:LEU:HD12	1.93	0.51
1:D:555:GLN:HA	1:D:558:PHE:HB3	1.93	0.51
1:A:516:VAL:O	1:A:520:VAL:HG23	2.11	0.51
1:A:573:LEU:HA	1:A:576:PHE:HB2	1.93	0.51
1:A:616:TYR:OH	1:D:244:SER:HA	2.10	0.51
1:B:294:LYS:HD3	1:B:308:PHE:O	2.11	0.51
1:B:359:GLY:HA2	1:B:366:TRP:CD1	2.45	0.51
1:C:634:PHE:O	1:C:637:PHE:N	2.43	0.51
1:D:279:PHE:O	1:D:282:PHE:HB3	2.11	0.51
1:D:541:ASP:OD1	1:D:542:GLN:N	2.44	0.51
1:D:659:ILE:O	1:D:663:THR:HG23	2.10	0.51
1:A:247:TYR:HE1	1:B:623:VAL:C	2.14	0.51
1:A:279:PHE:O	1:A:282:PHE:HB3	2.11	0.51
1:A:692:ALA:HA	1:A:695:LYS:HG2	1.92	0.51
1:A:379:HIS:HB3	1:A:423:PHE:CZ	2.45	0.50
1:A:463:ILE:HG13	1:A:465:TYR:O	2.11	0.50
1:A:570:TRP:O	1:A:573:LEU:HG	2.11	0.50
1:A:611:TYR:HB3	1:A:660:TYR:HE1	1.76	0.50
1:B:279:PHE:O	1:B:282:PHE:HB3	2.11	0.50
1:B:331:CYS:HB3	1:B:346:ASP:HB3	1.94	0.50
1:B:555:GLN:HA	1:B:558:PHE:HB3	1.93	0.50
1:C:639:ILE:HG12	1:C:644:ILE:HG21	1.92	0.50
1:D:254:SER:O	1:D:257:PHE:N	2.40	0.50
1:D:463:ILE:HG13	1:D:465:TYR:O	2.11	0.50
1:D:634:PHE:O	1:D:637:PHE:N	2.43	0.50
1:D:684:TYR:HA	1:D:687:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HD3	1:A:354:ASP:OD2	2.10	0.50
1:A:331:CYS:HB3	1:A:346:ASP:HB3	1.94	0.50
1:B:573:LEU:HA	1:B:576:PHE:HB2	1.93	0.50
1:C:573:LEU:O	1:C:577:ILE:N	2.33	0.50
1:C:684:TYR:HA	1:C:687:VAL:HG13	1.93	0.50
1:C:692:ALA:HA	1:C:695:LYS:HG2	1.92	0.50
1:D:288:LEU:HD11	1:D:402:THR:HG23	1.93	0.50
1:A:480:PHE:O	1:A:484:ILE:HD12	2.11	0.50
1:B:436:PHE:HB3	1:B:460:LEU:HB3	1.93	0.50
1:B:480:PHE:O	1:B:484:ILE:HD12	2.11	0.50
1:B:611:TYR:HB3	1:B:660:TYR:HE1	1.76	0.50
1:D:249:TYR:HE1	1:D:313:ASN:HD21	1.58	0.50
1:D:379:HIS:HB3	1:D:423:PHE:CZ	2.45	0.50
1:D:480:PHE:O	1:D:484:ILE:HD12	2.11	0.50
1:D:570:TRP:O	1:D:573:LEU:HG	2.11	0.50
1:D:573:LEU:O	1:D:577:ILE:N	2.33	0.50
1:B:322:ARG:N	1:B:423:PHE:O	2.28	0.50
1:B:432:ASN:ND2	1:C:447:ALA:O	2.41	0.50
1:B:532:VAL:HG21	1:B:551:LEU:HD21	1.94	0.50
1:B:541:ASP:OD1	1:B:542:GLN:N	2.44	0.50
1:B:573:LEU:O	1:B:577:ILE:N	2.33	0.50
1:C:327:ARG:HD3	1:C:354:ASP:OD2	2.10	0.50
1:C:463:ILE:HG13	1:C:465:TYR:O	2.11	0.50
1:C:532:VAL:HG21	1:C:551:LEU:HD21	1.94	0.50
1:A:448:THR:HB	1:D:249:TYR:HD1	1.76	0.50
1:B:516:VAL:O	1:B:520:VAL:HG23	2.11	0.50
1:C:398:THR:O	1:C:398:THR:CG2	2.58	0.50
1:D:436:PHE:HB3	1:D:460:LEU:HB3	1.93	0.50
1:D:611:TYR:HB3	1:D:660:TYR:HE1	1.76	0.50
1:A:634:PHE:O	1:A:637:PHE:N	2.44	0.50
1:B:580:ASN:O	1:B:581:ARG:NH1	2.40	0.50
1:C:361:ARG:C	3:C:1002:NAG:C8	2.79	0.50
1:B:224:LEU:O	1:B:228:LEU:N	2.38	0.50
1:B:675:MET:O	1:B:679:ILE:HD12	2.11	0.50
1:C:244:SER:HA	1:D:616:TYR:OH	2.11	0.50
1:C:541:ASP:OD1	1:C:542:GLN:N	2.44	0.50
1:D:314:LEU:HB3	1:D:429:TYR:CD2	2.26	0.50
1:D:331:CYS:HB3	1:D:346:ASP:HB3	1.94	0.50
1:D:639:ILE:HG12	1:D:644:ILE:HG21	1.93	0.50
1:B:639:ILE:HG12	1:B:644:ILE:HG21	1.92	0.50
1:C:555:GLN:HA	1:C:558:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:VAL:HG21	1:D:551:LEU:HD21	1.94	0.50
1:D:675:MET:O	1:D:679:ILE:HD12	2.11	0.50
1:A:684:TYR:HA	1:A:687:VAL:HG13	1.93	0.50
1:B:288:LEU:HD11	1:B:402:THR:HG23	1.93	0.50
1:C:331:CYS:HB3	1:C:346:ASP:HB3	1.93	0.50
1:C:401:GLU:HA	1:C:404:ALA:HB3	1.93	0.50
1:C:611:TYR:HB3	1:C:660:TYR:HE1	1.76	0.50
1:A:532:VAL:HG21	1:A:551:LEU:HD21	1.94	0.49
1:C:675:MET:O	1:C:679:ILE:HD12	2.11	0.49
1:C:677:LEU:O	1:D:674:ASN:ND2	2.45	0.49
1:D:294:LYS:NZ	1:D:308:PHE:O	2.41	0.49
1:A:288:LEU:HD11	1:A:402:THR:HG23	1.93	0.49
1:A:555:GLN:HA	1:A:558:PHE:HB3	1.93	0.49
1:A:577:ILE:HG12	1:B:602:ILE:HD13	1.94	0.49
1:C:307:SER:N	1:D:340:GLU:OE2	2.44	0.49
1:D:466:VAL:H	1:D:470:ASP:CB	2.20	0.49
1:D:603:MET:O	1:D:606:ILE:HG22	2.12	0.49
1:A:254:SER:O	1:A:257:PHE:N	2.39	0.49
1:A:514:ILE:HA	1:A:517:LEU:HD12	1.93	0.49
1:C:580:ASN:O	1:C:581:ARG:NH1	2.40	0.49
1:D:309:ILE:HD12	1:D:314:LEU:HA	1.94	0.49
1:C:331:CYS:SG	1:C:332:SER:N	2.83	0.49
1:C:567:PHE:O	1:C:571:ILE:HG23	2.13	0.49
4:C:1005:CHS:N	6:D:1010:PLM:O2	2.45	0.49
1:A:436:PHE:HB3	1:A:460:LEU:HB3	1.93	0.49
1:A:447:ALA:O	1:D:432:ASN:ND2	2.44	0.49
1:A:683:THR:O	1:A:687:VAL:HG13	2.13	0.49
1:B:401:GLU:HA	1:B:404:ALA:HB3	1.94	0.49
1:B:677:LEU:HD22	1:C:674:ASN:HB2	1.94	0.49
1:C:409:LEU:O	1:C:413:VAL:N	2.46	0.49
1:D:567:PHE:O	1:D:571:ILE:HG23	2.13	0.49
1:D:573:LEU:HA	1:D:576:PHE:HB2	1.93	0.49
1:A:309:ILE:HG12	1:A:314:LEU:HA	1.94	0.49
1:B:280:TRP:NE1	1:B:414:TRP:CD1	2.81	0.49
1:B:463:ILE:HG13	1:B:465:TYR:O	2.11	0.49
1:D:409:LEU:O	1:D:413:VAL:N	2.46	0.49
1:A:601:ALA:HB1	1:A:605:PHE:CZ	2.48	0.49
1:A:663:THR:O	1:A:667:PHE:N	2.28	0.49
1:C:280:TRP:NE1	1:C:414:TRP:CD1	2.81	0.49
1:C:573:LEU:HA	1:C:576:PHE:HB2	1.93	0.49
1:D:252:MET:HG3	1:D:253:MET:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:HA	1:A:404:ALA:HB3	1.93	0.49
1:B:230:PHE:CZ	1:B:484:ILE:HD11	2.48	0.49
1:B:331:CYS:SG	1:B:332:SER:N	2.83	0.49
1:B:683:THR:O	1:B:687:VAL:HG13	2.13	0.49
4:B:1005:CHS:N	6:C:1010:PLM:O2	2.45	0.49
1:C:399:ARG:HD3	1:C:402:THR:HG21	1.95	0.49
1:C:436:PHE:HB3	1:C:460:LEU:HB3	1.93	0.49
1:C:603:MET:O	1:C:606:ILE:HG22	2.13	0.49
1:D:401:GLU:HA	1:D:404:ALA:HB3	1.94	0.49
1:D:514:ILE:HA	1:D:517:LEU:HD12	1.93	0.49
1:A:335:GLN:OE1	1:D:467:THR:OG1	2.30	0.49
1:B:409:LEU:O	1:B:413:VAL:N	2.46	0.49
1:C:249:TYR:HD1	1:D:448:THR:HB	1.76	0.49
1:A:230:PHE:CZ	1:A:484:ILE:HD11	2.48	0.49
1:A:409:LEU:O	1:A:413:VAL:N	2.46	0.49
1:A:602:ILE:HD13	1:D:577:ILE:HG12	1.95	0.49
1:B:573:LEU:O	1:B:577:ILE:HG22	2.13	0.49
1:C:307:SER:HB3	1:C:397:ARG:HH21	1.77	0.49
1:C:322:ARG:N	1:C:423:PHE:O	2.28	0.49
1:C:683:THR:O	1:C:687:VAL:HG13	2.13	0.49
5:C:1007:PX6:H24	6:C:1010:PLM:HG2	1.95	0.49
1:D:230:PHE:CZ	1:D:484:ILE:HD11	2.48	0.49
1:D:513:VAL:O	1:D:517:LEU:HG	2.13	0.49
1:A:252:MET:HG3	1:A:253:MET:N	2.28	0.48
1:A:567:PHE:O	1:A:571:ILE:HG23	2.13	0.48
1:B:309:ILE:HG12	1:B:314:LEU:HA	1.94	0.48
1:C:601:ALA:HB1	1:C:605:PHE:CZ	2.48	0.48
1:D:399:ARG:HD3	1:D:402:THR:HG21	1.95	0.48
1:D:601:ALA:HB1	1:D:605:PHE:CZ	2.48	0.48
1:A:513:VAL:HG12	1:A:517:LEU:HD11	1.95	0.48
1:B:361:ARG:C	3:B:1002:NAG:C8	2.80	0.48
1:B:567:PHE:O	1:B:571:ILE:HG23	2.13	0.48
1:C:573:LEU:O	1:C:577:ILE:HG22	2.13	0.48
1:D:683:THR:O	1:D:687:VAL:HG13	2.13	0.48
1:B:532:VAL:O	1:B:536:LEU:HD13	2.14	0.48
1:B:601:ALA:HB1	1:B:605:PHE:CZ	2.48	0.48
1:C:252:MET:HG3	1:C:253:MET:N	2.28	0.48
1:C:288:LEU:HD11	1:C:402:THR:HG23	1.93	0.48
1:D:280:TRP:NE1	1:D:414:TRP:CD1	2.81	0.48
1:D:428:VAL:O	1:D:437:CYS:N	2.36	0.48
1:A:322:ARG:N	1:A:423:PHE:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:VAL:O	1:A:517:LEU:HG	2.13	0.48
1:B:513:VAL:O	1:B:517:LEU:HG	2.13	0.48
1:B:603:MET:O	1:B:606:ILE:HG22	2.12	0.48
1:C:230:PHE:CZ	1:C:484:ILE:HD11	2.48	0.48
1:C:238:THR:HA	1:C:241:MET:HG2	1.95	0.48
1:D:269:ASN:ND2	1:D:271:LYS:HB3	2.29	0.48
1:D:573:LEU:O	1:D:577:ILE:HG22	2.13	0.48
1:A:399:ARG:HD3	1:A:402:THR:HG21	1.95	0.48
1:A:406:VAL:HG13	1:A:414:TRP:NE1	2.24	0.48
1:A:624:ASP:C	1:A:626:PHE:N	2.67	0.48
5:A:1007:PX6:H46	5:A:1007:PX6:H53	1.60	0.48
1:B:269:ASN:ND2	1:B:271:LYS:HB3	2.29	0.48
1:B:640:ILE:HD12	1:B:672:LEU:CD2	2.44	0.48
1:C:249:TYR:CD1	1:D:448:THR:HB	2.48	0.48
1:C:269:ASN:ND2	1:C:271:LYS:HB3	2.29	0.48
1:C:319:PRO:HA	1:C:426:PHE:HB3	1.95	0.48
1:C:430:ASN:ND2	1:C:435:LEU:HB3	2.27	0.48
1:C:513:VAL:HG12	1:C:517:LEU:HD11	1.95	0.48
1:D:238:THR:HA	1:D:241:MET:HG2	1.96	0.48
1:D:640:ILE:HD12	1:D:672:LEU:CD2	2.44	0.48
1:A:223:GLU:OE1	1:A:227:TYR:CE2	2.66	0.48
1:A:238:THR:HA	1:A:241:MET:HG2	1.95	0.48
1:A:332:SER:HB3	1:D:432:ASN:HA	1.95	0.48
1:B:238:THR:HA	1:B:241:MET:HG2	1.96	0.48
1:B:513:VAL:HG12	1:B:517:LEU:HD11	1.95	0.48
6:C:1009:PLM:H61	6:C:1009:PLM:H92	1.73	0.48
1:D:223:GLU:OE1	1:D:227:TYR:CE2	2.66	0.48
1:D:513:VAL:HG12	1:D:517:LEU:HD11	1.95	0.48
1:A:323:GLN:NE2	1:A:415:LEU:O	2.44	0.48
1:B:223:GLU:OE1	1:B:227:TYR:CE2	2.66	0.48
1:C:223:GLU:OE1	1:C:227:TYR:CE2	2.66	0.48
1:C:577:ILE:HG12	1:D:602:ILE:HD13	1.96	0.48
1:D:294:LYS:HZ1	1:D:309:ILE:HA	1.71	0.48
1:A:603:MET:O	1:A:606:ILE:HG22	2.13	0.48
1:B:689:SER:HA	1:B:692:ALA:HB3	1.96	0.48
1:C:532:VAL:O	1:C:536:LEU:HD13	2.14	0.48
1:A:308:PHE:N	1:A:308:PHE:CD1	2.80	0.48
1:A:487:TYR:HD1	1:A:490:GLU:OE2	1.97	0.48
1:A:615:ALA:HA	1:A:619:PHE:CD2	2.49	0.48
1:A:640:ILE:HD12	1:A:672:LEU:CD2	2.44	0.48
1:B:466:VAL:H	1:B:470:ASP:CB	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:TYR:HD1	1:B:490:GLU:OE2	1.97	0.48
1:C:279:PHE:CE1	1:C:443:VAL:HG11	2.49	0.48
1:D:275:SER:HB2	1:D:278:ASP:OD2	2.14	0.48
1:D:639:ILE:O	1:D:642:GLY:N	2.47	0.48
1:A:279:PHE:CE1	1:A:443:VAL:HG11	2.49	0.48
1:A:280:TRP:NE1	1:A:414:TRP:CD1	2.81	0.48
1:A:573:LEU:O	1:A:577:ILE:HG22	2.13	0.48
1:B:249:TYR:HD1	1:C:448:THR:HB	1.79	0.48
1:B:323:GLN:NE2	1:B:415:LEU:O	2.44	0.48
1:C:689:SER:HA	1:C:692:ALA:HB3	1.95	0.48
1:D:279:PHE:CE1	1:D:443:VAL:HG11	2.48	0.48
1:D:331:CYS:SG	1:D:332:SER:N	2.83	0.48
1:B:254:SER:O	1:B:257:PHE:N	2.39	0.47
1:B:279:PHE:CE1	1:B:443:VAL:HG11	2.49	0.47
1:B:639:ILE:O	1:B:642:GLY:N	2.47	0.47
1:C:323:GLN:NE2	1:C:415:LEU:O	2.44	0.47
1:C:487:TYR:HD1	1:C:490:GLU:OE2	1.97	0.47
1:D:319:PRO:HA	1:D:426:PHE:HB3	1.96	0.47
1:D:398:THR:CB	3:D:1001:NAG:C6	2.85	0.47
1:D:487:TYR:HD1	1:D:490:GLU:OE2	1.97	0.47
1:A:571:ILE:O	1:A:574:PHE:HB3	2.14	0.47
1:A:604:PHE:O	1:A:607:ILE:HG22	2.14	0.47
1:A:639:ILE:O	1:A:642:GLY:N	2.47	0.47
1:B:399:ARG:HD3	1:B:402:THR:HG21	1.95	0.47
1:B:309:ILE:O	1:B:312:GLU:N	2.42	0.47
1:B:406:VAL:HG13	1:B:414:TRP:NE1	2.24	0.47
1:B:571:ILE:O	1:B:574:PHE:HB3	2.14	0.47
1:C:275:SER:HB2	1:C:278:ASP:OD2	2.14	0.47
1:C:513:VAL:O	1:C:517:LEU:HG	2.13	0.47
1:C:571:ILE:O	1:C:574:PHE:HB3	2.14	0.47
1:C:624:ASP:C	1:C:626:PHE:N	2.67	0.47
1:C:639:ILE:O	1:C:642:GLY:N	2.47	0.47
1:D:689:SER:HA	1:D:692:ALA:HB3	1.95	0.47
1:A:275:SER:HB2	1:A:278:ASP:OD2	2.14	0.47
1:A:466:VAL:H	1:A:470:ASP:CB	2.20	0.47
1:B:252:MET:HG3	1:B:253:MET:N	2.28	0.47
1:B:379:HIS:HA	1:B:440:ARG:NH2	2.29	0.47
1:B:400:GLU:OE1	1:B:400:GLU:N	2.36	0.47
1:C:573:LEU:HD12	1:D:606:ILE:HD13	1.89	0.47
1:B:624:ASP:C	1:B:626:PHE:N	2.67	0.47
1:D:619:PHE:C	1:D:621:THR:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:O	1:A:536:LEU:HD13	2.14	0.47
1:A:582:THR:O	1:A:586:LEU:HG	2.15	0.47
1:A:674:ASN:ND2	1:D:677:LEU:O	2.47	0.47
1:B:604:PHE:O	1:B:607:ILE:HG22	2.14	0.47
1:C:379:HIS:HA	1:C:440:ARG:NH2	2.29	0.47
1:C:524:ILE:HA	1:C:527:TYR:HB3	1.97	0.47
1:C:582:THR:O	1:C:586:LEU:HG	2.15	0.47
1:D:604:PHE:O	1:D:607:ILE:HG22	2.14	0.47
1:A:248:TYR:CE2	1:B:452:ILE:HD12	2.50	0.47
1:A:269:ASN:ND2	1:A:271:LYS:HB3	2.29	0.47
1:A:319:PRO:HA	1:A:426:PHE:HB3	1.96	0.47
1:A:323:GLN:HE22	1:A:415:LEU:HB2	1.79	0.47
1:A:417:ARG:HH11	1:D:311:TYR:HB3	1.78	0.47
1:A:627:SER:HB3	1:D:247:TYR:HB2	1.97	0.47
1:B:582:THR:O	1:B:586:LEU:HG	2.15	0.47
1:B:615:ALA:HA	1:B:619:PHE:CD2	2.49	0.47
1:B:630:GLN:O	1:B:633:ILE:HG22	2.15	0.47
1:B:677:LEU:O	1:C:674:ASN:ND2	2.45	0.47
1:C:401:GLU:O	1:C:405:GLN:N	2.27	0.47
1:C:612:ALA:HB2	1:C:636:GLN:OE1	2.15	0.47
1:C:640:ILE:HD12	1:C:672:LEU:CD2	2.44	0.47
1:C:641:LEU:HD21	1:D:642:GLY:HA2	1.96	0.47
5:C:1007:PX6:H46	5:C:1007:PX6:H53	1.63	0.47
1:D:323:GLN:HE22	1:D:415:LEU:HB2	1.80	0.47
1:D:379:HIS:HA	1:D:440:ARG:NH2	2.29	0.47
1:D:382:ILE:HG23	1:D:383:ILE:N	2.30	0.47
1:D:430:ASN:ND2	1:D:435:LEU:HB3	2.27	0.47
1:D:501:HIS:O	1:D:505:SER:OG	2.33	0.47
1:D:571:ILE:O	1:D:574:PHE:HB3	2.14	0.47
1:D:582:THR:O	1:D:586:LEU:HG	2.15	0.47
1:D:656:LEU:HA	1:D:657:GLY:HA2	1.34	0.47
5:D:1007:PX6:H24	6:D:1010:PLM:HG2	1.96	0.47
1:A:252:MET:SD	1:B:448:THR:OG1	2.60	0.47
1:A:448:THR:HB	1:D:249:TYR:CD1	2.50	0.47
1:B:663:THR:O	1:B:667:PHE:N	2.28	0.47
1:C:605:PHE:HZ	6:C:1009:PLM:HG3	1.80	0.47
1:C:652:ALA:O	1:C:653:ASN:ND2	2.48	0.47
1:A:652:ALA:O	1:A:653:ASN:ND2	2.48	0.47
1:C:501:HIS:O	1:C:505:SER:OG	2.33	0.47
1:C:630:GLN:O	1:C:633:ILE:HG22	2.15	0.47
1:D:624:ASP:C	1:D:626:PHE:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:GLN:O	1:D:633:ILE:HG22	2.15	0.47
1:A:244:SER:HA	1:B:616:TYR:OH	2.14	0.47
1:A:524:ILE:HA	1:A:527:TYR:HB3	1.97	0.47
1:A:689:SER:HA	1:A:692:ALA:HB3	1.96	0.47
1:B:275:SER:HB2	1:B:278:ASP:OD2	2.14	0.47
1:B:430:ASN:ND2	1:B:435:LEU:HB3	2.27	0.47
1:B:652:ALA:O	1:B:653:ASN:ND2	2.48	0.47
1:D:532:VAL:O	1:D:536:LEU:HD13	2.14	0.47
1:A:465:TYR:HA	1:A:470:ASP:OD2	2.15	0.46
1:B:382:ILE:HG23	1:B:383:ILE:N	2.30	0.46
4:B:1005:CHS:HD22	4:B:1006:CHS:HD23	1.98	0.46
1:D:652:ALA:O	1:D:653:ASN:ND2	2.48	0.46
1:A:379:HIS:HA	1:A:440:ARG:NH2	2.29	0.46
5:B:1007:PX6:H24	6:B:1010:PLM:HG2	1.97	0.46
1:D:406:VAL:HG13	1:D:414:TRP:NE1	2.24	0.46
1:A:382:ILE:HG23	1:A:383:ILE:N	2.30	0.46
1:B:612:ALA:HB2	1:B:636:GLN:OE1	2.15	0.46
1:D:406:VAL:O	1:D:410:LYS:N	2.47	0.46
1:A:325:ARG:NH2	1:A:355:ARG:HA	2.29	0.46
1:A:548:PHE:O	1:A:551:LEU:HB2	2.16	0.46
1:A:612:ALA:HB2	1:A:636:GLN:OE1	2.15	0.46
1:A:630:GLN:O	1:A:633:ILE:HG22	2.15	0.46
1:B:524:ILE:HA	1:B:527:TYR:HB3	1.97	0.46
1:C:247:TYR:HB2	1:D:627:SER:HB3	1.98	0.46
1:C:323:GLN:HE22	1:C:415:LEU:HB2	1.80	0.46
1:D:615:ALA:HA	1:D:619:PHE:CD2	2.49	0.46
1:A:328:ASN:OD1	1:A:343:GLU:HB3	2.15	0.46
1:B:249:TYR:CD1	1:C:448:THR:HB	2.51	0.46
1:C:604:PHE:O	1:C:607:ILE:HG22	2.14	0.46
1:B:244:SER:HA	1:C:616:TYR:OH	2.16	0.46
1:B:323:GLN:HE22	1:B:415:LEU:HB2	1.80	0.46
1:C:247:TYR:HB2	1:D:627:SER:CB	2.45	0.46
1:C:248:TYR:C	1:C:252:MET:HG2	2.36	0.46
1:C:465:TYR:HA	1:C:470:ASP:OD2	2.16	0.46
1:C:548:PHE:O	1:C:551:LEU:HB2	2.16	0.46
1:A:331:CYS:SG	1:A:332:SER:N	2.83	0.46
1:A:605:PHE:HZ	6:A:1009:PLM:HG3	1.79	0.46
1:B:294:LYS:HD2	1:B:294:LYS:N	2.31	0.46
1:B:319:PRO:HA	1:B:426:PHE:HB3	1.96	0.46
1:B:325:ARG:NH2	1:B:355:ARG:HA	2.29	0.46
1:C:294:LYS:N	1:C:294:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:SER:HB2	1:C:344:CYS:HB3	1.98	0.46
1:C:619:PHE:C	1:C:621:THR:N	2.67	0.46
1:D:332:SER:HB2	1:D:344:CYS:HB3	1.98	0.46
1:D:384:ALA:CA	1:D:385:THR:HG22	2.35	0.46
1:D:441:LEU:HD23	1:D:441:LEU:HA	1.74	0.46
1:B:577:ILE:HG12	1:C:602:ILE:CD1	2.45	0.46
1:C:615:ALA:HA	1:C:619:PHE:CD2	2.49	0.46
1:D:465:TYR:HA	1:D:470:ASP:OD2	2.15	0.46
6:D:1009:PLM:H71	6:D:1009:PLM:H42	1.60	0.46
1:A:309:ILE:HD11	1:A:314:LEU:C	2.28	0.46
1:A:332:SER:HB2	1:A:344:CYS:HB3	1.98	0.46
1:B:223:GLU:OE1	1:B:227:TYR:HE2	1.99	0.46
1:B:248:TYR:C	1:B:252:MET:HG2	2.36	0.46
1:B:465:TYR:HA	1:B:470:ASP:OD2	2.15	0.46
1:D:223:GLU:OE1	1:D:227:TYR:HE2	1.99	0.46
1:D:328:ASN:ND2	1:D:343:GLU:OE1	2.49	0.46
1:D:524:ILE:HA	1:D:527:TYR:HB3	1.97	0.46
1:A:223:GLU:OE1	1:A:227:TYR:HE2	1.99	0.46
1:B:573:LEU:HD12	1:C:606:ILE:HD13	1.83	0.46
6:B:1010:PLM:H42	6:B:1010:PLM:H71	1.56	0.46
1:C:293:TRP:CZ3	1:C:399:ARG:HG2	2.51	0.46
1:D:293:TRP:CZ3	1:D:399:ARG:HG2	2.51	0.46
1:D:294:LYS:HE2	1:D:309:ILE:HA	1.98	0.46
1:A:619:PHE:C	1:A:621:THR:N	2.67	0.45
1:C:223:GLU:OE1	1:C:227:TYR:HE2	1.99	0.45
1:C:382:ILE:HG23	1:C:383:ILE:N	2.30	0.45
1:C:466:VAL:H	1:C:470:ASP:CB	2.20	0.45
1:C:561:ILE:O	1:C:565:THR:HG23	2.17	0.45
1:D:328:ASN:OD1	1:D:343:GLU:HB3	2.15	0.45
1:A:294:LYS:N	1:A:294:LYS:HD2	2.31	0.45
1:A:328:ASN:ND2	1:A:343:GLU:OE1	2.49	0.45
1:B:247:TYR:HE1	1:C:623:VAL:C	2.19	0.45
1:B:458:GLN:HE21	1:B:459:PRO:HD2	1.81	0.45
1:B:619:PHE:C	1:B:621:THR:N	2.67	0.45
1:C:328:ASN:ND2	1:C:343:GLU:OE1	2.49	0.45
1:D:294:LYS:N	1:D:294:LYS:HD2	2.31	0.45
1:D:612:ALA:HB2	1:D:636:GLN:OE1	2.15	0.45
1:A:247:TYR:HB2	1:B:627:SER:CB	2.47	0.45
1:A:471:PHE:HA	1:A:474:ALA:HB3	1.98	0.45
1:B:328:ASN:OD1	1:B:343:GLU:HB3	2.15	0.45
1:B:501:HIS:O	1:B:505:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:CA	1:C:385:THR:HG22	2.35	0.45
1:A:293:TRP:CZ3	1:A:399:ARG:HG2	2.51	0.45
1:A:380:TRP:HB2	5:A:1007:PX6:H3	1.98	0.45
1:B:216:TYR:O	1:B:220:VAL:HG22	2.17	0.45
1:B:406:VAL:O	1:B:410:LYS:N	2.47	0.45
1:B:467:THR:OG1	1:C:335:GLN:OE1	2.34	0.45
1:B:471:PHE:HA	1:B:474:ALA:HB3	1.98	0.45
1:D:216:TYR:O	1:D:220:VAL:HG22	2.17	0.45
1:D:310:PHE:N	1:D:310:PHE:CD1	2.83	0.45
1:D:460:LEU:HD13	1:D:555:GLN:HG2	1.99	0.45
1:A:458:GLN:HE21	1:A:459:PRO:HD2	1.81	0.45
1:A:556:ILE:HG22	1:A:560:ASN:OD1	2.17	0.45
1:A:561:ILE:O	1:A:565:THR:HG23	2.17	0.45
1:B:220:VAL:O	1:B:224:LEU:HG	2.17	0.45
1:B:328:ASN:ND2	1:B:343:GLU:OE1	2.49	0.45
1:B:684:TYR:OH	1:C:679:ILE:HG12	2.16	0.45
1:C:328:ASN:OD1	1:C:343:GLU:HB3	2.15	0.45
1:C:591:SER:HA	1:C:594:ALA:CB	2.47	0.45
1:D:334:PRO:HB2	1:D:337:LEU:HB2	1.98	0.45
1:D:400:GLU:OE1	1:D:400:GLU:N	2.36	0.45
1:D:556:ILE:HG22	1:D:560:ASN:OD1	2.17	0.45
1:A:220:VAL:O	1:A:224:LEU:HG	2.17	0.45
1:A:378:SER:HB3	1:A:387:SER:HA	1.98	0.45
1:B:224:LEU:O	1:B:228:LEU:HG	2.17	0.45
1:B:227:TYR:O	1:B:231:LEU:HB2	2.17	0.45
1:B:548:PHE:O	1:B:551:LEU:HB2	2.16	0.45
1:C:254:SER:O	1:C:257:PHE:N	2.39	0.45
1:C:678:ALA:O	1:C:682:ASP:N	2.32	0.45
1:D:220:VAL:O	1:D:224:LEU:HG	2.17	0.45
1:D:248:TYR:C	1:D:252:MET:HG2	2.36	0.45
1:D:601:ALA:HB1	1:D:605:PHE:CE2	2.52	0.45
1:A:227:TYR:O	1:A:231:LEU:HB2	2.17	0.45
1:A:430:ASN:ND2	1:A:435:LEU:HB3	2.27	0.45
1:A:460:LEU:HD13	1:A:555:GLN:HG2	1.99	0.45
1:A:467:THR:HG21	1:B:333:ILE:HG22	1.98	0.45
1:B:293:TRP:CZ3	1:B:399:ARG:HG2	2.51	0.45
1:B:591:SER:HA	1:B:594:ALA:CB	2.47	0.45
1:B:633:ILE:HA	1:B:633:ILE:HD12	1.62	0.45
1:C:378:SER:HB3	1:C:387:SER:HA	1.98	0.45
1:C:406:VAL:O	1:C:410:LYS:N	2.47	0.45
1:D:249:TYR:OH	1:D:430:ASN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:PRO:HG3	1:D:426:PHE:CG	2.52	0.45
1:D:322:ARG:N	1:D:423:PHE:O	2.28	0.45
1:A:591:SER:HA	1:A:594:ALA:CB	2.47	0.45
1:A:601:ALA:HB1	1:A:605:PHE:CE2	2.52	0.45
1:B:332:SER:HB2	1:B:344:CYS:HB3	1.98	0.45
1:B:334:PRO:HB2	1:B:337:LEU:HB2	1.98	0.45
1:B:548:PHE:CD2	1:B:552:ALA:HB2	2.52	0.45
1:C:216:TYR:O	1:C:220:VAL:HG22	2.17	0.45
1:C:347:VAL:HG12	1:C:348:TYR:N	2.32	0.45
1:D:378:SER:HB3	1:D:387:SER:HA	1.98	0.45
1:D:548:PHE:O	1:D:551:LEU:HB2	2.16	0.45
1:A:216:TYR:O	1:A:220:VAL:HG22	2.17	0.45
1:A:680:ILE:CG2	1:B:674:ASN:HB3	2.47	0.45
1:B:319:PRO:HG3	1:B:426:PHE:CG	2.52	0.45
1:C:249:TYR:OH	1:C:430:ASN:HB3	2.17	0.45
1:C:319:PRO:HG3	1:C:426:PHE:CG	2.52	0.45
1:C:400:GLU:OE1	1:C:400:GLU:N	2.36	0.45
1:C:548:PHE:CD2	1:C:552:ALA:HB2	2.52	0.45
1:A:224:LEU:O	1:A:228:LEU:HG	2.17	0.45
1:A:248:TYR:C	1:A:252:MET:HG2	2.36	0.45
1:A:501:HIS:O	1:A:505:SER:OG	2.33	0.45
1:B:347:VAL:HG12	1:B:348:TYR:N	2.32	0.45
1:B:573:LEU:O	1:B:576:PHE:N	2.50	0.45
1:B:688:LYS:HA	1:B:691:LEU:HG	1.99	0.45
4:B:1006:CHS:O	4:B:1006:CHS:OH	2.22	0.45
1:C:385:THR:O	1:C:385:THR:HG23	2.17	0.45
1:D:548:PHE:CD2	1:D:552:ALA:HB2	2.52	0.45
1:A:262:VAL:O	1:A:263:SER:OG	2.31	0.44
1:A:371:GLU:OE1	1:A:378:SER:HB3	2.18	0.44
1:B:456:GLN:NE2	5:B:1007:PX6:O1	2.50	0.44
1:B:561:ILE:O	1:B:565:THR:HG23	2.17	0.44
1:C:220:VAL:O	1:C:224:LEU:HG	2.17	0.44
1:C:688:LYS:HA	1:C:691:LEU:HG	2.00	0.44
1:D:591:SER:HA	1:D:594:ALA:CB	2.47	0.44
1:A:334:PRO:HB2	1:A:337:LEU:HB2	1.98	0.44
1:A:347:VAL:HG12	1:A:348:TYR:N	2.32	0.44
1:A:385:THR:HG23	1:A:385:THR:O	2.17	0.44
1:A:436:PHE:CD1	1:A:460:LEU:HD23	2.53	0.44
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.74	0.44
1:B:460:LEU:HD13	1:B:555:GLN:HG2	1.99	0.44
1:B:556:ILE:HG22	1:B:560:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:SER:HB2	1:C:600:PHE:HE1	1.83	0.44
1:C:227:TYR:O	1:C:231:LEU:HB2	2.17	0.44
1:C:248:TYR:CE2	1:D:452:ILE:HD12	2.52	0.44
1:C:279:PHE:CE1	1:C:443:VAL:HG21	2.53	0.44
1:D:561:ILE:O	1:D:565:THR:HG23	2.16	0.44
1:D:573:LEU:O	1:D:576:PHE:N	2.50	0.44
1:A:319:PRO:HG3	1:A:426:PHE:CG	2.52	0.44
1:B:249:TYR:OH	1:B:430:ASN:HB3	2.17	0.44
1:C:323:GLN:NE2	1:C:415:LEU:HB2	2.33	0.44
1:C:377:SER:OG	1:C:378:SER:N	2.51	0.44
1:C:556:ILE:HG22	1:C:560:ASN:OD1	2.17	0.44
1:C:601:ALA:HB1	1:C:605:PHE:CE2	2.52	0.44
1:C:626:PHE:HA	1:C:632:CYS:SG	2.58	0.44
1:D:228:LEU:O	1:D:232:ILE:HD12	2.17	0.44
1:D:608:PHE:CZ	1:D:636:GLN:HB3	2.53	0.44
1:B:228:LEU:O	1:B:232:ILE:HD12	2.17	0.44
1:B:279:PHE:CE1	1:B:443:VAL:HG21	2.53	0.44
1:B:377:SER:OG	1:B:378:SER:N	2.51	0.44
1:B:667:PHE:O	1:B:671:ILE:N	2.31	0.44
1:C:355:ARG:HG2	1:C:368:TYR:CD1	2.53	0.44
1:C:471:PHE:HA	1:C:474:ALA:HB3	1.98	0.44
1:D:227:TYR:O	1:D:231:LEU:HB2	2.17	0.44
1:D:371:GLU:OE1	1:D:378:SER:HB3	2.17	0.44
1:A:228:LEU:O	1:A:232:ILE:HD12	2.17	0.44
1:A:536:LEU:O	1:A:540:GLU:HB3	2.17	0.44
1:A:573:LEU:HD12	1:B:606:ILE:HD13	1.84	0.44
1:A:573:LEU:O	1:A:576:PHE:N	2.50	0.44
1:B:378:SER:HB3	1:B:387:SER:HA	1.98	0.44
1:B:601:ALA:HB1	1:B:605:PHE:CE2	2.52	0.44
1:C:429:TYR:CE1	1:C:434:ASN:O	2.71	0.44
1:C:536:LEU:O	1:C:540:GLU:HB3	2.17	0.44
1:A:250:THR:OG1	1:B:622:GLN:HA	2.18	0.44
1:A:467:THR:HB	1:B:333:ILE:O	2.17	0.44
1:A:608:PHE:CZ	1:A:636:GLN:HB3	2.53	0.44
1:A:688:LYS:O	1:A:691:LEU:HG	2.18	0.44
6:A:1009:PLM:H61	6:A:1009:PLM:H92	1.73	0.44
1:B:295:MET:C	1:B:297:PRO:HD2	2.38	0.44
1:C:573:LEU:O	1:C:576:PHE:N	2.50	0.44
1:D:323:GLN:NE2	1:D:415:LEU:HB2	2.33	0.44
1:D:385:THR:HG23	1:D:385:THR:O	2.17	0.44
1:D:409:LEU:HD13	1:D:414:TRP:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:OH	1:A:430:ASN:HB3	2.17	0.44
1:A:627:SER:CB	1:D:247:TYR:HB2	2.47	0.44
1:B:429:TYR:CE1	1:B:434:ASN:O	2.71	0.44
1:B:536:LEU:O	1:B:540:GLU:HB3	2.17	0.44
5:B:1007:PX6:H53	5:B:1007:PX6:H46	1.65	0.44
1:C:228:LEU:O	1:C:232:ILE:HD12	2.17	0.44
1:C:460:LEU:HD13	1:C:555:GLN:HG2	1.99	0.44
1:C:608:PHE:CZ	1:C:636:GLN:HB3	2.53	0.44
1:D:325:ARG:NH2	1:D:355:ARG:HA	2.29	0.44
1:D:429:TYR:CE1	1:D:434:ASN:O	2.71	0.44
1:D:536:LEU:O	1:D:540:GLU:HB3	2.17	0.44
1:D:688:LYS:HA	1:D:691:LEU:HG	1.99	0.44
1:A:279:PHE:CE1	1:A:443:VAL:HG21	2.53	0.44
1:A:626:PHE:HA	1:A:632:CYS:SG	2.58	0.44
1:A:688:LYS:HA	1:A:691:LEU:HG	2.00	0.44
1:B:262:VAL:O	1:B:263:SER:OG	2.31	0.44
1:B:323:GLN:NE2	1:B:415:LEU:HB2	2.33	0.44
1:C:224:LEU:O	1:C:228:LEU:HG	2.17	0.44
1:D:295:MET:C	1:D:297:PRO:HD2	2.38	0.44
1:D:355:ARG:HG2	1:D:368:TYR:CD1	2.53	0.44
1:D:436:PHE:CD1	1:D:460:LEU:HD23	2.53	0.44
1:A:230:PHE:HE1	1:A:480:PHE:HB2	1.83	0.44
1:A:409:LEU:HD13	1:A:414:TRP:HD1	1.83	0.44
1:B:385:THR:HG23	1:B:385:THR:O	2.17	0.44
1:B:517:LEU:HA	1:B:561:ILE:HD11	2.00	0.44
1:B:597:LEU:O	1:B:601:ALA:HB2	2.18	0.44
6:B:1009:PLM:H71	6:B:1009:PLM:H42	1.60	0.44
1:C:295:MET:C	1:C:297:PRO:HD2	2.38	0.44
1:C:334:PRO:HB2	1:C:337:LEU:HB2	1.98	0.44
1:C:440:ARG:O	1:C:456:GLN:N	2.51	0.44
1:C:517:LEU:HA	1:C:561:ILE:HD11	2.00	0.44
1:D:224:LEU:O	1:D:228:LEU:HG	2.17	0.44
1:D:279:PHE:CE1	1:D:443:VAL:HG21	2.53	0.44
1:D:323:GLN:NE2	1:D:415:LEU:O	2.44	0.44
1:D:347:VAL:HG12	1:D:348:TYR:N	2.32	0.44
1:A:283:THR:HG1	1:A:284:GLU:H	1.63	0.43
1:A:323:GLN:NE2	1:A:415:LEU:HB2	2.33	0.43
1:A:355:ARG:HG2	1:A:368:TYR:CD1	2.53	0.43
1:A:440:ARG:O	1:A:456:GLN:N	2.51	0.43
1:A:548:PHE:CD2	1:A:552:ALA:HB2	2.52	0.43
1:B:296:GLN:N	1:B:297:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:LYS:O	1:B:691:LEU:HG	2.18	0.43
1:C:247:TYR:HE1	1:D:623:VAL:C	2.21	0.43
1:C:283:THR:HG1	1:C:284:GLU:H	1.65	0.43
1:C:296:GLN:N	1:C:297:PRO:HD2	2.33	0.43
1:C:309:ILE:HG13	1:C:313:ASN:C	2.38	0.43
1:C:406:VAL:HG13	1:C:414:TRP:NE1	2.24	0.43
1:C:460:LEU:CD1	1:C:555:GLN:HE21	2.31	0.43
1:D:458:GLN:HE21	1:D:459:PRO:HD2	1.81	0.43
1:D:460:LEU:CD1	1:D:555:GLN:HE21	2.31	0.43
1:D:688:LYS:O	1:D:691:LEU:HG	2.18	0.43
1:A:570:TRP:NE1	1:B:606:ILE:HG12	2.33	0.43
1:A:597:LEU:O	1:A:601:ALA:HB2	2.18	0.43
1:B:355:ARG:HG2	1:B:368:TYR:CD1	2.53	0.43
1:B:441:LEU:HA	1:B:441:LEU:HD23	1.74	0.43
1:B:542:GLN:HB3	1:B:544:THR:HG22	2.00	0.43
1:C:325:ARG:NH2	1:C:355:ARG:HA	2.29	0.43
1:C:379:HIS:HB3	1:C:423:PHE:CE2	2.53	0.43
1:D:377:SER:OG	1:D:378:SER:N	2.51	0.43
1:D:633:ILE:HD12	1:D:633:ILE:HA	1.62	0.43
1:A:249:TYR:CD1	1:B:448:THR:HB	2.53	0.43
1:A:429:TYR:CE1	1:A:434:ASN:O	2.71	0.43
5:A:1007:PX6:H24	6:A:1010:PLM:HG2	2.00	0.43
1:B:283:THR:OG1	1:B:284:GLU:N	2.51	0.43
1:C:458:GLN:CG	1:C:556:ILE:HG12	2.49	0.43
5:C:1007:PX6:H61	5:C:1007:PX6:H54	1.89	0.43
1:D:379:HIS:HB3	1:D:423:PHE:CE2	2.54	0.43
1:D:462:LEU:HD12	1:D:463:ILE:N	2.33	0.43
1:D:471:PHE:HA	1:D:474:ALA:HB3	1.98	0.43
1:A:377:SER:OG	1:A:378:SER:N	2.51	0.43
1:B:427:SER:CB	1:B:438:VAL:HA	2.49	0.43
1:C:371:GLU:OE1	1:C:378:SER:HB3	2.18	0.43
1:C:399:ARG:HD3	1:C:399:ARG:HA	1.80	0.43
1:C:427:SER:CB	1:C:438:VAL:HA	2.49	0.43
1:C:688:LYS:O	1:C:691:LEU:HG	2.18	0.43
1:D:296:GLN:N	1:D:297:PRO:HD2	2.33	0.43
1:A:460:LEU:CD1	1:A:555:GLN:HE21	2.31	0.43
1:A:677:LEU:C	1:B:674:ASN:HD22	2.22	0.43
1:B:371:GLU:OE1	1:B:378:SER:HB3	2.17	0.43
1:B:440:ARG:O	1:B:456:GLN:N	2.51	0.43
1:B:460:LEU:CD1	1:B:555:GLN:HE21	2.31	0.43
1:B:462:LEU:HD12	1:B:463:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:PHE:HA	1:B:485:PHE:HB3	2.01	0.43
1:B:608:PHE:C	1:B:636:GLN:HE22	2.15	0.43
1:B:676:PHE:O	1:B:680:ILE:HG13	2.19	0.43
1:C:230:PHE:HE1	1:C:480:PHE:HB2	1.83	0.43
1:C:349:SER:OG	1:C:350:VAL:N	2.52	0.43
1:D:327:ARG:NH1	1:D:351:SER:O	2.30	0.43
1:D:458:GLN:CG	1:D:556:ILE:HG12	2.49	0.43
1:D:517:LEU:HA	1:D:561:ILE:HD11	2.00	0.43
1:A:283:THR:OG1	1:A:284:GLU:N	2.51	0.43
1:A:306:ARG:CD	1:A:308:PHE:HZ	2.32	0.43
1:A:359:GLY:HA2	1:A:366:TRP:NE1	2.34	0.43
1:B:264:LYS:HG2	1:B:264:LYS:O	2.19	0.43
1:B:479:ILE:HA	1:B:482:PHE:CE2	2.54	0.43
1:C:283:THR:OG1	1:C:284:GLU:N	2.51	0.43
1:C:542:GLN:HB3	1:C:544:THR:HG22	2.00	0.43
1:C:597:LEU:O	1:C:601:ALA:HB2	2.18	0.43
1:D:440:ARG:O	1:D:456:GLN:N	2.51	0.43
1:A:532:VAL:HG11	1:A:551:LEU:HD11	2.00	0.43
1:A:532:VAL:HG12	1:A:536:LEU:HD13	2.01	0.43
1:A:536:LEU:HD21	1:A:548:PHE:CD1	2.54	0.43
1:A:542:GLN:HB3	1:A:544:THR:HG22	2.00	0.43
1:B:349:SER:OG	1:B:350:VAL:N	2.52	0.43
1:C:436:PHE:CD1	1:C:460:LEU:HD23	2.53	0.43
1:D:536:LEU:HD21	1:D:548:PHE:CD1	2.54	0.43
1:D:599:GLY:O	1:D:602:ILE:HG22	2.19	0.43
1:D:618:VAL:HG13	1:D:656:LEU:HD11	2.00	0.43
1:D:626:PHE:HA	1:D:632:CYS:SG	2.58	0.43
1:A:228:LEU:O	1:A:231:LEU:HB3	2.19	0.43
1:A:295:MET:C	1:A:297:PRO:HD2	2.38	0.43
1:A:321:ILE:N	1:A:393:LEU:O	2.49	0.43
1:A:322:ARG:NH1	1:A:371:GLU:OE2	2.52	0.43
1:A:327:ARG:NH1	1:A:351:SER:O	2.30	0.43
1:A:517:LEU:HA	1:A:561:ILE:HD11	2.00	0.43
1:A:566:VAL:HG21	1:B:617:LEU:HD21	2.00	0.43
1:A:618:VAL:HG13	1:A:656:LEU:HD11	2.00	0.43
1:A:676:PHE:O	1:A:680:ILE:HG13	2.19	0.43
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.87	0.43
1:B:436:PHE:CD1	1:B:460:LEU:HD23	2.53	0.43
1:C:462:LEU:HD12	1:C:463:ILE:N	2.34	0.43
1:C:633:ILE:HA	1:C:633:ILE:HD12	1.62	0.43
1:D:349:SER:OG	1:D:350:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:LEU:O	1:D:601:ALA:HB2	2.18	0.43
1:A:264:LYS:O	1:A:264:LYS:HG2	2.19	0.43
1:B:228:LEU:O	1:B:231:LEU:HB3	2.19	0.43
1:B:359:GLY:HA2	1:B:366:TRP:NE1	2.34	0.43
1:B:432:ASN:HA	1:C:332:SER:HB3	2.01	0.43
1:C:428:VAL:N	1:C:437:CYS:O	2.50	0.43
4:C:1005:CHS:HD22	4:C:1006:CHS:HD23	2.01	0.43
1:D:427:SER:CB	1:D:438:VAL:HA	2.49	0.43
1:A:249:TYR:HD1	1:B:448:THR:HB	1.84	0.43
1:A:379:HIS:HB3	1:A:423:PHE:CE2	2.53	0.43
1:A:560:ASN:O	1:A:564:VAL:HG23	2.19	0.43
1:B:230:PHE:HE1	1:B:480:PHE:HB2	1.83	0.43
1:B:379:HIS:HB3	1:B:423:PHE:CE2	2.53	0.43
1:B:458:GLN:CG	1:B:556:ILE:HG12	2.49	0.43
1:B:578:ASN:OD1	1:B:578:ASN:N	2.52	0.43
1:B:605:PHE:HZ	6:B:1009:PLM:HG3	1.84	0.43
1:B:626:PHE:HA	1:B:632:CYS:SG	2.58	0.43
1:C:536:LEU:HD21	1:C:548:PHE:CD1	2.54	0.43
1:C:676:PHE:O	1:C:680:ILE:HG13	2.19	0.43
6:C:1009:PLM:H42	6:C:1009:PLM:H71	1.59	0.43
1:A:296:GLN:N	1:A:297:PRO:HD2	2.33	0.42
1:A:406:VAL:O	1:A:410:LYS:N	2.47	0.42
1:A:458:GLN:CG	1:A:556:ILE:HG12	2.49	0.42
1:A:479:ILE:HA	1:A:482:PHE:CE2	2.54	0.42
1:A:532:VAL:HG12	1:A:536:LEU:CD1	2.49	0.42
1:A:605:PHE:CZ	6:A:1009:PLM:HG3	2.53	0.42
1:B:433:ILE:O	1:B:434:ASN:OD1	2.37	0.42
1:B:532:VAL:HG11	1:B:551:LEU:HD11	2.00	0.42
1:B:532:VAL:HG12	1:B:536:LEU:HD13	2.01	0.42
1:B:599:GLY:O	1:B:602:ILE:HG22	2.19	0.42
1:B:608:PHE:CZ	1:B:636:GLN:HB3	2.53	0.42
1:B:618:VAL:HG13	1:B:656:LEU:HD11	2.00	0.42
1:B:680:ILE:CG2	1:C:674:ASN:HB3	2.49	0.42
1:C:458:GLN:HE21	1:C:459:PRO:HD2	1.81	0.42
1:C:560:ASN:O	1:C:564:VAL:HG23	2.19	0.42
4:C:1005:CHS:HE23	6:D:1010:PLM:H61	2.01	0.42
1:D:283:THR:OG1	1:D:284:GLU:N	2.51	0.42
1:A:462:LEU:HD12	1:A:463:ILE:N	2.33	0.42
1:A:482:PHE:HA	1:A:485:PHE:HB3	2.01	0.42
1:A:557:GLN:O	1:A:561:ILE:HG22	2.19	0.42
1:B:309:ILE:HD11	1:B:314:LEU:C	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:GLY:O	1:C:602:ILE:HG22	2.19	0.42
1:C:618:VAL:HG13	1:C:656:LEU:HD11	2.00	0.42
6:C:1008:PLM:HF1	6:C:1008:PLM:HB2	2.01	0.42
1:D:249:TYR:CZ	1:D:430:ASN:HB3	2.54	0.42
1:D:409:LEU:HD13	1:D:414:TRP:CD1	2.54	0.42
1:D:560:ASN:O	1:D:564:VAL:HG23	2.19	0.42
1:A:349:SER:OG	1:A:350:VAL:N	2.52	0.42
1:A:409:LEU:HD13	1:A:414:TRP:CD1	2.54	0.42
1:A:667:PHE:O	1:A:671:ILE:N	2.31	0.42
1:B:409:LEU:HD13	1:B:414:TRP:CD1	2.54	0.42
1:B:460:LEU:HD21	1:B:462:LEU:HA	2.02	0.42
1:B:536:LEU:HD21	1:B:548:PHE:CD1	2.54	0.42
1:B:557:GLN:O	1:B:561:ILE:HG22	2.19	0.42
1:C:322:ARG:NH1	1:C:371:GLU:OE2	2.52	0.42
1:C:359:GLY:HA2	1:C:366:TRP:NE1	2.34	0.42
1:C:668:MET:O	1:C:672:LEU:N	2.33	0.42
1:D:322:ARG:NH1	1:D:371:GLU:OE2	2.52	0.42
1:D:359:GLY:HA2	1:D:366:TRP:NE1	2.34	0.42
1:D:416:ASP:OD1	1:D:419:THR:OG1	2.38	0.42
1:D:479:ILE:HA	1:D:482:PHE:CE2	2.54	0.42
1:D:532:VAL:HG12	1:D:536:LEU:HD13	2.01	0.42
1:A:427:SER:CB	1:A:438:VAL:HA	2.49	0.42
1:B:311:TYR:HB3	1:C:417:ARG:HH11	1.84	0.42
1:C:320:ARG:NH1	1:C:547:ASN:HB2	2.35	0.42
1:C:409:LEU:HD13	1:C:414:TRP:CD1	2.54	0.42
1:C:479:ILE:HA	1:C:482:PHE:CE2	2.54	0.42
1:D:321:ILE:N	1:D:393:LEU:O	2.49	0.42
1:D:433:ILE:O	1:D:434:ASN:OD1	2.37	0.42
1:D:532:VAL:HG12	1:D:536:LEU:CD1	2.49	0.42
1:A:433:ILE:O	1:A:434:ASN:OD1	2.37	0.42
1:A:623:VAL:HG13	1:A:626:PHE:HB2	2.02	0.42
1:A:651:GLU:OE1	1:D:271:LYS:NZ	2.50	0.42
1:C:228:LEU:O	1:C:231:LEU:HB3	2.19	0.42
1:C:237:LEU:HB3	1:C:241:MET:HE2	2.02	0.42
1:C:264:LYS:O	1:C:264:LYS:HG2	2.19	0.42
1:C:532:VAL:HG11	1:C:551:LEU:HD11	2.00	0.42
1:D:623:VAL:HG13	1:D:626:PHE:HB2	2.02	0.42
1:A:599:GLY:O	1:A:602:ILE:HG22	2.19	0.42
1:A:681:ASN:O	1:A:685:SER:N	2.36	0.42
1:B:247:TYR:HB2	1:C:627:SER:CB	2.50	0.42
1:B:320:ARG:NH1	1:B:547:ASN:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ASN:O	1:B:564:VAL:HG23	2.19	0.42
1:C:416:ASP:OD1	1:C:419:THR:OG1	2.38	0.42
1:C:460:LEU:HD21	1:C:462:LEU:HA	2.02	0.42
1:C:482:PHE:HA	1:C:485:PHE:HB3	2.01	0.42
1:C:604:PHE:CZ	1:C:608:PHE:CD1	3.08	0.42
1:D:341:ILE:HD13	1:D:344:CYS:SG	2.60	0.42
1:D:532:VAL:HG11	1:D:551:LEU:HD11	2.00	0.42
1:A:361:ARG:C	3:A:1002:NAG:C8	2.80	0.42
1:B:321:ILE:N	1:B:393:LEU:O	2.49	0.42
1:B:428:VAL:N	1:B:437:CYS:O	2.50	0.42
1:B:532:VAL:HG12	1:B:536:LEU:CD1	2.50	0.42
1:B:587:SER:HB2	1:C:600:PHE:CE1	2.54	0.42
1:C:532:VAL:HG12	1:C:536:LEU:HD13	2.01	0.42
1:C:557:GLN:O	1:C:561:ILE:HG22	2.19	0.42
6:C:1010:PLM:H71	6:C:1010:PLM:H42	1.56	0.42
1:D:228:LEU:O	1:D:231:LEU:HB3	2.19	0.42
1:D:230:PHE:HE1	1:D:480:PHE:HB2	1.83	0.42
1:D:320:ARG:NH1	1:D:547:ASN:HB2	2.35	0.42
1:D:676:PHE:O	1:D:680:ILE:HG13	2.19	0.42
1:A:269:ASN:OD1	1:A:271:LYS:N	2.53	0.42
1:A:323:GLN:OE1	1:A:415:LEU:HB2	2.20	0.42
6:A:1009:PLM:H42	6:A:1009:PLM:H71	1.60	0.42
1:B:323:GLN:OE1	1:B:415:LEU:HB2	2.20	0.42
1:B:383:ILE:CD1	1:B:446:PRO:HG3	2.50	0.42
1:B:577:ILE:CG1	1:C:602:ILE:HD13	2.49	0.42
1:B:604:PHE:CZ	1:B:608:PHE:CD1	3.08	0.42
6:B:1008:PLM:HB2	6:B:1008:PLM:HF1	2.02	0.42
1:C:323:GLN:OE1	1:C:415:LEU:HB2	2.20	0.42
1:C:623:VAL:HG13	1:C:626:PHE:HB2	2.02	0.42
1:C:628:THR:O	1:C:631:GLU:N	2.51	0.42
1:D:323:GLN:OE1	1:D:415:LEU:HB2	2.20	0.42
1:D:460:LEU:HD21	1:D:462:LEU:HA	2.02	0.42
1:A:460:LEU:HD21	1:A:462:LEU:HA	2.02	0.42
1:B:249:TYR:CZ	1:B:430:ASN:HB3	2.54	0.42
1:C:249:TYR:CZ	1:C:430:ASN:HB3	2.54	0.42
1:C:269:ASN:OD1	1:C:271:LYS:N	2.53	0.42
1:C:341:ILE:HD13	1:C:344:CYS:SG	2.60	0.42
1:C:432:ASN:HA	1:D:332:SER:HB3	2.02	0.42
1:C:605:PHE:CZ	6:C:1009:PLM:HG3	2.54	0.42
1:D:262:VAL:O	1:D:263:SER:OG	2.31	0.42
1:D:557:GLN:O	1:D:561:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ILE:O	1:D:574:PHE:N	2.53	0.42
5:D:1007:PX6:H53	5:D:1007:PX6:H46	1.65	0.42
1:A:416:ASP:OD1	1:A:419:THR:OG1	2.38	0.42
1:A:467:THR:HG23	1:B:335:GLN:HB3	2.02	0.42
1:A:605:PHE:O	1:A:609:LEU:N	2.35	0.42
1:B:408:SER:O	1:B:411:LYS:HB3	2.20	0.42
1:C:409:LEU:HD13	1:C:414:TRP:HD1	1.83	0.42
1:C:667:PHE:O	1:C:671:ILE:N	2.31	0.42
1:D:264:LYS:O	1:D:264:LYS:HG2	2.19	0.42
1:A:383:ILE:CD1	1:A:446:PRO:HG3	2.50	0.41
1:A:408:SER:O	1:A:411:LYS:HB3	2.20	0.41
1:A:633:ILE:HD12	1:A:633:ILE:HA	1.62	0.41
1:B:409:LEU:HD13	1:B:414:TRP:HD1	1.83	0.41
1:C:433:ILE:O	1:C:434:ASN:OD1	2.37	0.41
1:C:571:ILE:O	1:C:574:PHE:N	2.53	0.41
1:A:320:ARG:NH1	1:A:547:ASN:HB2	2.35	0.41
1:A:604:PHE:CZ	1:A:608:PHE:CD1	3.08	0.41
1:B:247:TYR:HB2	1:C:627:SER:HB3	2.03	0.41
1:B:322:ARG:NH1	1:B:371:GLU:OE2	2.52	0.41
1:B:623:VAL:HG13	1:B:626:PHE:HB2	2.02	0.41
1:B:628:THR:O	1:B:631:GLU:N	2.51	0.41
1:C:532:VAL:HG12	1:C:536:LEU:CD1	2.50	0.41
1:C:550:HIS:O	1:C:553:TYR:HB3	2.20	0.41
1:D:380:TRP:HB2	5:D:1007:PX6:H3	2.03	0.41
1:D:383:ILE:CD1	1:D:446:PRO:HG3	2.50	0.41
1:D:542:GLN:HB3	1:D:544:THR:HG22	2.00	0.41
1:D:604:PHE:CZ	1:D:608:PHE:CD1	3.08	0.41
1:A:249:TYR:CZ	1:A:430:ASN:HB3	2.54	0.41
1:A:341:ILE:HD13	1:A:344:CYS:SG	2.60	0.41
1:A:628:THR:O	1:A:631:GLU:N	2.51	0.41
1:A:680:ILE:HG21	1:B:674:ASN:HB3	2.02	0.41
1:B:327:ARG:NH1	1:B:351:SER:O	2.31	0.41
1:C:325:ARG:NH2	1:C:356:ALA:H	2.17	0.41
1:D:398:THR:CB	3:D:1001:NAG:O6	2.69	0.41
1:D:605:PHE:O	1:D:609:LEU:N	2.35	0.41
1:A:237:LEU:HB3	1:A:241:MET:HE2	2.03	0.41
1:A:292:TYR:HB3	1:A:310:PHE:HE1	1.85	0.41
6:A:1008:PLM:HF1	6:A:1008:PLM:HB2	2.02	0.41
1:B:269:ASN:OD1	1:B:271:LYS:N	2.53	0.41
1:B:292:TYR:HB3	1:B:310:PHE:HE1	1.86	0.41
1:B:380:TRP:HB2	5:B:1007:PX6:H3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ASP:OD1	1:B:419:THR:OG1	2.38	0.41
1:D:269:ASN:OD1	1:D:271:LYS:N	2.53	0.41
1:D:325:ARG:NH2	1:D:356:ALA:H	2.17	0.41
1:D:378:SER:OG	1:D:386:TYR:O	2.26	0.41
6:A:1010:PLM:H61	4:D:1005:CHS:HE23	2.02	0.41
1:B:502:TYR:HB2	1:B:508:ASN:HB2	2.03	0.41
6:B:1009:PLM:H61	6:B:1009:PLM:H92	1.73	0.41
1:C:292:TYR:HB3	1:C:310:PHE:HE1	1.86	0.41
1:C:608:PHE:CD2	1:C:633:ILE:HD11	2.55	0.41
1:D:237:LEU:HB3	1:D:241:MET:HE2	2.02	0.41
1:D:655:VAL:C	1:D:658:PRO:HD2	2.41	0.41
1:A:379:HIS:CG	1:A:380:TRP:N	2.88	0.41
1:A:423:PHE:HD1	1:A:423:PHE:HA	1.72	0.41
1:A:608:PHE:CD2	1:A:633:ILE:HD11	2.55	0.41
1:A:615:ALA:O	1:A:619:PHE:N	2.37	0.41
1:C:327:ARG:NH1	1:C:351:SER:O	2.30	0.41
1:C:461:LYS:HG3	1:C:461:LYS:O	2.21	0.41
1:D:461:LYS:HG3	1:D:461:LYS:O	2.21	0.41
1:B:461:LYS:HG3	1:B:461:LYS:O	2.21	0.41
1:B:643:ASP:OD1	1:B:643:ASP:C	2.59	0.41
5:B:1007:PX6:H61	5:B:1007:PX6:H54	1.89	0.41
1:C:321:ILE:N	1:C:393:LEU:O	2.49	0.41
1:C:383:ILE:CD1	1:C:446:PRO:HG3	2.50	0.41
1:C:466:VAL:HB	1:C:470:ASP:H	1.86	0.41
1:D:379:HIS:CG	1:D:380:TRP:N	2.88	0.41
1:D:482:PHE:HA	1:D:485:PHE:HB3	2.01	0.41
1:A:396:SER:OG	1:A:402:THR:HB	2.21	0.41
1:A:642:GLY:HA2	1:D:641:LEU:HD21	2.02	0.41
1:D:628:THR:O	1:D:631:GLU:N	2.51	0.41
6:D:1008:PLM:HF1	6:D:1008:PLM:HB2	2.02	0.41
1:A:277:GLU:HA	1:A:280:TRP:HE3	1.86	0.41
1:A:325:ARG:HH21	1:A:356:ALA:N	2.18	0.41
1:A:325:ARG:NH2	1:A:356:ALA:H	2.17	0.41
1:A:335:GLN:HG2	1:A:336:ASP:N	2.36	0.41
1:A:550:HIS:O	1:A:553:TYR:HB3	2.20	0.41
1:A:570:TRP:CE3	1:B:613:GLN:OE1	2.74	0.41
1:B:237:LEU:O	1:B:241:MET:HG2	2.21	0.41
1:B:237:LEU:HB3	1:B:241:MET:HE2	2.03	0.41
1:B:455:TRP:CH2	1:C:651:GLU:CD	2.94	0.41
1:B:550:HIS:O	1:B:553:TYR:HB3	2.20	0.41
1:B:586:LEU:HD21	1:B:691:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:MET:HG3	1:B:604:PHE:N	2.36	0.41
1:B:608:PHE:CD2	1:B:633:ILE:HD11	2.56	0.41
1:C:237:LEU:O	1:C:241:MET:HG2	2.21	0.41
1:C:319:PRO:HG3	1:C:426:PHE:CD1	2.56	0.41
1:C:326:VAL:HG12	1:C:327:ARG:N	2.36	0.41
1:C:502:TYR:HB2	1:C:508:ASN:HB2	2.03	0.41
1:C:653:ASN:C	1:C:656:LEU:H	2.23	0.41
1:D:221:LEU:O	1:D:225:VAL:HG23	2.21	0.41
1:D:277:GLU:HA	1:D:280:TRP:HE3	1.86	0.41
1:D:361:ARG:C	3:D:1002:NAG:C8	2.80	0.41
1:D:399:ARG:HD3	1:D:399:ARG:HA	1.80	0.41
1:D:550:HIS:O	1:D:553:TYR:HB3	2.20	0.41
1:D:653:ASN:C	1:D:656:LEU:H	2.23	0.41
1:A:655:VAL:C	1:A:658:PRO:HD2	2.41	0.41
1:B:341:ILE:HD13	1:B:344:CYS:SG	2.60	0.41
1:B:357:PRO:O	1:B:366:TRP:HB3	2.21	0.41
1:C:251:ARG:O	1:C:254:SER:N	2.51	0.41
1:C:262:VAL:CG1	1:C:266:GLU:HB3	2.51	0.41
1:D:335:GLN:HG2	1:D:336:ASP:N	2.36	0.41
1:D:608:PHE:CD2	1:D:633:ILE:HD11	2.55	0.41
1:D:674:ASN:O	1:D:678:ALA:N	2.49	0.41
1:A:311:TYR:HB3	1:B:417:ARG:NH1	2.35	0.40
1:A:461:LYS:HG3	1:A:461:LYS:O	2.21	0.40
1:A:466:VAL:HB	1:A:470:ASP:H	1.86	0.40
1:A:502:TYR:HB2	1:A:508:ASN:HB2	2.03	0.40
1:B:248:TYR:CE2	1:C:452:ILE:HD12	2.57	0.40
1:B:308:PHE:CD1	1:B:308:PHE:N	2.86	0.40
1:B:326:VAL:HG12	1:B:327:ARG:N	2.36	0.40
1:C:309:ILE:HD11	1:C:315:LEU:CA	2.50	0.40
1:C:529:THR:O	1:C:533:GLU:HG3	2.21	0.40
1:D:529:THR:O	1:D:533:GLU:HG3	2.21	0.40
1:A:221:LEU:O	1:A:225:VAL:HG23	2.21	0.40
1:A:262:VAL:CG1	1:A:266:GLU:HB3	2.51	0.40
1:A:326:VAL:HG12	1:A:327:ARG:N	2.36	0.40
1:A:509:CYS:HA	1:A:512:VAL:HG22	2.03	0.40
1:A:529:THR:O	1:A:533:GLU:HG3	2.21	0.40
1:B:306:ARG:CG	1:B:308:PHE:HE1	2.30	0.40
1:B:503:PHE:C	1:B:505:SER:H	2.25	0.40
1:C:311:TYR:HB3	1:D:417:ARG:HH11	1.85	0.40
1:C:357:PRO:O	1:C:366:TRP:HB3	2.21	0.40
1:C:509:CYS:HA	1:C:512:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:ASP:OD1	1:C:643:ASP:C	2.59	0.40
1:D:254:SER:O	1:D:256:LEU:N	2.54	0.40
1:D:262:VAL:CG1	1:D:266:GLU:HB3	2.51	0.40
1:D:509:CYS:HA	1:D:512:VAL:HG22	2.04	0.40
1:D:586:LEU:HD21	1:D:691:LEU:HB3	2.03	0.40
1:A:237:LEU:O	1:A:241:MET:HG2	2.21	0.40
1:A:247:TYR:HB2	1:B:627:SER:HB3	2.03	0.40
1:B:254:SER:O	1:B:256:LEU:N	2.55	0.40
1:C:379:HIS:CG	1:C:380:TRP:N	2.89	0.40
1:C:396:SER:OG	1:C:402:THR:HB	2.21	0.40
1:D:310:PHE:C	1:D:312:GLU:H	2.25	0.40
1:D:357:PRO:O	1:D:366:TRP:HB3	2.21	0.40
1:A:549:GLU:O	1:A:552:ALA:N	2.54	0.40
1:B:221:LEU:O	1:B:225:VAL:HG23	2.21	0.40
1:B:262:VAL:CG1	1:B:266:GLU:HB3	2.51	0.40
1:B:306:ARG:CD	1:B:308:PHE:HZ	2.33	0.40
1:B:316:LEU:HD21	1:B:428:VAL:HA	2.04	0.40
1:B:325:ARG:NH2	1:B:356:ALA:H	2.17	0.40
1:B:335:GLN:HG2	1:B:336:ASP:N	2.36	0.40
1:B:577:ILE:CG1	1:C:602:ILE:CD1	2.99	0.40
1:B:655:VAL:C	1:B:658:PRO:HD2	2.41	0.40
1:C:503:PHE:C	1:C:505:SER:H	2.25	0.40
1:C:655:VAL:C	1:C:658:PRO:HD2	2.41	0.40
1:D:337:LEU:HD23	1:D:337:LEU:HA	1.85	0.40
1:D:408:SER:O	1:D:411:LYS:HB3	2.20	0.40
1:D:502:TYR:HB2	1:D:508:ASN:HB2	2.03	0.40
1:D:643:ASP:OD1	1:D:643:ASP:C	2.59	0.40
1:D:677:LEU:HD23	1:D:677:LEU:HA	1.88	0.40
1:A:586:LEU:HD21	1:A:691:LEU:HB3	2.03	0.40
1:A:643:ASP:OD1	1:A:643:ASP:C	2.59	0.40
1:A:653:ASN:C	1:A:656:LEU:H	2.23	0.40
1:A:682:ASP:CG	1:A:683:THR:N	2.75	0.40
1:B:319:PRO:HG3	1:B:426:PHE:CD1	2.56	0.40
1:B:364:THR:HG23	1:B:392:TYR:CE1	2.57	0.40
1:B:379:HIS:CG	1:B:380:TRP:N	2.89	0.40
1:B:653:ASN:C	1:B:656:LEU:H	2.23	0.40
1:C:254:SER:O	1:C:256:LEU:N	2.54	0.40
1:C:408:SER:O	1:C:411:LYS:HB3	2.20	0.40
1:C:438:VAL:HG22	1:C:458:GLN:O	2.22	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	471/968 (49%)	382 (81%)	87 (18%)	2 (0%)	34	72
1	B	471/968 (49%)	383 (81%)	86 (18%)	2 (0%)	34	72
1	C	471/968 (49%)	381 (81%)	88 (19%)	2 (0%)	34	72
1	D	471/968 (49%)	381 (81%)	87 (18%)	3 (1%)	25	65
All	All	1884/3872 (49%)	1527 (81%)	348 (18%)	9 (0%)	32	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	TYR
1	A	258	LEU
1	B	258	LEU
1	C	258	LEU
1	D	258	LEU
1	A	623	VAL
1	B	623	VAL
1	C	623	VAL
1	D	623	VAL

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	429/837 (51%)	426 (99%)	3 (1%)	84	90
1	B	429/837 (51%)	426 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	429/837 (51%)	426 (99%)	3 (1%)	84 90
1	D	429/837 (51%)	425 (99%)	4 (1%)	78 88
All	All	1716/3348 (51%)	1703 (99%)	13 (1%)	82 89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	A	415	LEU
1	A	577	ILE
1	B	309	ILE
1	B	415	LEU
1	B	577	ILE
1	C	308	PHE
1	C	415	LEU
1	C	577	ILE
1	D	309	ILE
1	D	310	PHE
1	D	415	LEU
1	D	577	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	458	GLN
1	A	501	HIS
1	A	550	HIS
1	A	622	GLN
1	A	653	ASN
1	A	693	GLN
1	B	456	GLN
1	B	458	GLN
1	B	501	HIS
1	B	537	GLN
1	B	550	HIS
1	B	622	GLN
1	B	653	ASN
1	B	693	GLN
1	C	456	GLN

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Mol	Chain	Res	Type
1	C	458	GLN
1	C	501	HIS
1	C	537	GLN
1	C	550	HIS
1	C	613	GLN
1	C	622	GLN
1	C	653	ASN
1	C	693	GLN
1	D	456	GLN
1	D	458	GLN
1	D	501	HIS
1	D	537	GLN
1	D	550	HIS
1	D	622	GLN
1	D	653	ASN
1	D	693	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 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	E	1	1,2	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	1	1,2	14,14,15	0.52	0	17,19,21	1.14	2 (11%)
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.47	0	17,19,21	1.14	2 (11%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	1.18	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C8-C7-N2	2.35	120.07	116.10
2	E	1	NAG	C8-C7-N2	2.33	120.05	116.10
2	E	2	NAG	C8-C7-N2	2.33	120.04	116.10
2	F	2	NAG	C8-C7-N2	2.32	120.03	116.10
2	F	1	NAG	C8-C7-N2	2.31	120.01	116.10
2	G	1	NAG	C8-C7-N2	2.29	119.98	116.10
2	G	1	NAG	C2-N2-C7	-2.07	119.96	122.90
2	E	1	NAG	C2-N2-C7	-2.04	120.00	122.90
2	F	1	NAG	C2-N2-C7	-2.04	120.00	122.90
2	G	2	NAG	C2-N2-C7	-2.03	120.01	122.90
2	E	2	NAG	C2-N2-C7	-2.03	120.02	122.90
2	F	2	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

There are no torsion outliers.

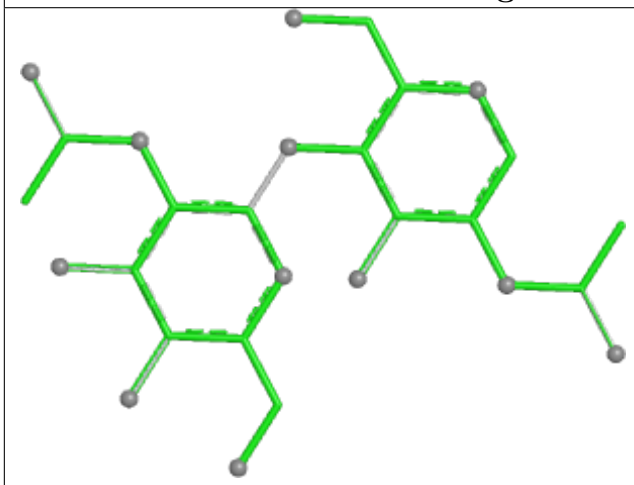
There are no ring outliers.

3 monomers are involved in 6 short contacts:

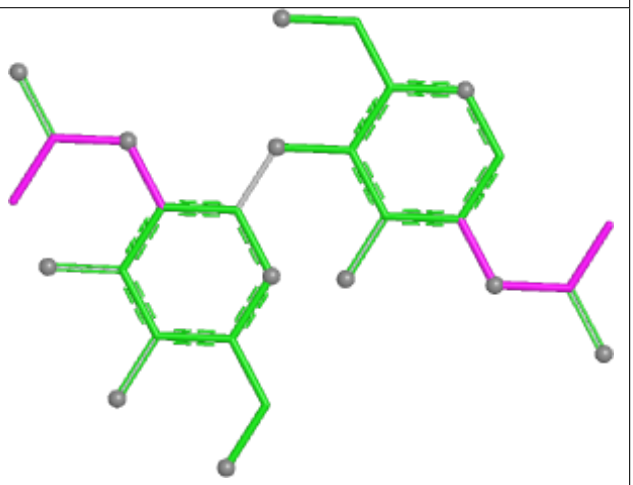
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	2	0
2	F	2	NAG	2	0
2	E	2	NAG	2	0

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

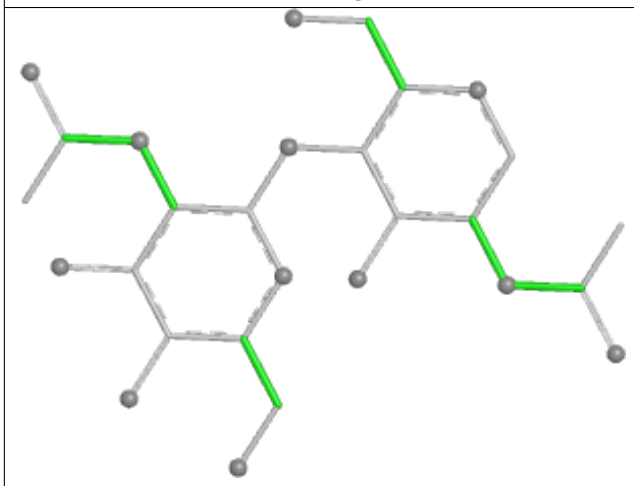
Oligosaccharide Chain E



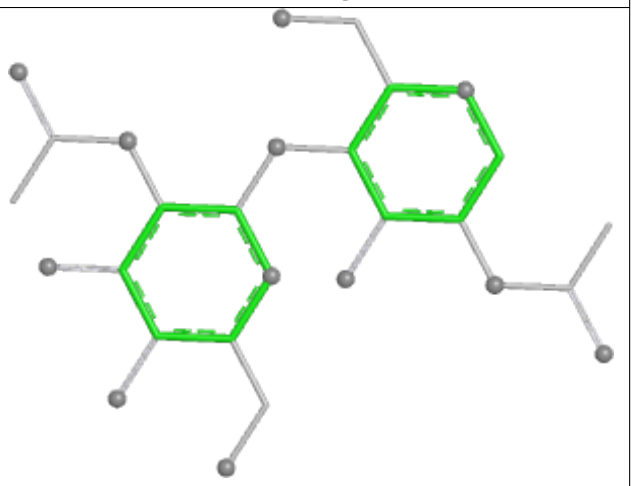
Bond lengths



Bond angles

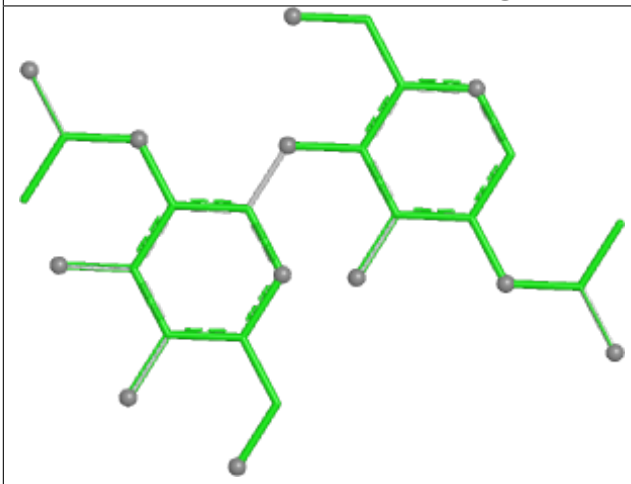


Torsions

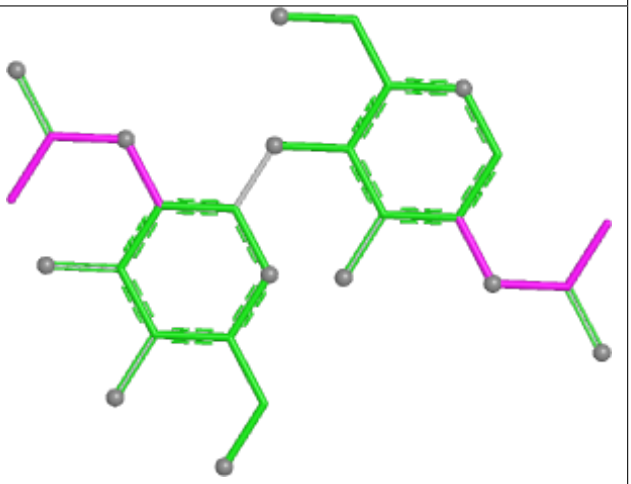


Rings

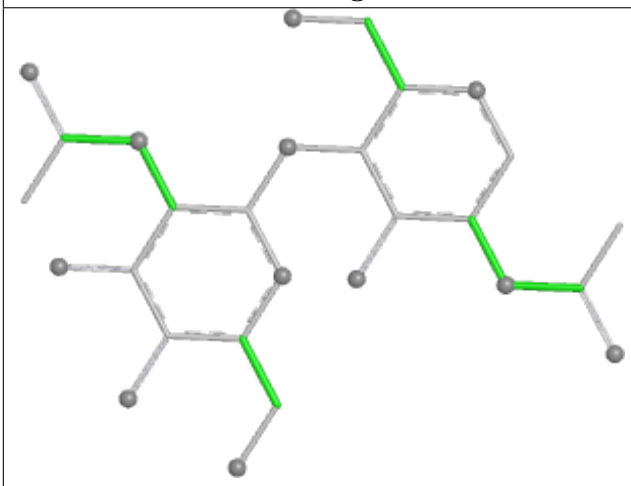
Oligosaccharide Chain F



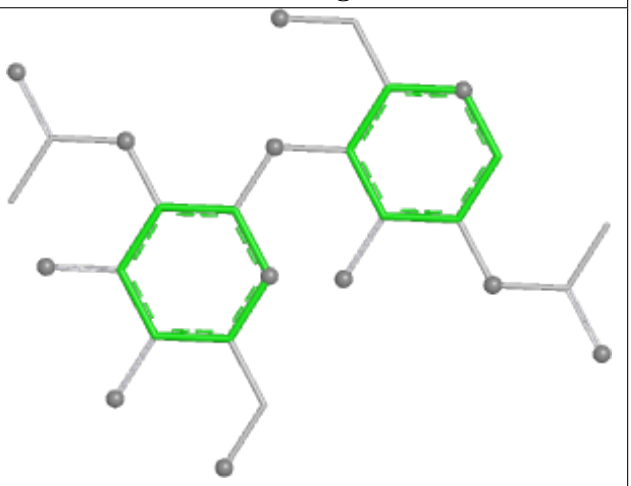
Bond lengths



Bond angles

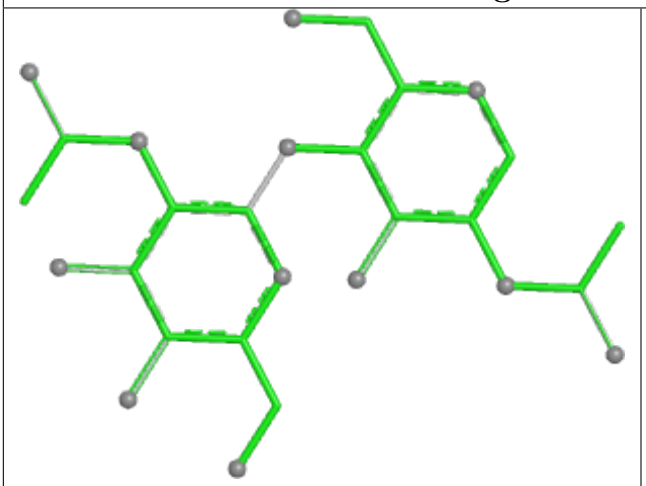


Torsions

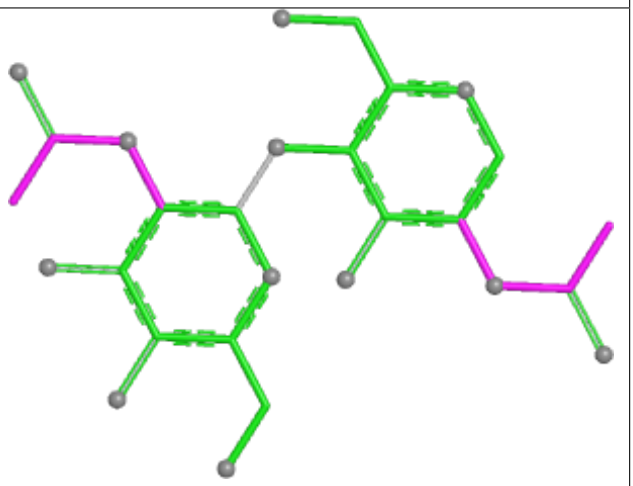


Rings

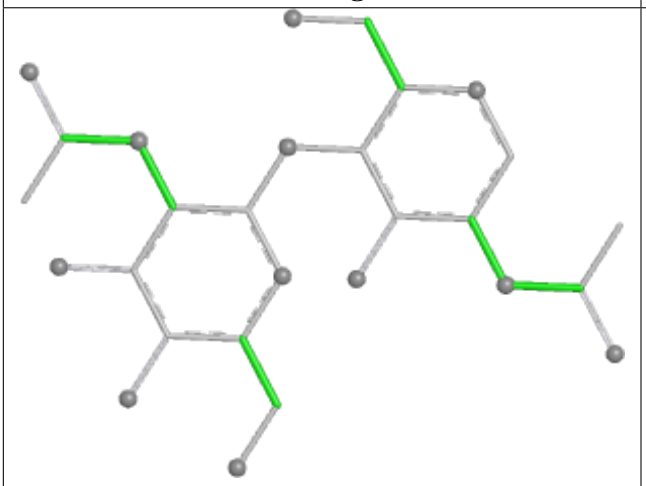
Oligosaccharide Chain G



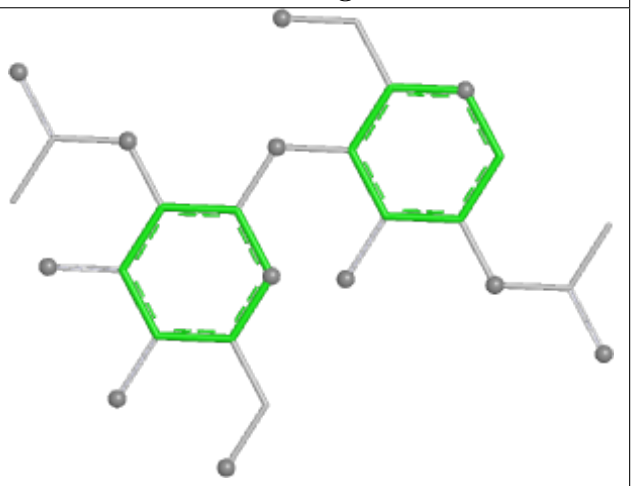
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
4	CHS	A	1005	-	15,15,15	0.52	0	15,19,19	0.83	0
6	PLM	A	1009	-	17,17,17	0.50	0	17,17,17	0.97	0
6	PLM	D	1008	-	17,17,17	0.57	0	17,17,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PLM	D	1009	-	17,17,17	0.50	0	17,17,17	0.96	0
3	NAG	C	1001	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
4	CHS	D	1006	-	15,15,15	0.59	0	15,19,19	0.99	1 (6%)
4	CHS	B	1005	-	15,15,15	0.52	0	15,19,19	0.84	0
6	PLM	B	1009	-	17,17,17	0.51	0	17,17,17	0.97	0
6	PLM	D	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
5	PX6	A	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	3 (6%)
5	PX6	D	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	4 (9%)
6	PLM	C	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
3	NAG	B	1002	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	D	1001	1	14,14,15	0.86	1 (7%)	17,19,21	0.82	1 (5%)
4	CHS	D	1005	-	15,15,15	0.51	0	15,19,19	0.83	0
5	PX6	B	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	4 (9%)
6	PLM	B	1008	-	17,17,17	0.57	0	17,17,17	0.75	0
4	CHS	C	1005	-	15,15,15	0.51	0	15,19,19	0.82	0
4	CHS	A	1006	-	15,15,15	0.59	0	15,19,19	1.01	1 (6%)
4	CHS	C	1006	-	15,15,15	0.58	0	15,19,19	1.01	1 (6%)
3	NAG	B	1001	1	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
3	NAG	D	1003	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
6	PLM	C	1008	-	17,17,17	0.56	0	17,17,17	0.75	0
6	PLM	B	1010	-	17,17,17	0.53	0	17,17,17	0.77	0
6	PLM	C	1009	-	17,17,17	0.50	0	17,17,17	0.97	0
3	NAG	C	1002	1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
3	NAG	D	1002	1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
3	NAG	D	1004	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
5	PX6	C	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.51	4 (9%)
6	PLM	A	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
3	NAG	A	1002	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	CHS	B	1006	-	15,15,15	0.57	0	15,19,19	1.03	1 (6%)
6	PLM	A	1008	-	17,17,17	0.57	0	17,17,17	0.74	0
3	NAG	A	1001	1	14,14,15	0.70	1 (7%)	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHS	A	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	A	1009	-	-	7/15/15/15	-
6	PLM	D	1008	-	-	11/15/15/15	-
6	PLM	D	1009	-	-	6/15/15/15	-
3	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
4	CHS	D	1006	-	-	5/12/20/20	0/1/1/1
4	CHS	B	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	B	1009	-	-	6/15/15/15	-
6	PLM	D	1010	-	-	12/15/15/15	-
5	PX6	A	1007	-	-	17/41/41/45	-
5	PX6	D	1007	-	-	19/41/41/45	-
6	PLM	C	1010	-	-	12/15/15/15	-
3	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
4	CHS	D	1005	-	-	5/12/20/20	0/1/1/1
5	PX6	B	1007	-	-	19/41/41/45	-
6	PLM	B	1008	-	-	11/15/15/15	-
4	CHS	C	1005	-	-	5/12/20/20	0/1/1/1
4	CHS	A	1006	-	-	4/12/20/20	0/1/1/1
4	CHS	C	1006	-	-	4/12/20/20	0/1/1/1
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
6	PLM	C	1008	-	-	11/15/15/15	-
6	PLM	B	1010	-	-	12/15/15/15	-
6	PLM	C	1009	-	-	6/15/15/15	-
3	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1004	-	-	0/6/23/26	0/1/1/1
5	PX6	C	1007	-	-	17/41/41/45	-
6	PLM	A	1010	-	-	12/15/15/15	-
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
4	CHS	B	1006	-	-	5/12/20/20	0/1/1/1
6	PLM	A	1008	-	-	11/15/15/15	-
3	NAG	A	1001	1	-	2/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1007	PX6	P1-O2	4.62	1.65	1.50
5	D	1007	PX6	P1-O2	4.62	1.65	1.50
5	A	1007	PX6	P1-O2	4.61	1.65	1.50
5	C	1007	PX6	P1-O2	4.59	1.65	1.50
5	A	1007	PX6	O7-C2	-3.11	1.38	1.46
5	D	1007	PX6	O7-C2	-3.09	1.38	1.46
5	C	1007	PX6	O7-C2	-3.08	1.38	1.46
5	B	1007	PX6	O7-C2	-3.06	1.38	1.46
3	D	1001	NAG	C1-C2	3.01	1.56	1.52
5	B	1007	PX6	O5-C4	2.99	1.42	1.33
5	C	1007	PX6	O5-C4	2.99	1.42	1.33
5	D	1007	PX6	O5-C4	2.99	1.42	1.33
5	A	1007	PX6	O5-C4	2.99	1.42	1.33
5	D	1007	PX6	P1-O3	-2.38	1.45	1.54
5	C	1007	PX6	P1-O3	-2.37	1.45	1.54
5	B	1007	PX6	P1-O3	-2.37	1.45	1.54
5	A	1007	PX6	P1-O3	-2.36	1.45	1.54
5	D	1007	PX6	O7-C20	2.35	1.41	1.34
5	C	1007	PX6	O7-C20	2.35	1.40	1.34
5	A	1007	PX6	O7-C20	2.35	1.40	1.34
5	B	1007	PX6	O7-C20	2.34	1.40	1.34
5	C	1007	PX6	P1-O1	-2.26	1.46	1.54
5	B	1007	PX6	P1-O1	-2.26	1.46	1.54
5	A	1007	PX6	P1-O1	-2.25	1.46	1.54
5	D	1007	PX6	P1-O1	-2.25	1.46	1.54
3	A	1001	NAG	C1-C2	2.15	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1007	PX6	O5-C3-C2	7.59	130.54	108.43
5	D	1007	PX6	O5-C3-C2	7.55	130.42	108.43
5	A	1007	PX6	O5-C3-C2	7.55	130.40	108.43
5	C	1007	PX6	O5-C3-C2	7.51	130.30	108.43
5	D	1007	PX6	O7-C20-C21	2.90	117.74	111.50
3	A	1001	NAG	C1-O5-C5	2.88	116.09	112.19
5	B	1007	PX6	O7-C20-C21	2.88	117.70	111.50
5	D	1007	PX6	O5-C4-C5	2.80	120.70	111.91
5	B	1007	PX6	O5-C4-C5	2.79	120.66	111.91
4	B	1006	CHS	CH-CM-C	-2.79	107.89	114.03
5	C	1007	PX6	O5-C4-C5	2.78	120.64	111.91
5	A	1007	PX6	O5-C4-C5	2.77	120.61	111.91
3	B	1001	NAG	C1-O5-C5	2.76	115.93	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1007	PX6	O7-C20-C21	2.71	117.33	111.50
4	C	1006	CHS	CH-CM-C	-2.70	108.08	114.03
3	D	1001	NAG	C1-O5-C5	2.70	115.85	112.19
5	A	1007	PX6	O7-C20-C21	2.68	117.27	111.50
4	A	1006	CHS	CH-CM-C	-2.66	108.18	114.03
4	D	1006	CHS	CH-CM-C	-2.52	108.48	114.03
3	D	1002	NAG	C8-C7-N2	2.33	120.04	116.10
3	A	1002	NAG	C8-C7-N2	2.33	120.04	116.10
3	D	1003	NAG	C8-C7-N2	2.32	120.03	116.10
3	D	1004	NAG	C8-C7-N2	2.32	120.03	116.10
3	B	1002	NAG	C8-C7-N2	2.32	120.03	116.10
3	C	1002	NAG	C8-C7-N2	2.32	120.02	116.10
3	C	1001	NAG	C1-O5-C5	2.23	115.21	112.19
5	B	1007	PX6	O1-P1-O4	2.06	112.22	106.73
5	C	1007	PX6	O1-P1-O4	2.05	112.18	106.73
3	D	1004	NAG	C2-N2-C7	-2.04	120.00	122.90
3	C	1002	NAG	C2-N2-C7	-2.02	120.03	122.90
3	D	1003	NAG	C2-N2-C7	-2.01	120.04	122.90
3	B	1002	NAG	C2-N2-C7	-2.00	120.05	122.90
5	D	1007	PX6	O1-P1-O4	2.00	112.06	106.73
3	D	1002	NAG	C2-N2-C7	-2.00	120.06	122.90

There are no chirality outliers.

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1005	CHS	N-CA-CB-CG
4	A	1005	CHS	N-CA-CH-CM
4	A	1005	CHS	CB-CA-CH-CM
4	B	1005	CHS	N-CA-CB-CG
4	B	1005	CHS	N-CA-CH-CM
4	B	1005	CHS	CB-CA-CH-CM
4	C	1005	CHS	N-CA-CB-CG
4	C	1005	CHS	N-CA-CH-CM
4	C	1005	CHS	CB-CA-CH-CM
4	D	1005	CHS	N-CA-CB-CG
4	D	1005	CHS	N-CA-CH-CM
4	D	1005	CHS	CB-CA-CH-CM
5	B	1007	PX6	O8-C20-O7-C2
5	C	1007	PX6	O8-C20-O7-C2
5	D	1007	PX6	O8-C20-O7-C2
3	D	1001	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1007	PX6	C21-C20-O7-C2
5	C	1007	PX6	C21-C20-O7-C2
5	D	1007	PX6	C21-C20-O7-C2
3	A	1001	NAG	O5-C5-C6-O6
3	B	1001	NAG	O5-C5-C6-O6
3	C	1001	NAG	O5-C5-C6-O6
5	A	1007	PX6	C21-C20-O7-C2
3	C	1001	NAG	C4-C5-C6-O6
3	D	1001	NAG	C4-C5-C6-O6
5	A	1007	PX6	O8-C20-O7-C2
3	A	1001	NAG	C4-C5-C6-O6
3	B	1001	NAG	C4-C5-C6-O6
6	C	1009	PLM	C6-C7-C8-C9
6	A	1009	PLM	C6-C7-C8-C9
6	B	1009	PLM	C6-C7-C8-C9
6	D	1009	PLM	C6-C7-C8-C9
6	A	1008	PLM	C1-C2-C3-C4
6	B	1008	PLM	C1-C2-C3-C4
6	C	1008	PLM	C1-C2-C3-C4
6	D	1008	PLM	C1-C2-C3-C4
5	A	1007	PX6	C7-C8-C9-C10
5	B	1007	PX6	C7-C8-C9-C10
5	D	1007	PX6	C7-C8-C9-C10
5	C	1007	PX6	C7-C8-C9-C10
6	B	1010	PLM	C7-C8-C9-CA
5	A	1007	PX6	C6-C7-C8-C9
5	B	1007	PX6	C6-C7-C8-C9
5	C	1007	PX6	C6-C7-C8-C9
5	D	1007	PX6	C6-C7-C8-C9
6	A	1010	PLM	C7-C8-C9-CA
6	B	1010	PLM	C2-C3-C4-C5
6	C	1010	PLM	C2-C3-C4-C5
6	C	1010	PLM	C7-C8-C9-CA
6	D	1010	PLM	C7-C8-C9-CA
6	A	1010	PLM	C2-C3-C4-C5
6	D	1010	PLM	C2-C3-C4-C5
5	D	1007	PX6	C28-C29-C30-C31
6	D	1008	PLM	C3-C4-C5-C6
5	A	1007	PX6	C28-C29-C30-C31
5	B	1007	PX6	C28-C29-C30-C31
5	C	1007	PX6	C28-C29-C30-C31
6	C	1008	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	A	1008	PLM	C3-C4-C5-C6
6	A	1008	PLM	C6-C7-C8-C9
6	B	1008	PLM	C3-C4-C5-C6
6	C	1008	PLM	C8-C9-CA-CB
6	B	1008	PLM	C6-C7-C8-C9
6	C	1008	PLM	C6-C7-C8-C9
6	D	1008	PLM	C6-C7-C8-C9
5	B	1007	PX6	C22-C23-C24-C25
6	A	1008	PLM	C8-C9-CA-CB
6	B	1008	PLM	C8-C9-CA-CB
6	C	1008	PLM	C7-C8-C9-CA
6	D	1010	PLM	C4-C5-C6-C7
5	D	1007	PX6	C22-C23-C24-C25
6	D	1008	PLM	C7-C8-C9-CA
6	D	1010	PLM	C1-C2-C3-C4
5	B	1007	PX6	C26-C27-C28-C29
5	C	1007	PX6	C22-C23-C24-C25
5	D	1007	PX6	C26-C27-C28-C29
6	A	1008	PLM	C7-C8-C9-CA
6	A	1009	PLM	C7-C8-C9-CA
6	B	1008	PLM	C7-C8-C9-CA
6	B	1009	PLM	C7-C8-C9-CA
6	B	1010	PLM	C4-C5-C6-C7
6	C	1009	PLM	C7-C8-C9-CA
6	C	1010	PLM	C4-C5-C6-C7
6	D	1008	PLM	C8-C9-CA-CB
5	C	1007	PX6	C26-C27-C28-C29
6	A	1010	PLM	C4-C5-C6-C7
6	D	1009	PLM	C7-C8-C9-CA
5	A	1007	PX6	C26-C27-C28-C29
6	A	1010	PLM	C5-C6-C7-C8
6	B	1008	PLM	C4-C5-C6-C7
6	B	1010	PLM	C5-C6-C7-C8
6	D	1008	PLM	C4-C5-C6-C7
6	D	1008	PLM	C5-C6-C7-C8
6	D	1010	PLM	C5-C6-C7-C8
6	A	1010	PLM	C1-C2-C3-C4
6	A	1008	PLM	C4-C5-C6-C7
6	C	1008	PLM	C4-C5-C6-C7
6	C	1010	PLM	C5-C6-C7-C8
6	B	1008	PLM	CB-CC-CD-CE
6	C	1008	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	D	1008	PLM	CB-CC-CD-CE
6	A	1008	PLM	CB-CC-CD-CE
6	C	1008	PLM	CB-CC-CD-CE
5	A	1007	PX6	C22-C23-C24-C25
6	A	1008	PLM	C5-C6-C7-C8
6	C	1010	PLM	C1-C2-C3-C4
5	D	1007	PX6	C24-C25-C26-C27
6	B	1008	PLM	C5-C6-C7-C8
5	B	1007	PX6	C24-C25-C26-C27
6	B	1010	PLM	C1-C2-C3-C4
5	C	1007	PX6	C24-C25-C26-C27
5	A	1007	PX6	C24-C25-C26-C27
6	A	1010	PLM	C9-CA-CB-CC
5	D	1007	PX6	C21-C22-C23-C24
6	C	1009	PLM	C2-C3-C4-C5
6	D	1010	PLM	C9-CA-CB-CC
6	C	1010	PLM	C9-CA-CB-CC
6	D	1009	PLM	C2-C3-C4-C5
6	B	1010	PLM	C9-CA-CB-CC
5	C	1007	PX6	C32-C33-C34-C35
5	A	1007	PX6	C32-C33-C34-C35
5	D	1007	PX6	C32-C33-C34-C35
5	B	1007	PX6	C32-C33-C34-C35
5	B	1007	PX6	C21-C22-C23-C24
5	A	1007	PX6	C25-C26-C27-C28
4	A	1005	CHS	CB-CA-CH-OH
4	A	1006	CHS	CB-CA-CH-OH
4	B	1005	CHS	CB-CA-CH-OH
4	B	1006	CHS	CB-CA-CH-OH
4	C	1005	CHS	CB-CA-CH-OH
4	C	1006	CHS	CB-CA-CH-OH
4	D	1005	CHS	CB-CA-CH-OH
4	D	1006	CHS	CB-CA-CH-OH
5	D	1007	PX6	C25-C26-C27-C28
6	B	1009	PLM	C2-C3-C4-C5
5	C	1007	PX6	C25-C26-C27-C28
6	A	1009	PLM	C2-C3-C4-C5
5	B	1007	PX6	C25-C26-C27-C28
4	B	1006	CHS	CA-CB-CG-CD2
4	C	1006	CHS	CA-CB-CG-CD1
6	B	1010	PLM	C8-C9-CA-CB
6	C	1010	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	B	1010	PLM	C3-C4-C5-C6
6	C	1009	PLM	C4-C5-C6-C7
5	C	1007	PX6	C21-C22-C23-C24
6	C	1010	PLM	C8-C9-CA-CB
4	B	1006	CHS	N-CA-CH-CM
4	D	1006	CHS	N-CA-CH-CM
6	A	1010	PLM	C3-C4-C5-C6
6	D	1010	PLM	C8-C9-CA-CB
6	D	1009	PLM	C4-C5-C6-C7
5	A	1007	PX6	C12-C13-C14-C15
6	A	1010	PLM	C8-C9-CA-CB
6	A	1009	PLM	C4-C5-C6-C7
5	B	1007	PX6	C12-C13-C14-C15
6	B	1009	PLM	C4-C5-C6-C7
6	D	1010	PLM	C3-C4-C5-C6
6	D	1009	PLM	CC-CD-CE-CF
5	C	1007	PX6	C12-C13-C14-C15
5	D	1007	PX6	C12-C13-C14-C15
6	D	1010	PLM	C6-C7-C8-C9
4	A	1006	CHS	OH-CH-CM-C
4	B	1006	CHS	OH-CH-CM-C
4	C	1006	CHS	OH-CH-CM-C
4	D	1006	CHS	OH-CH-CM-C
6	B	1009	PLM	CC-CD-CE-CF
4	A	1006	CHS	CA-CB-CG-CD1
4	A	1006	CHS	CA-CB-CG-CD2
4	B	1006	CHS	CA-CB-CG-CD1
4	C	1006	CHS	CA-CB-CG-CD2
4	D	1006	CHS	CA-CB-CG-CD2
6	A	1010	PLM	C6-C7-C8-C9
6	B	1010	PLM	C6-C7-C8-C9
6	C	1009	PLM	C3-C4-C5-C6
5	A	1007	PX6	C21-C22-C23-C24
6	A	1009	PLM	C3-C4-C5-C6
6	B	1009	PLM	C3-C4-C5-C6
6	D	1009	PLM	C3-C4-C5-C6
6	C	1010	PLM	C6-C7-C8-C9
6	B	1010	PLM	CA-CB-CC-CD
6	D	1010	PLM	CA-CB-CC-CD
5	B	1007	PX6	C2-C1-O4-P1
6	A	1010	PLM	CA-CB-CC-CD
6	C	1009	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
5	D	1007	PX6	C23-C24-C25-C26
5	A	1007	PX6	C5-C6-C7-C8
6	C	1010	PLM	CA-CB-CC-CD
5	B	1007	PX6	C23-C24-C25-C26
5	A	1007	PX6	C2-C1-O4-P1
5	C	1007	PX6	C2-C1-O4-P1
5	D	1007	PX6	C2-C1-O4-P1
6	A	1008	PLM	O2-C1-C2-C3
6	B	1008	PLM	O2-C1-C2-C3
5	C	1007	PX6	C5-C6-C7-C8
4	D	1006	CHS	CA-CB-CG-CD1
6	C	1008	PLM	O2-C1-C2-C3
5	D	1007	PX6	C5-C6-C7-C8
6	D	1008	PLM	CC-CD-CE-CF
5	B	1007	PX6	C5-C6-C7-C8
6	A	1008	PLM	O1-C1-C2-C3
6	B	1008	PLM	O1-C1-C2-C3
6	D	1008	PLM	O2-C1-C2-C3
6	C	1008	PLM	O1-C1-C2-C3
6	D	1008	PLM	O1-C1-C2-C3
5	A	1007	PX6	C11-C12-C13-C14
6	B	1008	PLM	CC-CD-CE-CF
6	A	1008	PLM	CC-CD-CE-CF
6	D	1010	PLM	O1-C1-C2-C3
6	B	1010	PLM	O1-C1-C2-C3
6	A	1010	PLM	O1-C1-C2-C3
6	C	1010	PLM	O1-C1-C2-C3
6	A	1009	PLM	CD-CE-CF-CG
6	D	1010	PLM	O2-C1-C2-C3
6	C	1008	PLM	CC-CD-CE-CF
6	A	1010	PLM	O2-C1-C2-C3
5	D	1007	PX6	C11-C12-C13-C14
6	B	1010	PLM	O2-C1-C2-C3
6	C	1010	PLM	O2-C1-C2-C3
4	A	1005	CHS	N-CA-CH-OH
4	B	1005	CHS	N-CA-CH-OH
4	C	1005	CHS	N-CA-CH-OH
4	D	1005	CHS	N-CA-CH-OH
5	A	1007	PX6	O5-C4-C5-C6
5	B	1007	PX6	C11-C12-C13-C14
5	B	1007	PX6	O5-C4-C5-C6
5	C	1007	PX6	O5-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	D	1007	PX6	O5-C4-C5-C6
5	C	1007	PX6	C11-C12-C13-C14
5	D	1007	PX6	C29-C30-C31-C32
5	A	1007	PX6	O6-C4-C5-C6
6	A	1009	PLM	CC-CD-CE-CF
5	B	1007	PX6	O6-C4-C5-C6
5	C	1007	PX6	O6-C4-C5-C6
5	D	1007	PX6	O6-C4-C5-C6
5	B	1007	PX6	C29-C30-C31-C32

There are no ring outliers.

30 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	CHS	2	0
6	A	1009	PLM	4	0
6	D	1008	PLM	2	0
6	D	1009	PLM	1	0
4	D	1006	CHS	2	0
4	B	1005	CHS	3	0
6	B	1009	PLM	3	0
6	D	1010	PLM	3	0
5	A	1007	PX6	3	0
5	D	1007	PX6	4	0
6	C	1010	PLM	3	0
3	B	1002	NAG	8	0
3	D	1001	NAG	6	0
4	D	1005	CHS	3	0
5	B	1007	PX6	6	0
6	B	1008	PLM	2	0
4	C	1005	CHS	4	0
4	A	1006	CHS	2	0
4	C	1006	CHS	3	0
6	C	1008	PLM	2	0
6	B	1010	PLM	3	0
6	C	1009	PLM	4	0
3	C	1002	NAG	8	0
3	D	1002	NAG	8	0
3	D	1004	NAG	2	0
5	C	1007	PX6	4	0
6	A	1010	PLM	3	0
3	A	1002	NAG	8	0

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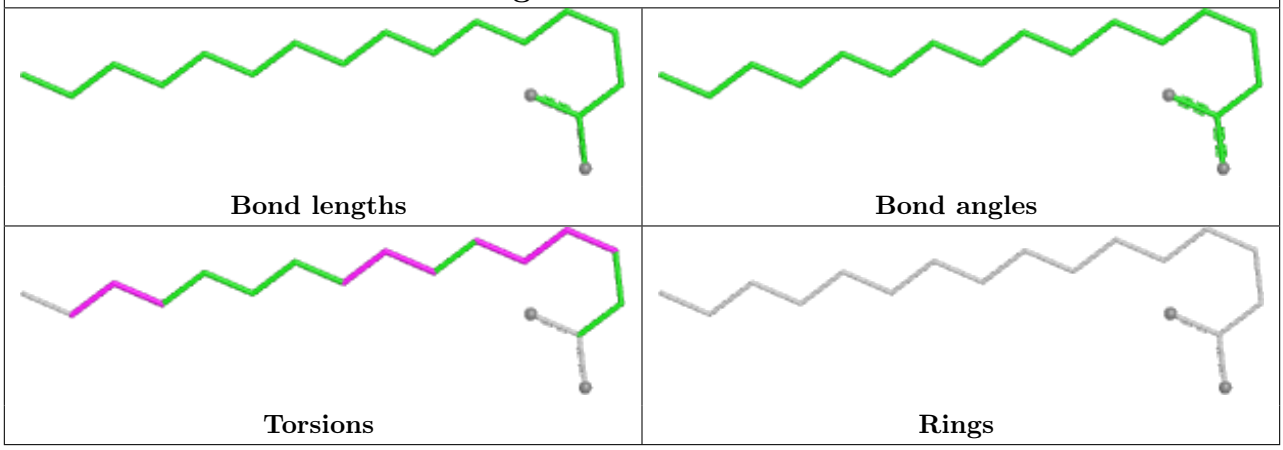
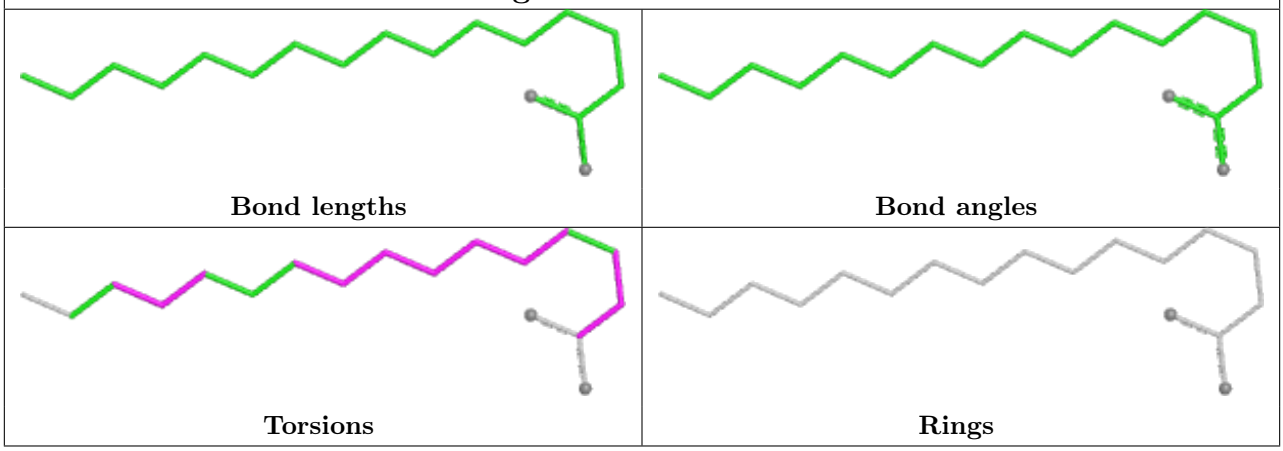
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1006	CHS	3	0
6	A	1008	PLM	2	0

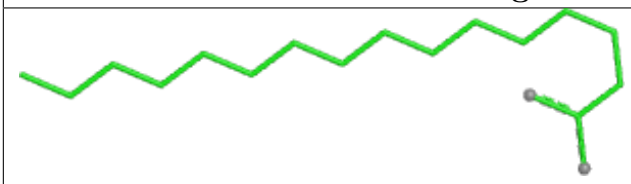
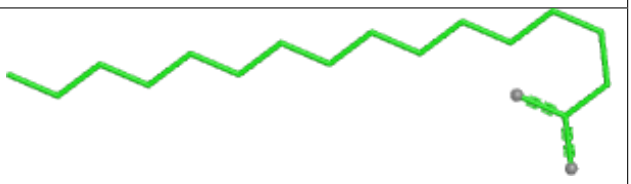
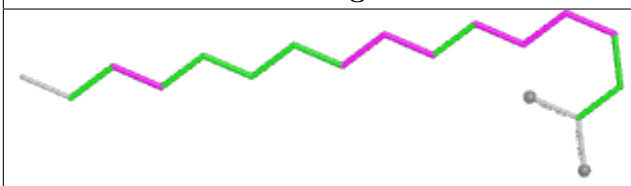
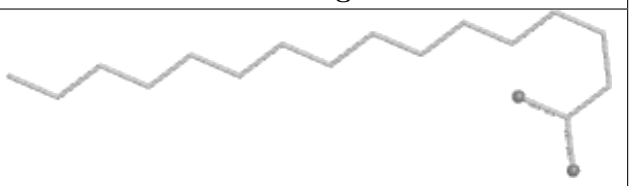
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

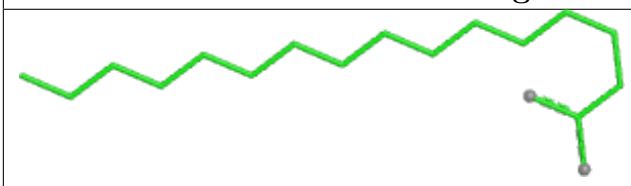
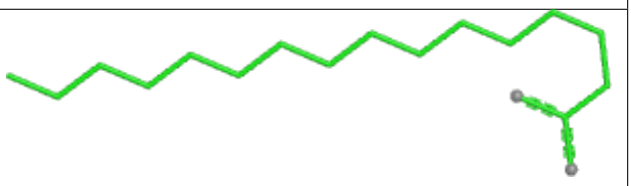
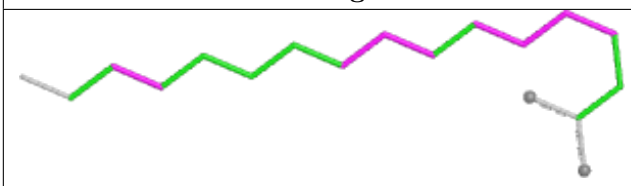
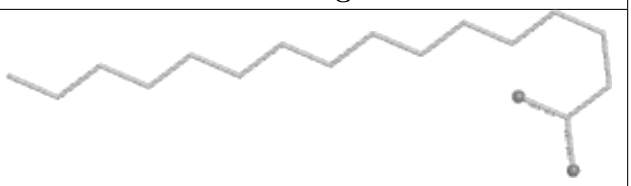
Ligand PLM A 1009

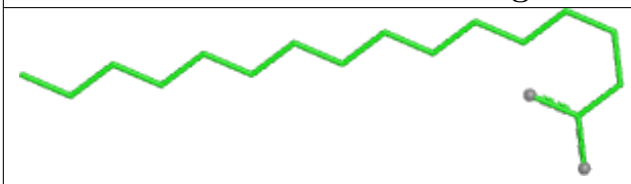
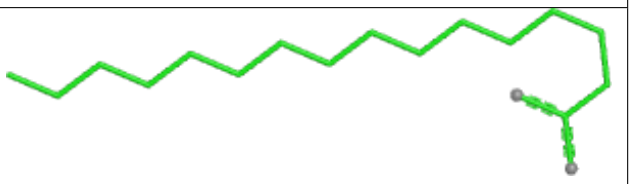
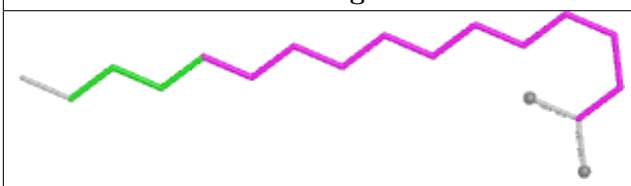
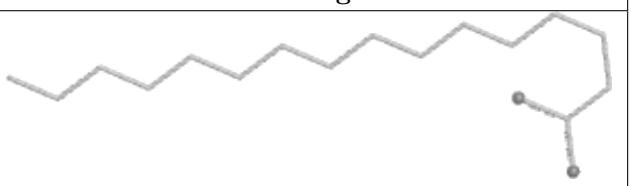


Ligand PLM D 1008

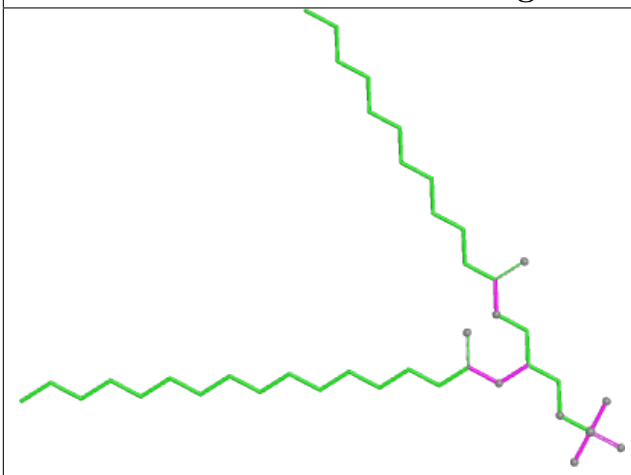


Ligand PLM D 1009	
 Bond lengths	 Bond angles
 Torsions	 Rings

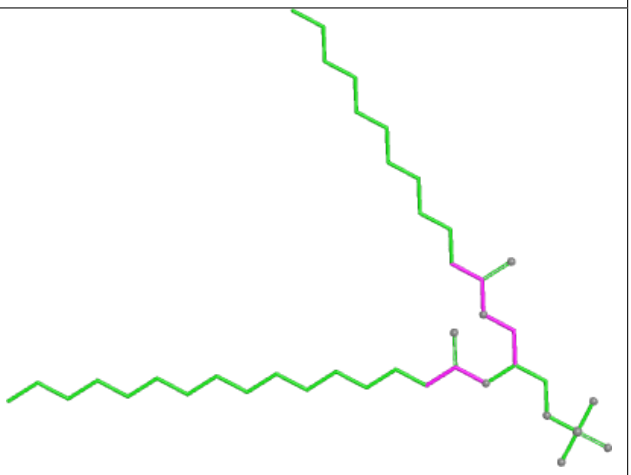
Ligand PLM B 1009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM D 1010	
 Bond lengths	 Bond angles
 Torsions	 Rings

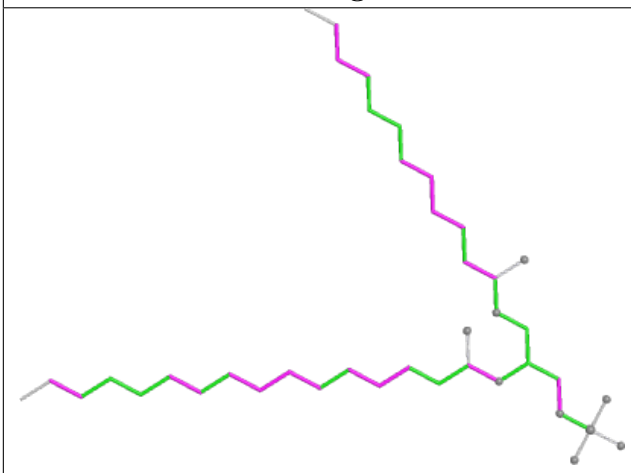
Ligand PX6 A 1007



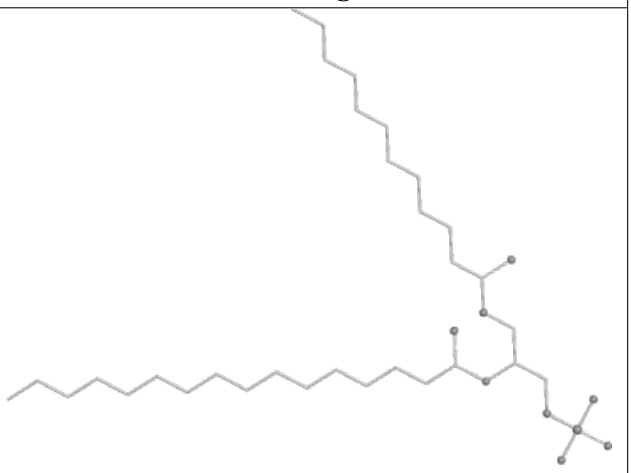
Bond lengths



Bond angles

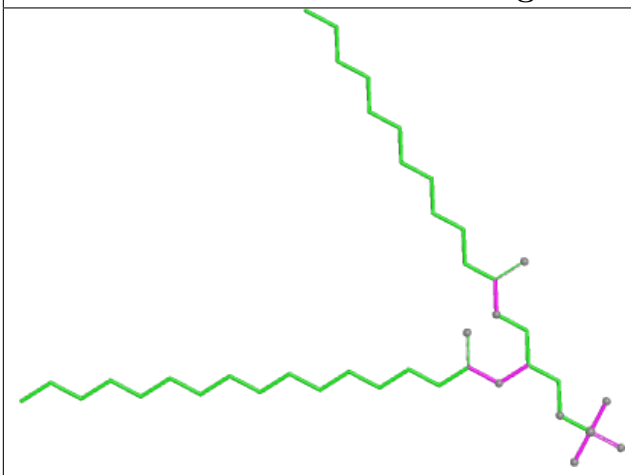


Torsions



Rings

Ligand PX6 D 1007



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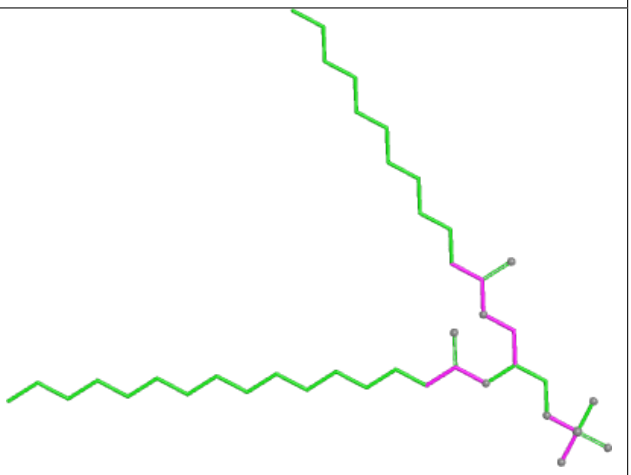

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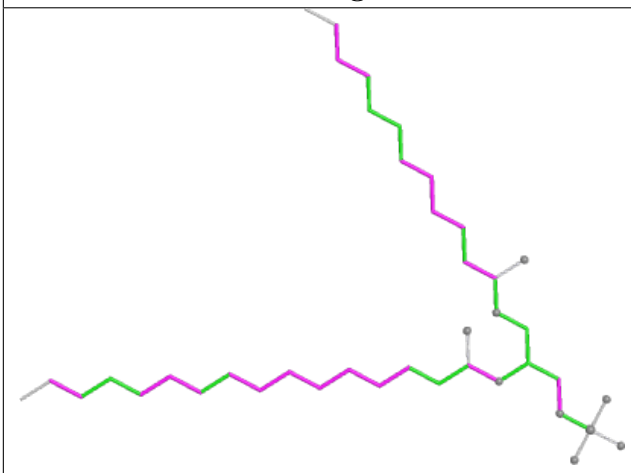

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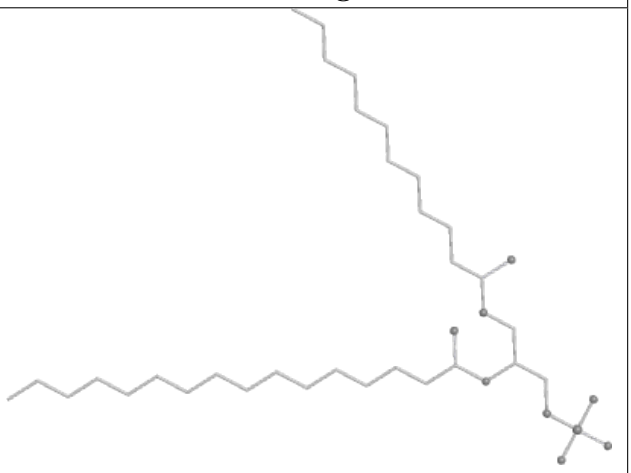
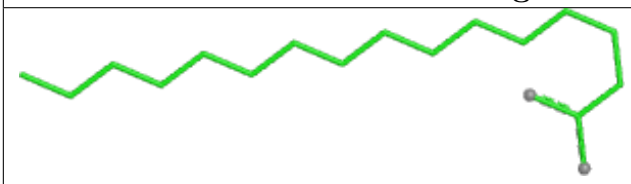


Rings

Ligand PLM C 1010



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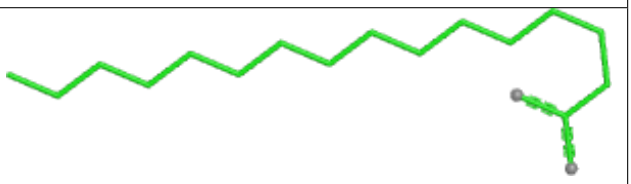

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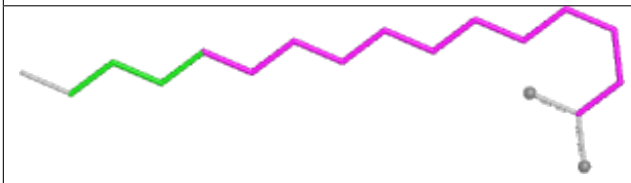

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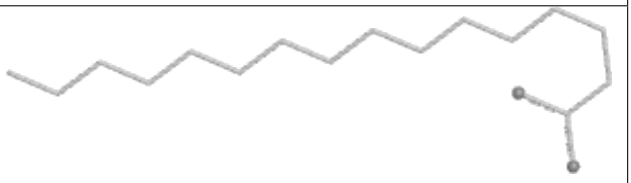
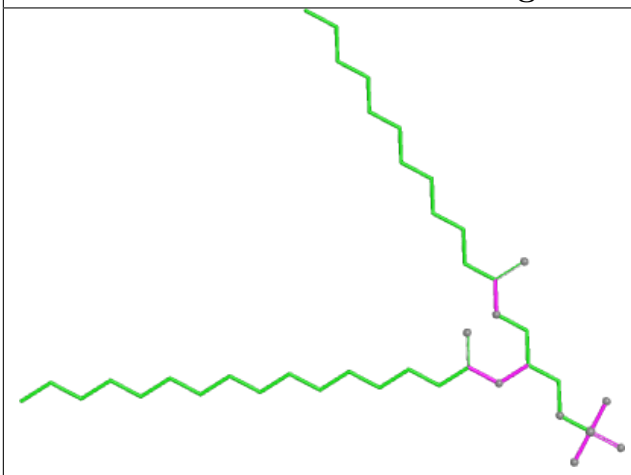


Rings

Ligand PX6 B 1007



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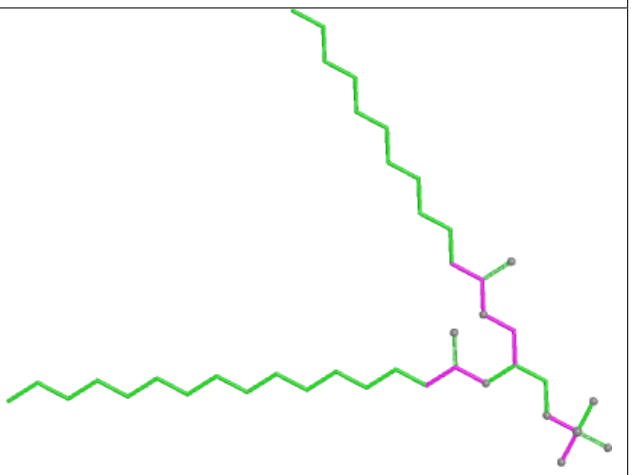

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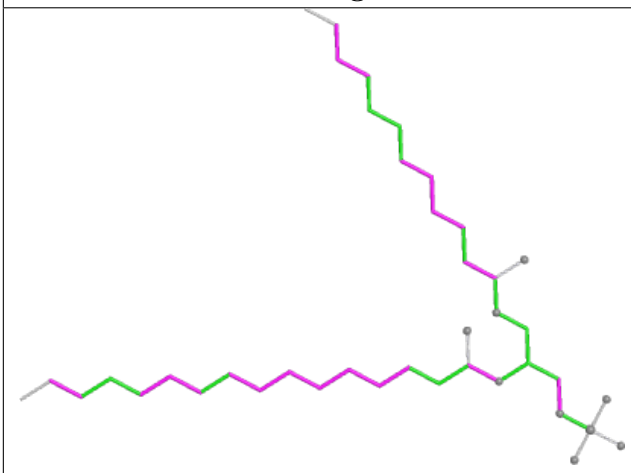

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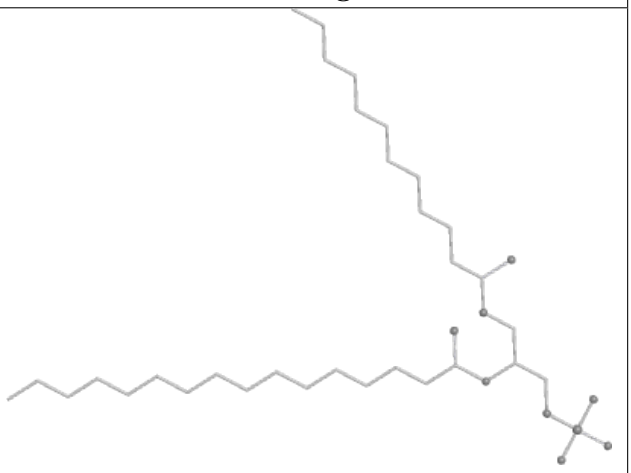
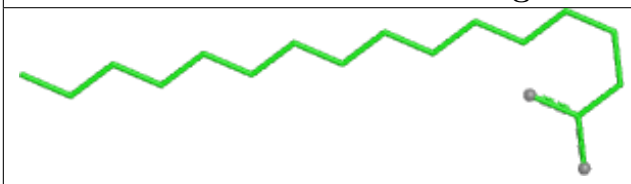


Rings

Ligand PLM B 1008



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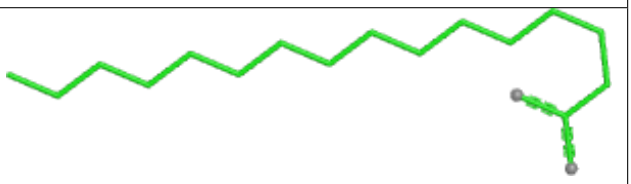
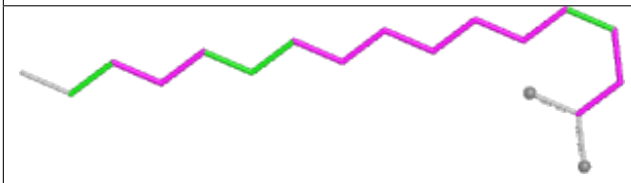


Bond angles



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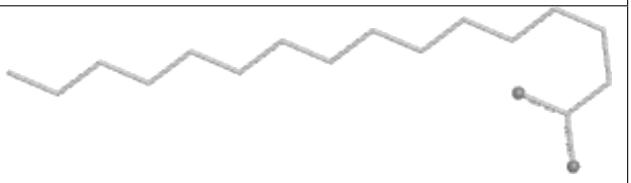
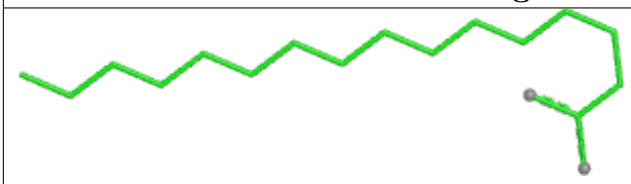
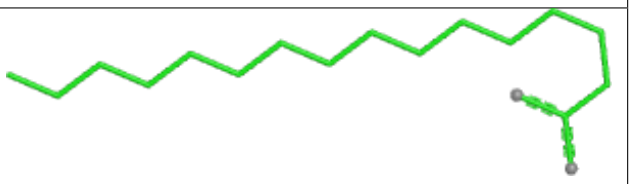
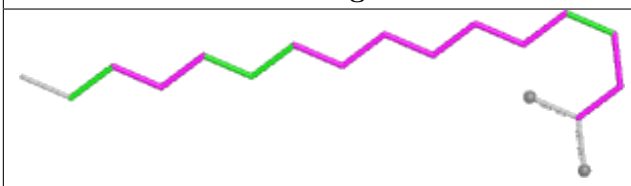
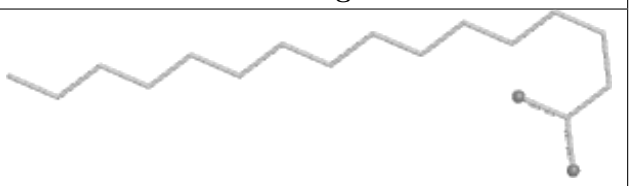
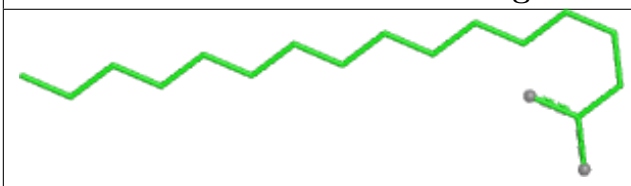
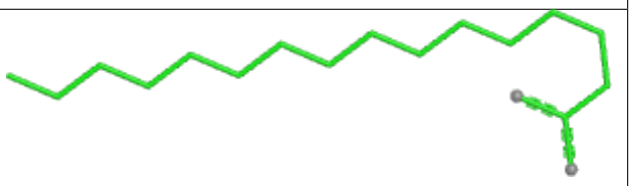
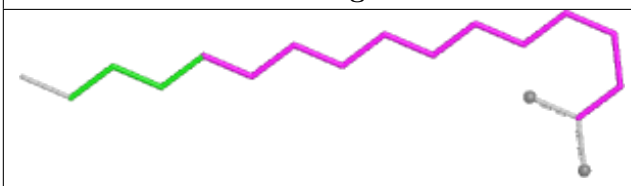
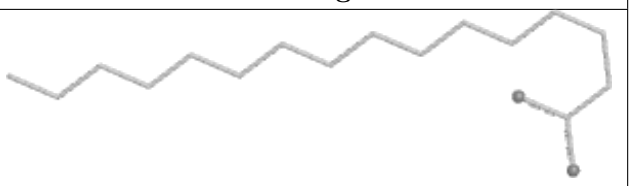
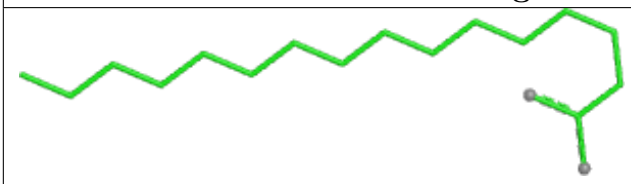
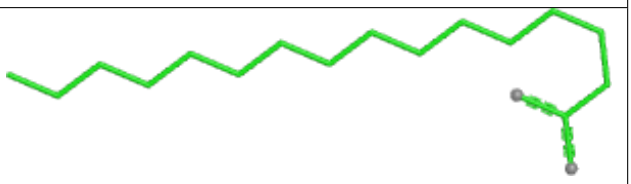
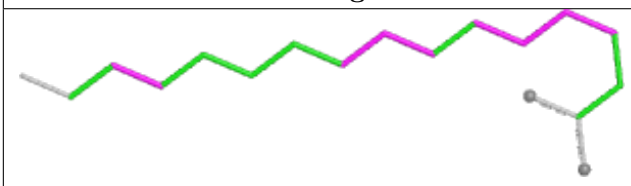
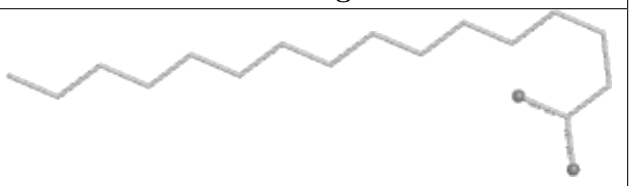


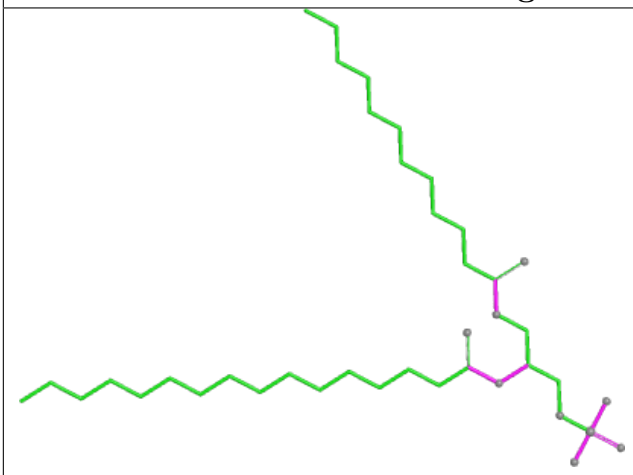
Rings

Ligand PLM C 1008	
 Bond lengths	 Bond angles
 Torsions	 Rings

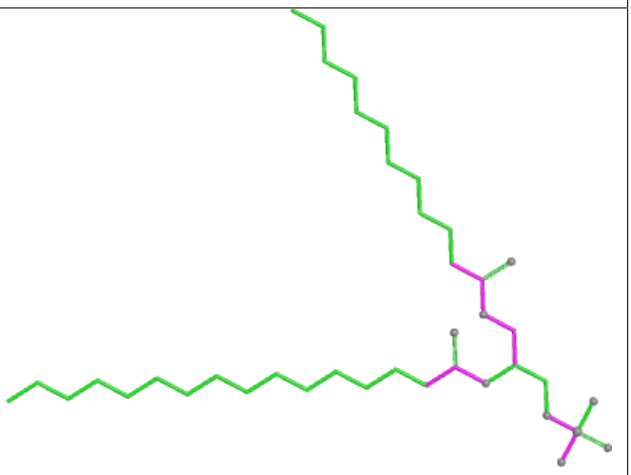
Ligand PLM B 1010	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM C 1009	
 Bond lengths	 Bond angles
 Torsions	 Rings

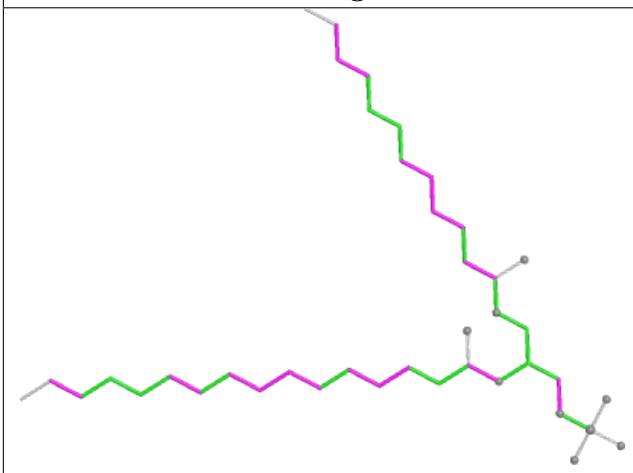
Ligand PX6 C 1007



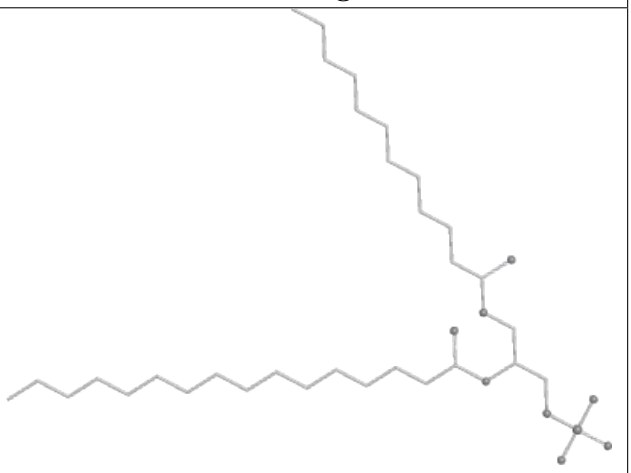
Bond lengths



Bond angles

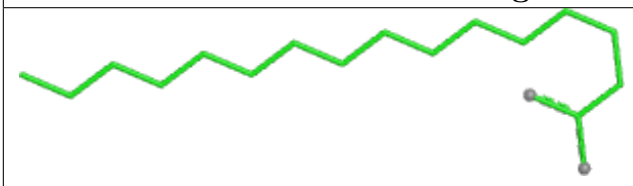


Torsions

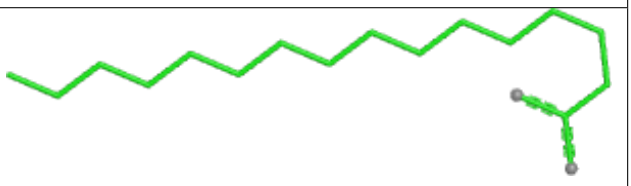


Rings

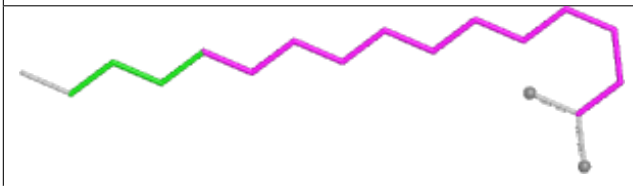
Ligand PLM A 1010



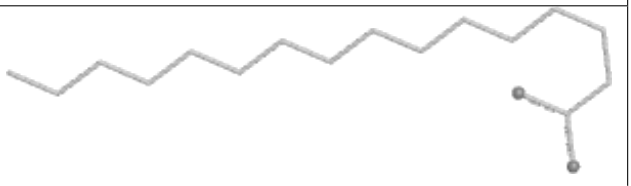
Bond lengths



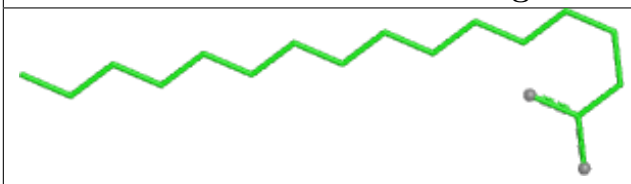
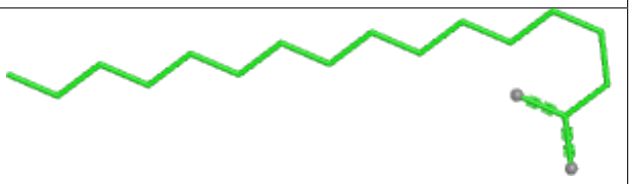
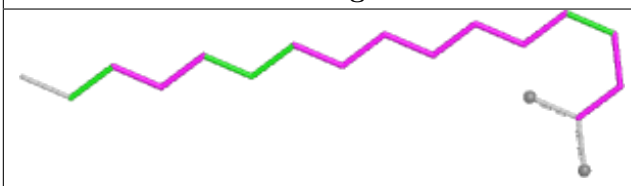
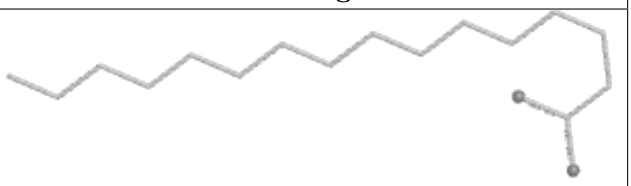
Bond angles



Torsions



Rings

Ligand PLM A 1008	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

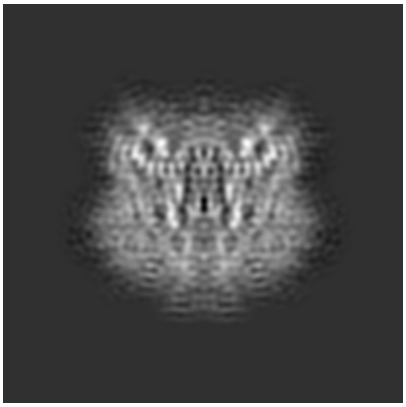
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3523. These allow visual inspection of the internal detail of the map and identification of artifacts.

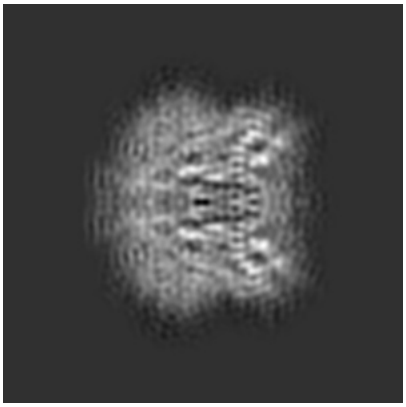
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

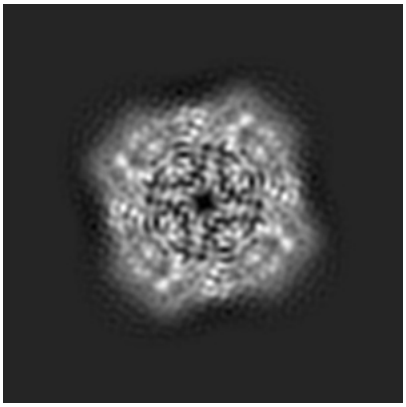
6.1.1 Primary map



X



Y



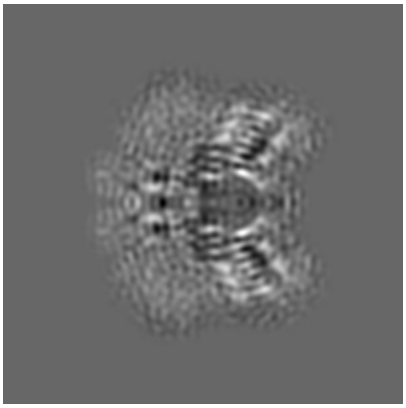
Z

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

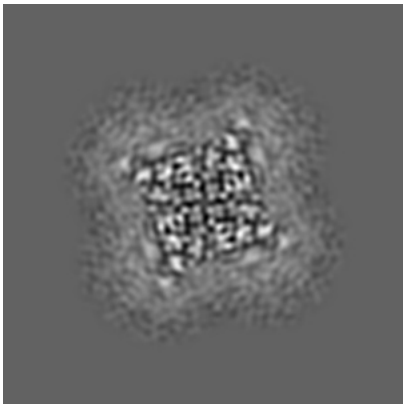
6.2 Central slices

6.2.1 Primary map

X Index: 84



Y Index: 84

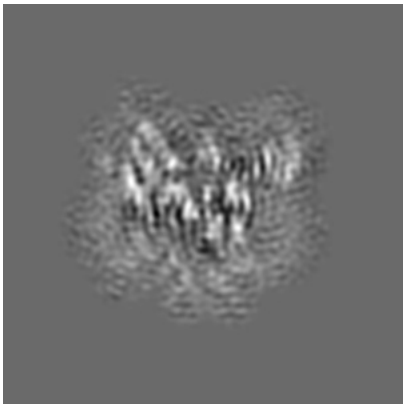


Z Index: 84

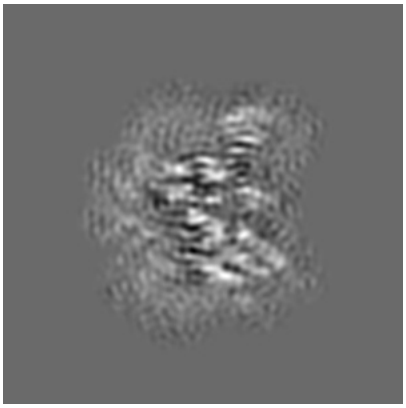
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

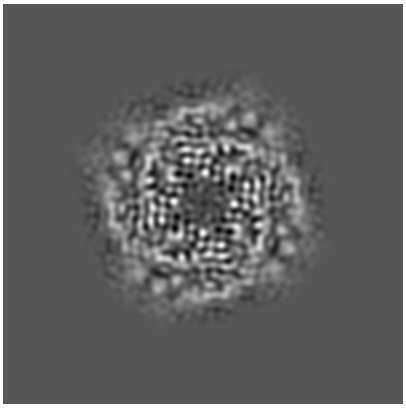
6.3.1 Primary map



X Index: 74



Y Index: 94

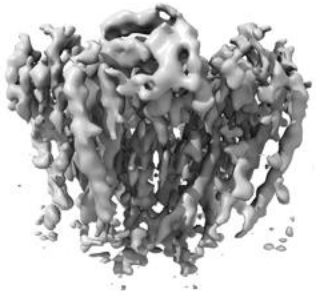


Z Index: 100

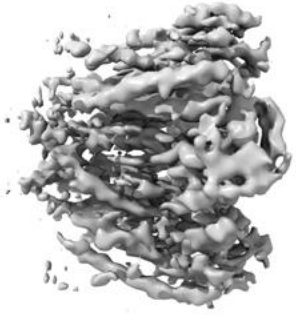
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

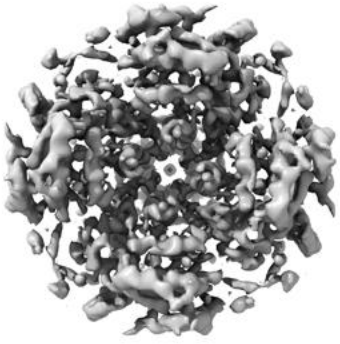
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0345. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

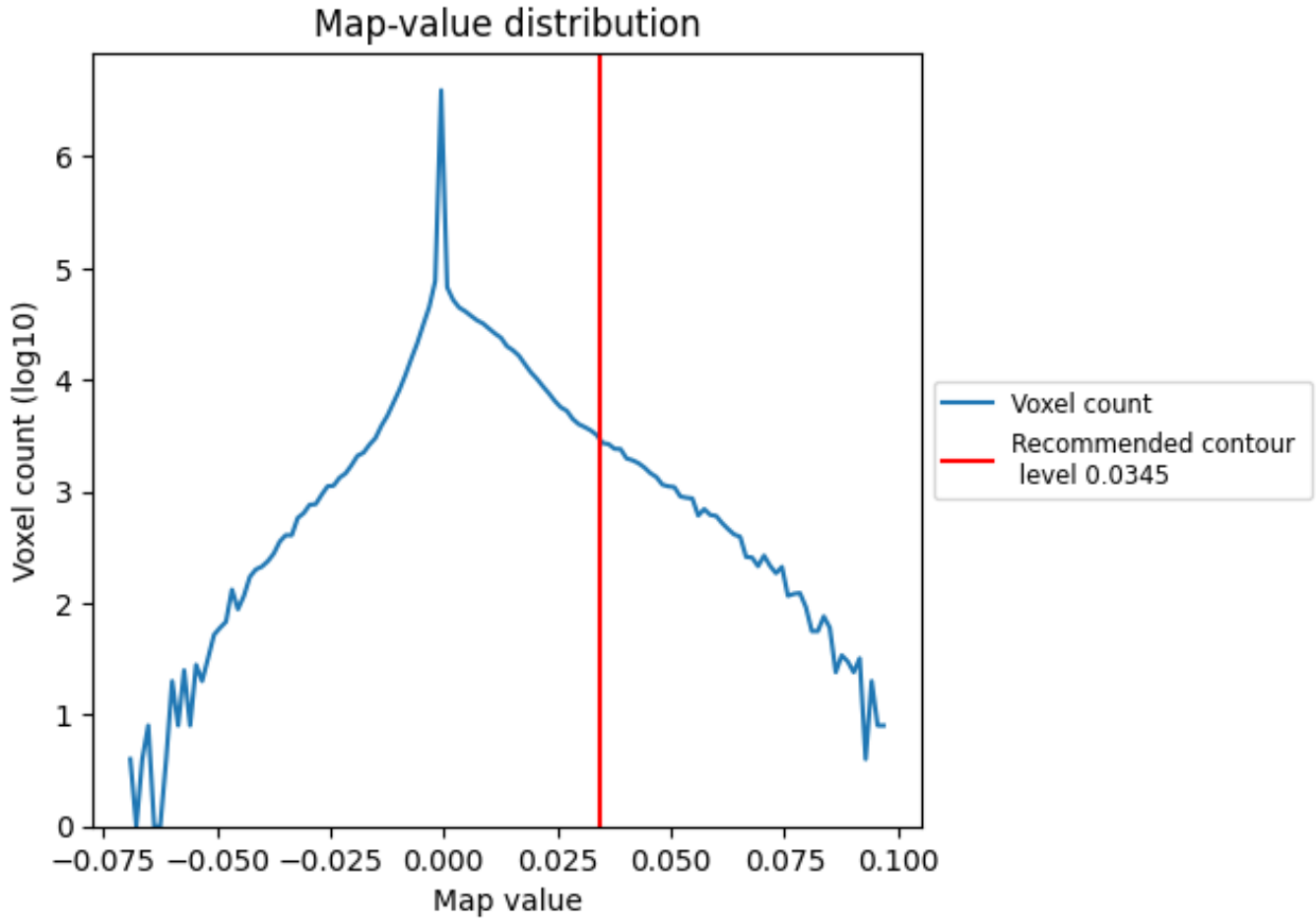
6.5 Mask visualisation (i)

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

7 Map analysis

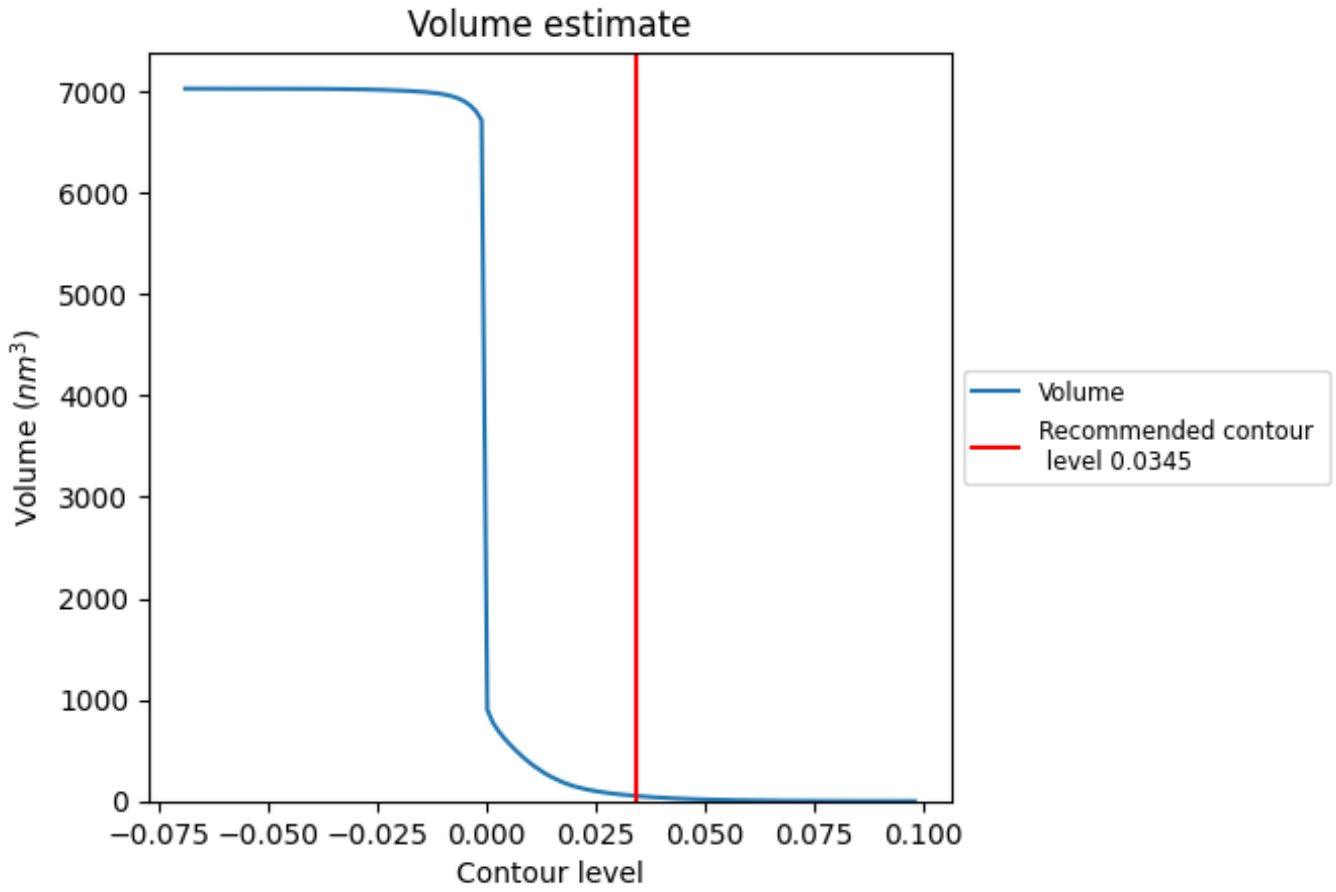
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

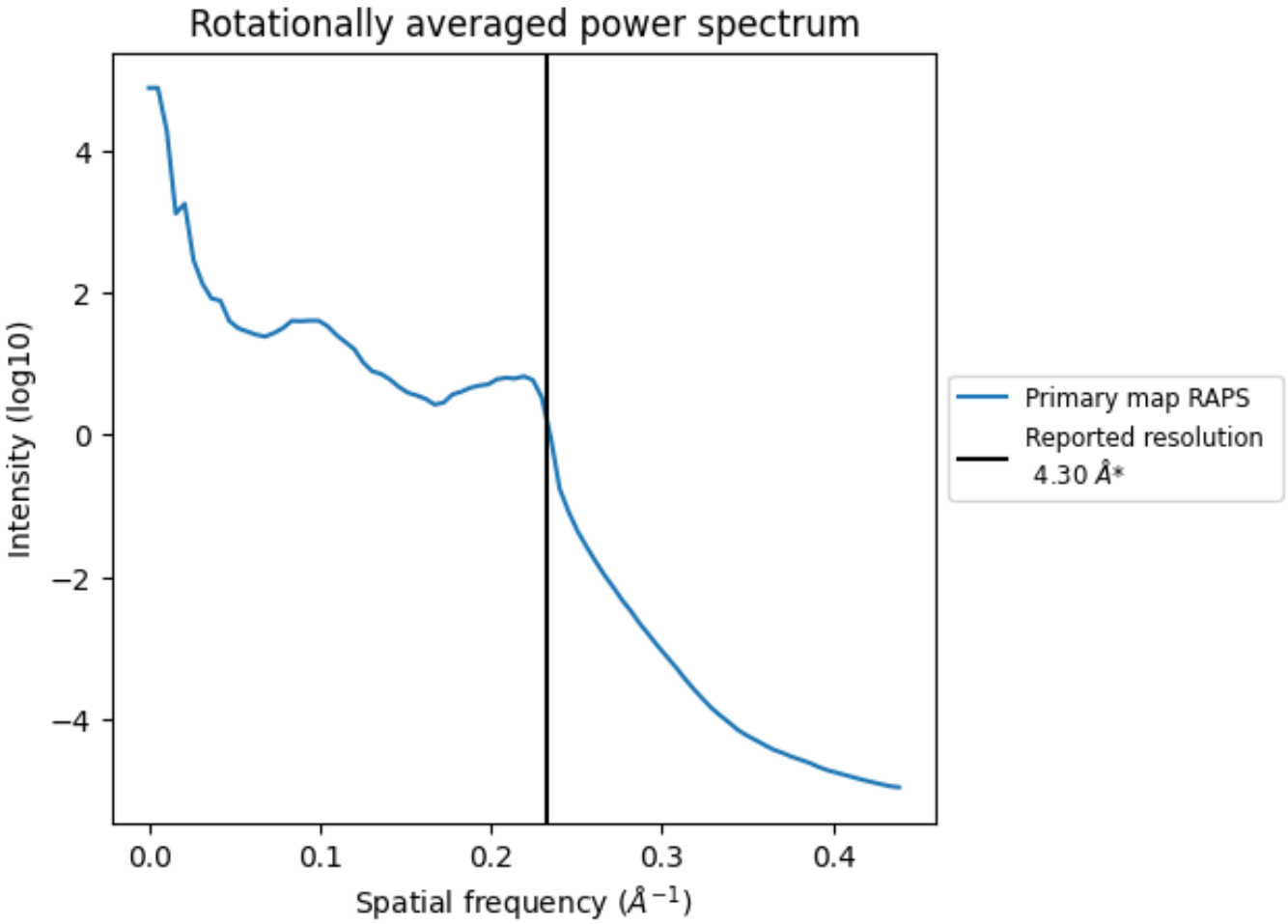
7.2 Volume estimate



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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 0.233 $Å^{-1}$

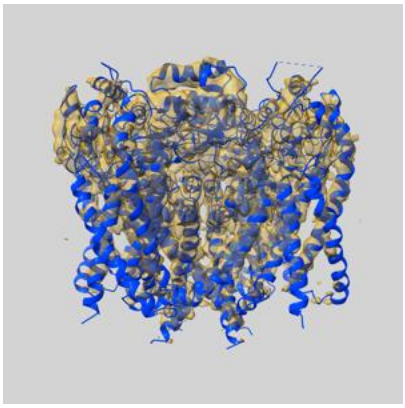
8 Fourier-Shell correlation

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

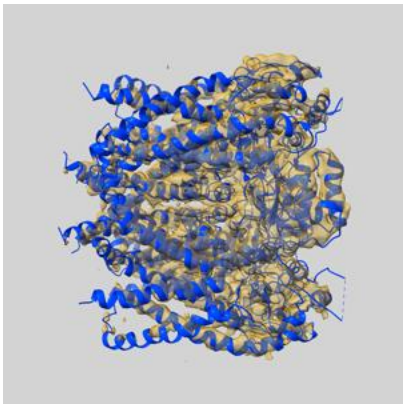
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3523 and PDB model 5MKE. Per-residue inclusion information can be found in section 3 on page 9.

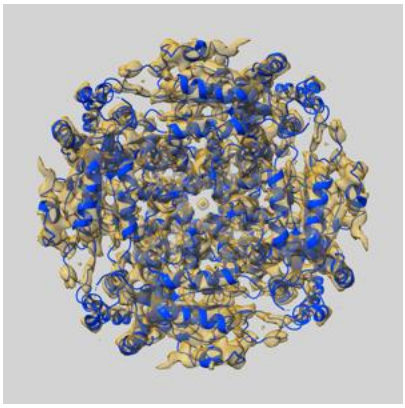
9.1 Map-model overlay



X



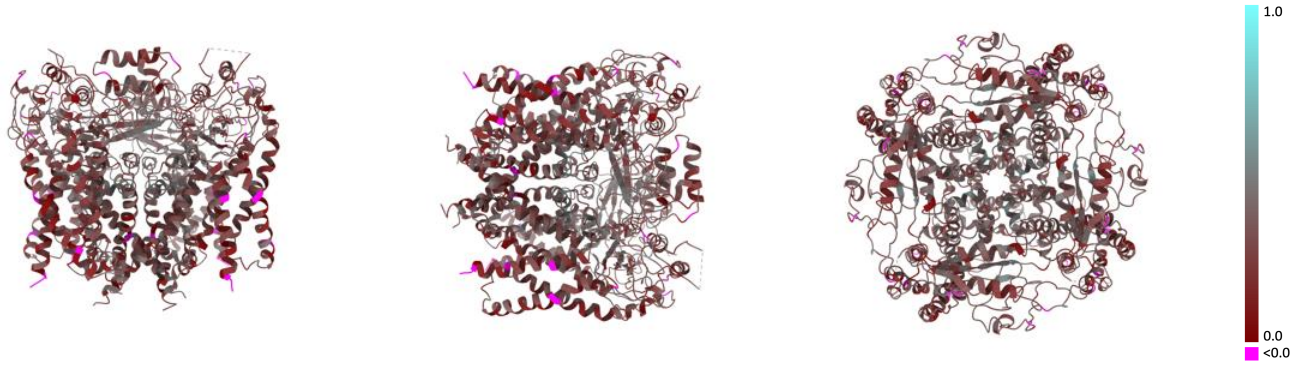
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0345 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.

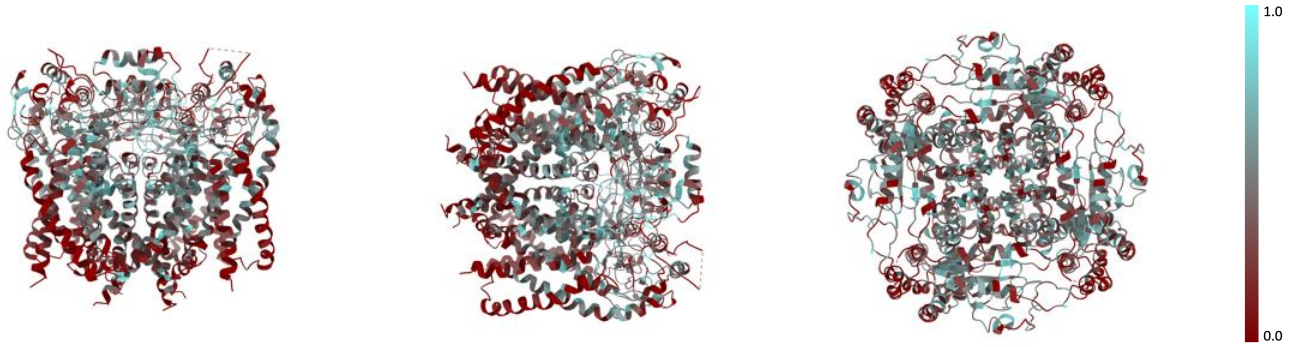
9.2 Q-score mapped to coordinate model (i)



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.

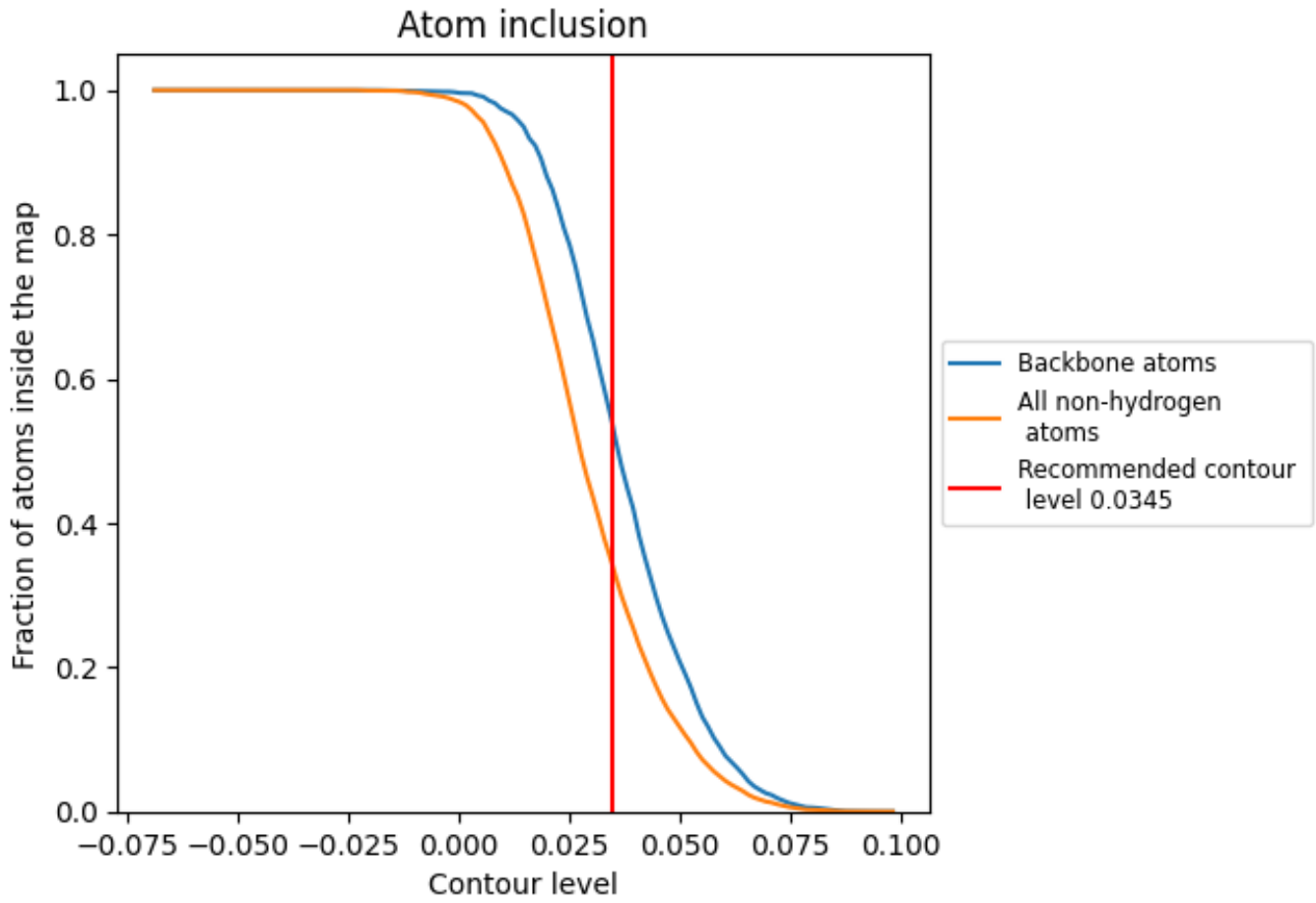
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0345).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 35% 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 (0.0345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3457	0.3030
A	0.3463	0.3040
B	0.3483	0.3040
C	0.3465	0.3020
D	0.3471	0.3030
E	0.1071	0.2280
F	0.0714	0.2390
G	0.1071	0.2180