



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 PM UTC

PDB ID : 1PXX / pdb_00001pxx
Title : CRYSTAL STRUCTURE OF DICLOFENAC BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2
Authors : Kiefer, J.R.; Rowlinson, S.W.; Prusakiewicz, J.J.; Pawlitz, J.L.; Kozak, K.R.; Kalgutkar, A.S.; Stallings, W.C.; Marnett, L.J.; Kurumbail, R.G.
Deposited on : 2003-07-07
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

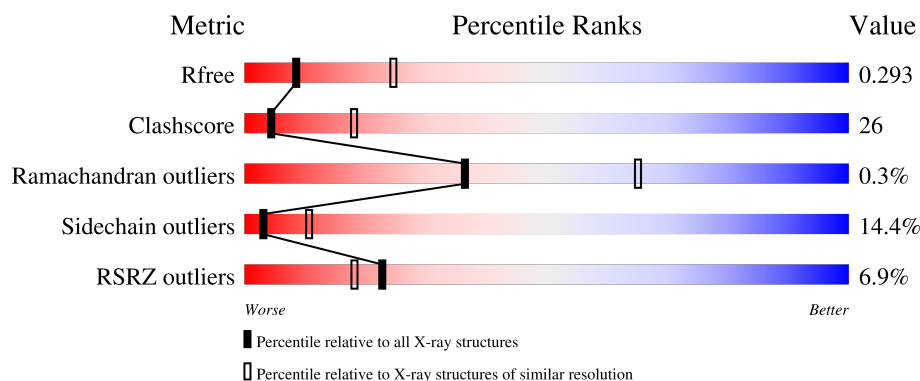
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	604	5% 48% 33% 10% 9%
1	B	604	7% 47% 35% 10% 9%
1	C	604	3% 48% 33% 10% 9%
1	D	604	9% 46% 36% 9% 9%

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Mol	Chain	Length	Quality of chain	
2	E	3		
2	F	3		
2	G	3		
2	H	3		

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	C	2661	-	-	X	-
4	BOG	D	3703	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18778 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4472	2885	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



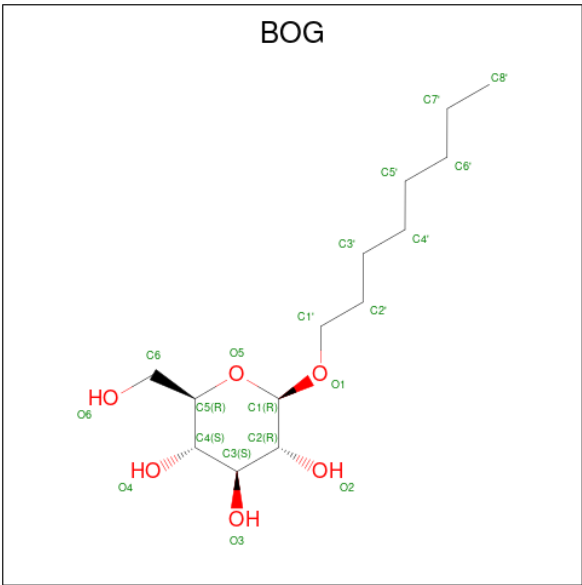
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	F	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	G	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	H	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



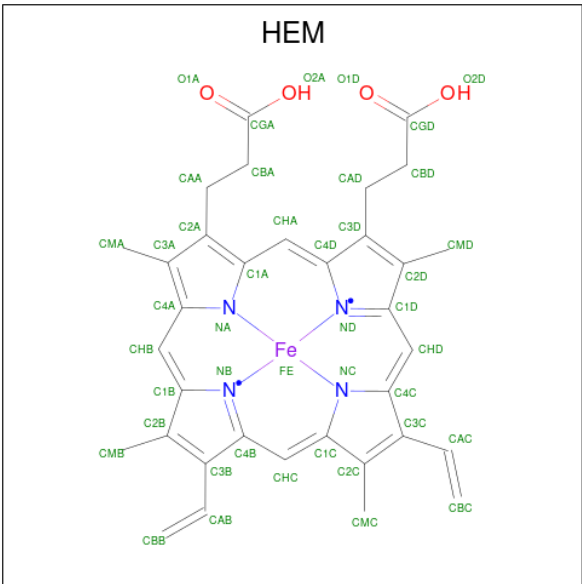
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			20	14	6			
4	D	1	Total	C	O		0	0
			19	13	6			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



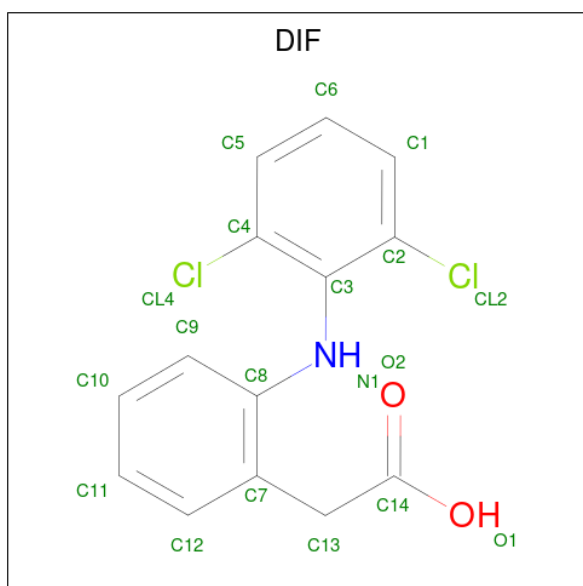
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETIC ACID (CCD ID: DIF) (formula: $C_{14}H_{11}Cl_2NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	B	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	C	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	D	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	60	Total O	0	0
			60 60		
7	B	93	Total O	0	0
			93 93		

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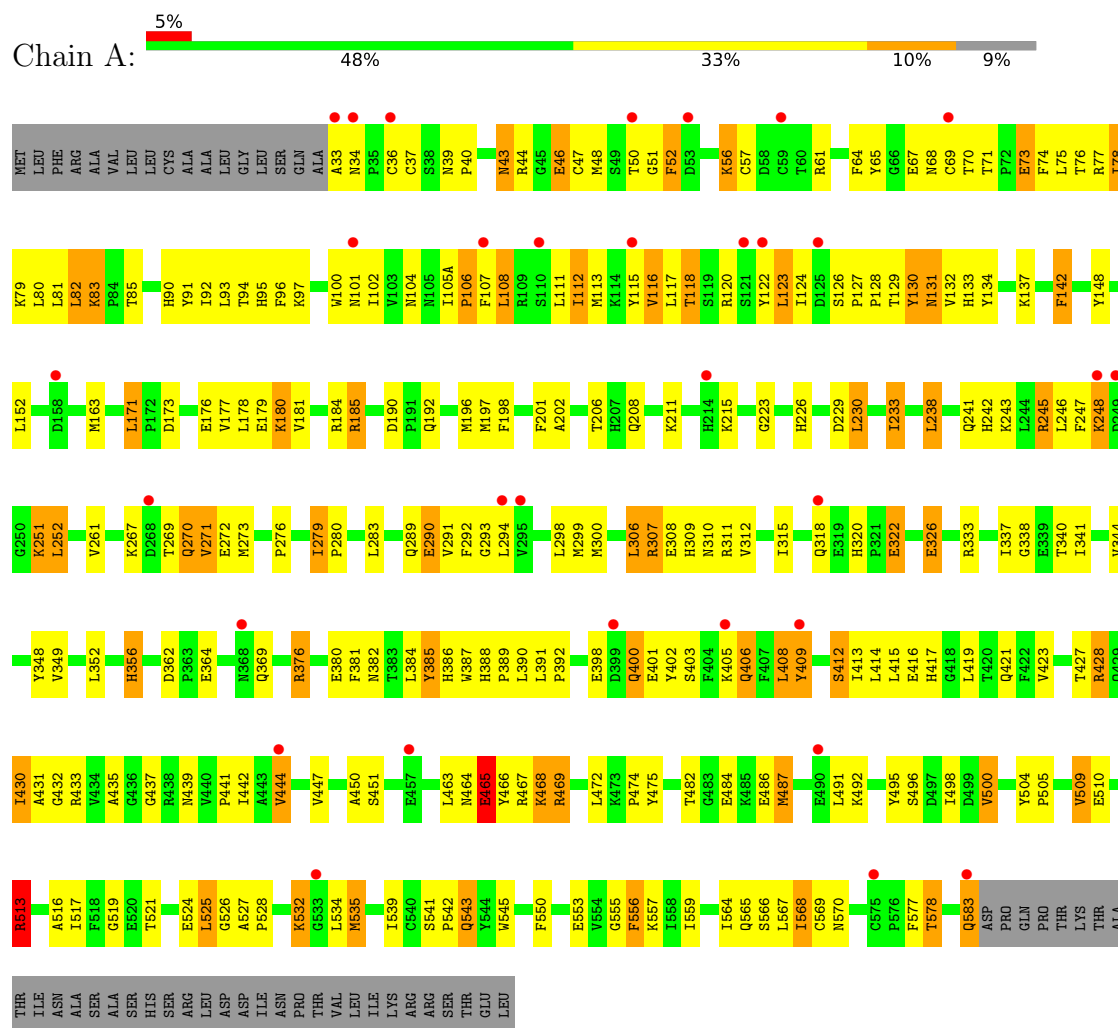
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	69	Total	O	0	0
			69	69		
7	D	95	Total	O	0	0
			95	95		

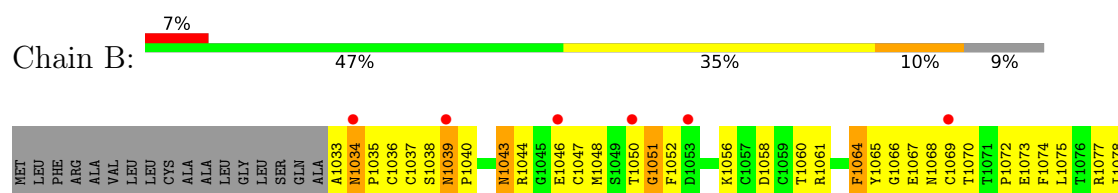
3 Residue-property plots

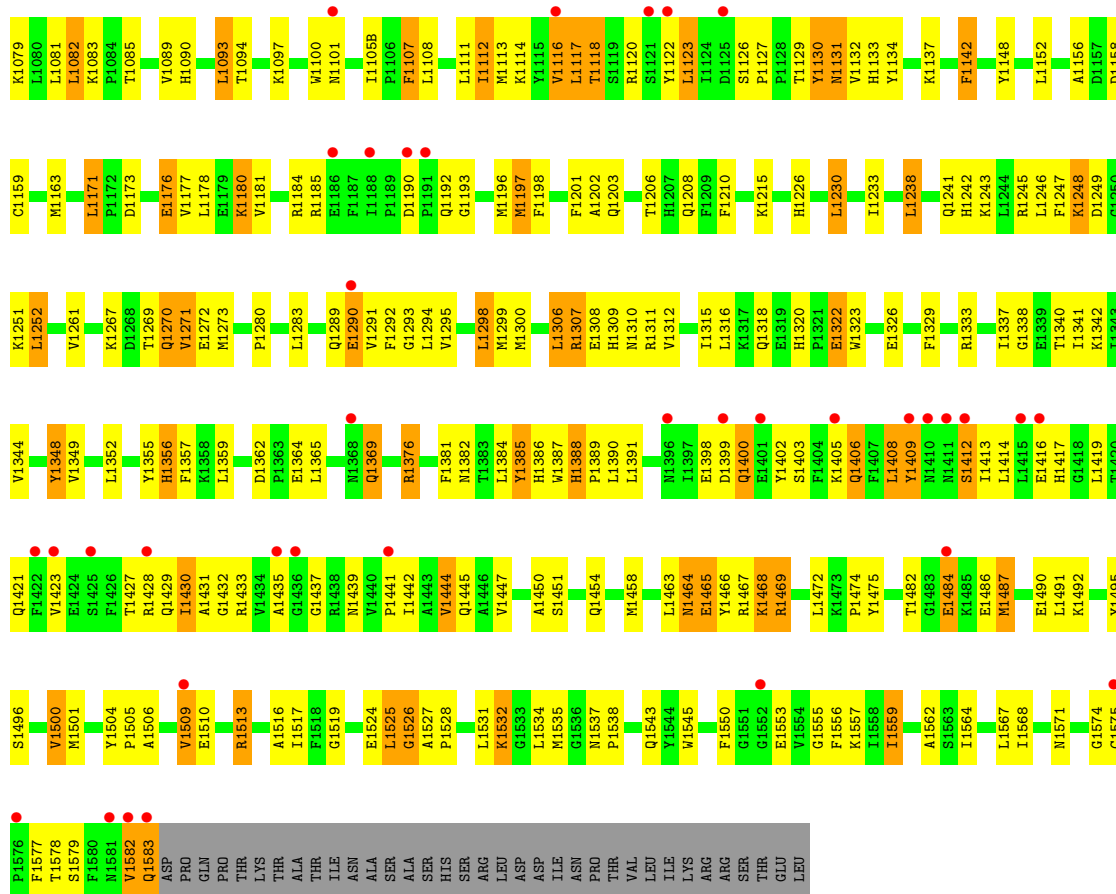
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Prostaglandin G/H synthase 2

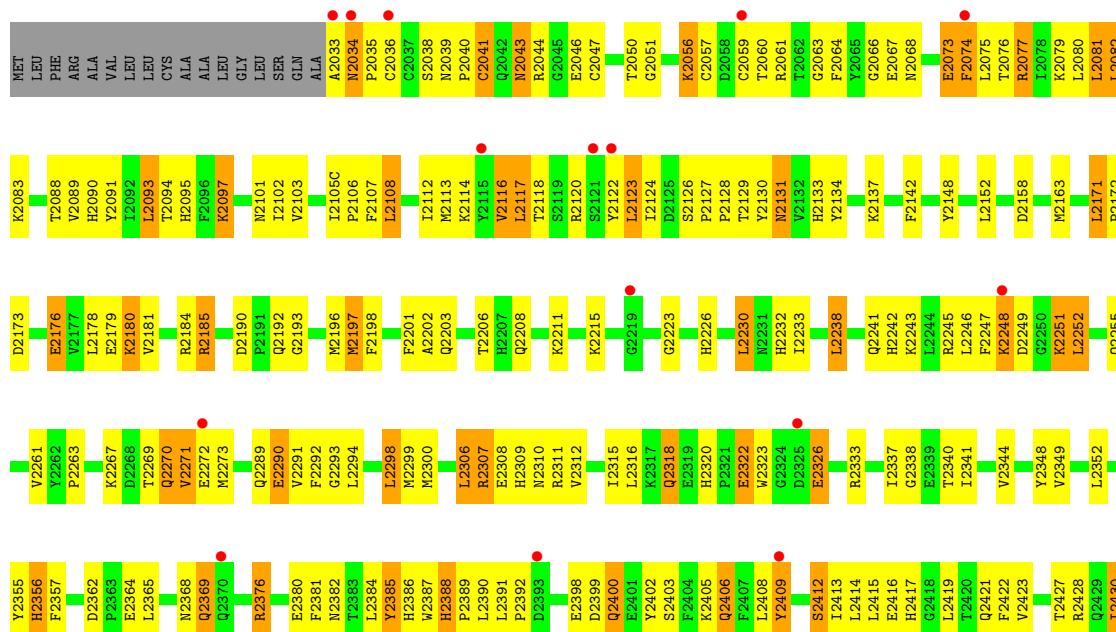


• Molecule 1: Prostaglandin G/H synthase 2





• Molecule 1: Prostaglandin G/H synthase 2



Chain E:  33% 67%



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

Chain F:  33% 67%



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

Chain G:  33% 67%



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

Chain H:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	181.15Å 135.09Å 124.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.6 (20.00-2.90) 83.3 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.254 , 0.302 0.244 , 0.293	Depositor DCC
R_{free} test set	5475 reflections (9.63%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18778	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4672e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, HEM, NAG, DIF

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	0.60	0/4598	1.04	30/6232 (0.5%)
1	B	0.60	0/4601	1.04	24/6239 (0.4%)
1	C	0.60	0/4601	1.04	22/6239 (0.4%)
1	D	0.60	0/4601	1.04	23/6239 (0.4%)
All	All	0.60	0/18401	1.04	99/24949 (0.4%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1148	TYR	N-CA-C	-8.56	95.57	109.96
1	D	3148	TYR	N-CA-C	-8.08	96.38	109.96
1	C	2148	TYR	N-CA-C	-8.03	96.47	109.96
1	A	148	TYR	N-CA-C	-7.91	96.67	109.96
1	B	1043	ASN	N-CA-C	6.86	121.02	112.24
1	A	513	ARG	N-CA-C	-6.73	100.30	110.39
1	D	3356	HIS	N-CA-C	-6.71	105.12	113.38
1	B	1051	GLY	N-CA-C	-6.65	105.25	112.04
1	D	3437	GLY	N-CA-C	-6.65	105.36	112.08
1	D	3513	ARG	N-CA-C	-6.59	100.71	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2356	HIS	N-CA-C	-6.59	105.28	113.38
1	C	2208	GLN	N-CA-C	-6.57	105.40	113.41
1	C	2388	HIS	ND1-CE1-NE2	6.51	114.92	108.40
1	A	567	LEU	N-CA-C	-6.48	103.84	111.03
1	B	1208	GLN	N-CA-C	-6.47	105.51	113.41
1	C	2041	CYS	N-CA-C	6.47	119.66	109.96
1	A	356	HIS	N-CA-C	-6.41	105.47	113.28
1	A	400	GLN	N-CA-C	6.39	118.11	110.19
1	A	208	GLN	N-CA-C	-6.33	105.69	113.41
1	B	1356	HIS	N-CA-C	-6.30	105.59	113.28
1	A	306	LEU	N-CA-C	-6.29	104.34	111.14
1	D	3432	GLY	N-CA-C	6.20	120.47	112.54
1	C	2063	GLY	N-CA-C	-6.17	106.53	114.85
1	B	1180	LYS	N-CA-C	6.13	118.05	111.36
1	C	2388	HIS	CA-CB-CG	-6.09	107.71	113.80
1	C	2043	ASN	N-CA-C	6.09	119.94	111.90
1	A	437	GLY	N-CA-C	-6.08	105.94	112.08
1	C	2513	ARG	N-CA-C	-6.08	101.28	110.39
1	D	3039	ASN	CA-C-N	6.07	125.79	119.05
1	D	3039	ASN	C-N-CA	6.07	125.79	119.05
1	A	118	THR	N-CA-C	6.07	117.69	111.14
1	B	1400	GLN	N-CA-C	6.06	117.71	110.19
1	D	3400	GLN	N-CA-C	6.03	117.67	110.19
1	B	1039	ASN	CA-C-N	5.99	125.20	118.97
1	B	1039	ASN	C-N-CA	5.99	125.20	118.97
1	D	3486	GLU	N-CA-C	5.98	117.67	111.03
1	B	1513	ARG	N-CA-C	-5.96	101.62	110.20
1	D	3043	ASN	N-CA-C	5.95	119.86	112.24
1	A	500	VAL	N-CA-C	-5.92	107.49	113.47
1	C	2400	GLN	N-CA-C	5.92	117.53	110.19
1	D	3197	MET	N-CA-C	-5.89	104.99	111.82
1	D	3208	GLN	N-CA-C	-5.81	106.32	113.41
1	B	1130	TYR	N-CA-C	5.79	117.99	110.53
1	C	2388	HIS	ND1-CG-CD2	5.71	111.81	106.10
1	A	179	GLU	N-CA-C	5.71	117.58	111.36
1	B	1197	MET	N-CA-C	-5.70	105.21	111.82
1	D	3073	GLU	N-CA-C	-5.66	102.91	110.55
1	B	1306	LEU	N-CA-C	-5.64	105.05	111.14
1	A	251	LYS	N-CA-C	5.64	118.16	110.55
1	D	3180	LYS	N-CA-C	5.58	117.45	111.36
1	A	43	ASN	N-CA-C	5.58	119.13	111.54
1	B	1500	VAL	N-CA-C	-5.57	107.84	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3179	GLU	N-CA-C	5.55	117.41	111.36
1	D	3306	LEU	N-CA-C	-5.54	105.15	111.14
1	A	142	PHE	N-CA-C	5.53	118.07	111.71
1	C	2437	GLY	N-CA-C	-5.51	106.51	112.08
1	C	2180	LYS	N-CA-C	5.51	117.36	111.36
1	A	73	GLU	N-CA-C	-5.49	102.64	110.59
1	C	2073	GLU	N-CA-C	-5.48	103.15	110.55
1	A	465	GLU	N-CA-C	-5.46	105.25	111.14
1	C	2559	ILE	CB-CA-C	-5.46	104.83	111.87
1	A	233	ILE	CB-CA-C	-5.43	106.28	111.44
1	A	180	LYS	N-CA-C	5.41	117.26	111.36
1	C	2500	VAL	N-CA-C	-5.40	108.02	113.47
1	C	2197	MET	N-CA-C	-5.39	105.56	111.82
1	D	3109	ARG	N-CA-C	-5.37	105.33	111.07
1	D	3500	VAL	N-CA-C	-5.36	108.06	113.47
1	D	3412	SER	N-CA-C	-5.35	105.61	111.82
1	C	2306	LEU	N-CA-C	-5.35	105.37	111.14
1	B	1486	GLU	N-CA-C	5.34	116.96	111.03
1	A	412	SER	N-CA-C	-5.32	105.65	111.82
1	B	1052	PHE	N-CA-C	5.26	118.80	112.38
1	B	1412	SER	N-CA-C	-5.24	105.74	111.82
1	B	1432	GLY	N-CA-C	5.23	119.23	112.54
1	B	1142	PHE	N-CA-C	5.22	117.71	111.71
1	C	2251	LYS	N-CA-C	5.22	117.60	110.55
1	C	2412	SER	N-CA-C	-5.22	105.77	111.82
1	D	3498	ILE	N-CA-C	-5.20	105.28	112.50
1	A	279	ILE	CA-C-N	5.19	125.44	119.83
1	A	279	ILE	C-N-CA	5.19	125.44	119.83
1	B	1437	GLY	N-CA-C	-5.19	106.84	112.08
1	A	432	GLY	N-CA-C	5.16	119.14	112.54
1	B	1388	HIS	ND1-CG-CD2	5.16	111.26	106.10
1	D	3388	HIS	ND1-CG-CD2	5.13	111.23	106.10
1	A	486	GLU	N-CA-C	5.13	116.72	111.03
1	B	1559	ILE	CB-CA-C	-5.13	105.30	112.02
1	C	2179	GLU	N-CA-C	5.09	116.91	111.36
1	D	3142	PHE	N-CA-C	5.09	117.57	111.71
1	A	229	ASP	N-CA-C	-5.08	106.49	113.30
1	A	52	PHE	N-CA-C	5.08	118.25	111.75
1	A	245	ARG	N-CA-C	5.08	118.22	110.20
1	B	1526	GLY	N-CA-C	5.07	119.26	112.77
1	D	3045	GLY	N-CA-C	-5.07	105.60	112.14
1	B	1388	HIS	ND1-CE1-NE2	5.05	113.45	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ILE	N-CA-C	-5.04	105.50	112.50
1	C	2465	GLU	N-CA-C	-5.03	105.70	111.14
1	A	130	TYR	N-CA-C	5.00	117.85	110.59
1	A	83	LYS	CA-C-N	5.00	124.76	119.76
1	A	83	LYS	C-N-CA	5.00	124.76	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1348	TYR	Sidechain
1	D	3348	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4366	235	0
1	B	4474	0	4372	249	1
1	C	4474	0	4372	240	1
1	D	4474	0	4372	240	0
2	E	42	0	37	3	0
2	F	42	0	37	1	0
2	G	42	0	37	2	0
2	H	42	0	37	3	0
3	A	28	0	26	5	0
3	B	28	0	26	6	0
3	C	28	0	26	7	0
3	D	28	0	26	4	0
4	A	20	0	28	5	1
4	D	19	0	25	9	1
5	A	43	0	30	4	0
5	B	43	0	30	7	0
5	C	43	0	30	4	0
5	D	43	0	30	4	0
6	A	19	0	10	3	0
6	B	19	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	19	0	10	4	0
6	D	19	0	10	1	0
7	A	60	0	0	9	0
7	B	93	0	0	9	0
7	C	69	0	0	8	0
7	D	95	0	0	7	0
All	All	18778	0	17947	964	2

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 26.

All (964) 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:D:3294:LEU:HD22	1:D:3409:TYR:HD2	1.03	1.15
1:A:294:LEU:HD22	1:A:409:TYR:CD2	1.80	1.14
1:D:3294:LEU:HD22	1:D:3409:TYR:CD2	1.84	1.12
1:A:294:LEU:HD22	1:A:409:TYR:HD2	1.00	1.11
1:D:3442:ILE:HD13	4:D:3703:BOG:H62	1.34	1.08
1:C:2105(C):ILE:CG2	1:C:2108:LEU:HB2	1.84	1.07
1:C:2294:LEU:HD22	1:C:2409:TYR:HD2	1.13	1.07
1:B:1294:LEU:HD22	1:B:1409:TYR:HD2	1.18	1.07
1:C:2105(C):ILE:HG22	1:C:2108:LEU:HB2	1.32	1.06
1:C:2294:LEU:HD22	1:C:2409:TYR:CD2	1.92	1.03
1:B:1294:LEU:HD22	1:B:1409:TYR:CD2	1.93	1.02
1:D:3113:MET:O	1:D:3116:VAL:HG22	1.59	1.01
1:A:442:ILE:HD13	4:A:703:BOG:H62	1.41	0.99
1:B:1398:GLU:HG3	1:B:1421:GLN:CD	1.88	0.99
1:A:398:GLU:HG3	1:A:421:GLN:CD	1.88	0.98
1:C:2398:GLU:HG3	1:C:2421:GLN:CD	1.89	0.97
1:D:3447:VAL:HG13	5:D:3601:HEM:HBA1	1.49	0.93
1:B:1181:VAL:HG12	1:B:1487:MET:HG2	1.52	0.92
1:D:3398:GLU:HG3	1:D:3421:GLN:CD	1.95	0.92
1:A:33:ALA:C	1:A:34:ASN:CA	2.43	0.91
1:B:1184:ARG:HB2	1:B:1439:ASN:HA	1.51	0.91
1:A:105(A):ILE:CG2	1:A:108:LEU:HB2	1.99	0.91
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.53	0.91
1:D:3184:ARG:HB2	1:D:3439:ASN:HA	1.53	0.90
1:C:2039:ASN:HB3	7:C:5138:HOH:O	1.72	0.90
1:C:2447:VAL:HG13	5:C:2601:HEM:HBA2	1.54	0.90
1:B:1447:VAL:HG13	5:B:1601:HEM:HBA1	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:O	1:A:299:MET:HE2	1.72	0.89
1:C:2322:GLU:HG2	1:D:3051:GLY:C	1.98	0.89
1:C:2181:VAL:HG12	1:C:2487:MET:HG2	1.54	0.88
1:A:294:LEU:CD2	1:A:409:TYR:HD2	1.85	0.88
1:C:2184:ARG:HB2	1:C:2439:ASN:HA	1.53	0.87
1:B:1105(B):ILE:HD13	1:B:1108:LEU:HD12	1.55	0.86
1:D:3294:LEU:CD2	1:D:3409:TYR:HD2	1.86	0.86
1:D:3075:LEU:CG	1:D:3079:LYS:HE3	2.06	0.85
1:B:1206:THR:HG21	1:B:1385:TYR:CE2	2.13	0.84
1:D:3075:LEU:HG	1:D:3079:LYS:HE3	1.59	0.84
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.18	0.84
1:A:293:GLY:HA2	1:A:299:MET:CE	2.08	0.83
1:C:2105(C):ILE:HG22	1:C:2105(C):ILE:O	1.78	0.83
1:B:1387:TRP:HB2	5:B:1601:HEM:HAC	1.61	0.83
1:B:1292:PHE:O	1:B:1299:MET:HE2	1.78	0.83
1:B:1385:TYR:OH	6:B:1701:DIF:H132	1.78	0.83
1:B:1472:LEU:HD21	1:B:1524:GLU:HG3	1.62	0.82
1:B:1113:MET:HE3	1:B:1116:VAL:CG2	2.08	0.82
1:D:3206:THR:HG21	1:D:3385:TYR:CE2	2.15	0.82
1:C:2292:PHE:O	1:C:2299:MET:HE2	1.78	0.82
1:B:1113:MET:HE3	1:B:1116:VAL:HG21	1.61	0.82
1:D:3074:PHE:O	1:D:3078:ILE:HD12	1.79	0.81
1:B:1246:LEU:HG	1:B:1248:LYS:HG3	1.62	0.81
1:D:3419:LEU:O	1:D:3423:VAL:HG23	1.80	0.81
1:B:1465:GLU:OE1	1:B:1465:GLU:HA	1.81	0.81
1:C:2123:LEU:O	1:C:2469:ARG:NH2	2.14	0.81
1:D:3293:GLY:HA2	1:D:3299:MET:CE	2.11	0.80
1:A:185:ARG:HH11	4:A:703:BOG:H4'1	1.47	0.80
1:B:1293:GLY:HA2	1:B:1299:MET:CE	2.12	0.80
1:B:1131:ASN:HD22	1:B:1131:ASN:C	1.89	0.80
1:C:2131:ASN:HD22	1:C:2131:ASN:C	1.90	0.80
1:A:123:LEU:O	1:A:469:ARG:NH2	2.15	0.80
1:B:1123:LEU:O	1:B:1469:ARG:NH2	2.15	0.79
1:D:3123:LEU:O	1:D:3469:ARG:NH2	2.15	0.79
1:D:3516:ALA:HB1	7:D:5034:HOH:O	1.83	0.79
1:C:2246:LEU:HG	1:C:2248:LYS:HG3	1.65	0.79
1:D:3181:VAL:HG12	1:D:3487:MET:HG2	1.63	0.79
1:D:3427:THR:HG22	1:D:3583:GLN:HE22	1.47	0.79
1:D:3131:ASN:C	1:D:3131:ASN:HD22	1.91	0.79
1:D:3202:ALA:O	1:D:3206:THR:HG23	1.83	0.79
1:C:2294:LEU:CD2	1:C:2409:TYR:HD2	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2198:PHE:CZ	1:C:2352:LEU:HD13	2.19	0.78
1:C:2472:LEU:HD21	1:C:2524:GLU:HG3	1.64	0.78
1:A:427:THR:HG22	1:A:583:GLN:HE22	1.48	0.78
1:C:2293:GLY:HA2	1:C:2299:MET:CE	2.13	0.78
1:B:1294:LEU:CD2	1:B:1409:TYR:HD2	1.96	0.78
1:D:3292:PHE:O	1:D:3299:MET:HE2	1.84	0.77
1:A:105(A):ILE:HG22	1:A:108:LEU:HB2	1.65	0.77
1:B:1163:MET:CE	1:B:1171:LEU:HD21	2.14	0.77
1:D:3472:LEU:HD21	1:D:3524:GLU:HG3	1.64	0.77
1:C:2051:GLY:O	1:D:3322:GLU:HG2	1.85	0.77
1:B:1427:THR:HG22	1:B:1583:GLN:HE22	1.49	0.77
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.67	0.76
1:A:40:PRO:HA	3:A:661:NAG:H83	1.66	0.76
1:B:1202:ALA:O	1:B:1206:THR:HG23	1.84	0.76
1:D:3039:ASN:N	1:D:3040:PRO:HD3	1.99	0.76
1:D:3162:PRO:HD2	7:D:5121:HOH:O	1.84	0.76
1:A:56:LYS:HG3	1:A:57:CYS:N	2.00	0.76
1:C:2202:ALA:O	1:C:2206:THR:HG23	1.85	0.76
1:A:525:LEU:HD21	7:A:5160:HOH:O	1.86	0.76
1:B:1034:ASN:ND2	1:B:1036:CYS:H	1.82	0.76
1:C:2465:GLU:OE1	1:C:2465:GLU:HA	1.86	0.75
1:B:1034:ASN:HD22	1:B:1036:CYS:H	1.32	0.75
1:A:444:VAL:O	1:A:444:VAL:HG13	1.86	0.75
1:A:34:ASN:HD22	1:A:36:CYS:H	1.33	0.75
1:C:2206:THR:HG21	1:C:2385:TYR:CE2	2.21	0.75
1:B:1241:GLN:NE2	1:B:1245:ARG:HH11	1.85	0.75
1:D:3113:MET:HE3	1:D:3116:VAL:HG21	1.69	0.74
1:C:2163:MET:HE2	1:C:2171:LEU:HD21	1.69	0.74
1:C:2163:MET:CE	1:C:2171:LEU:HD21	2.18	0.74
1:D:3246:LEU:HG	1:D:3248:LYS:HG3	1.69	0.74
1:C:2113:MET:HA	1:C:2116:VAL:HG13	1.69	0.74
1:D:3230:LEU:HG	1:D:3337:ILE:HG12	1.70	0.74
1:D:3465:GLU:OE1	1:D:3465:GLU:HA	1.87	0.73
1:A:130:TYR:HB3	1:A:134:TYR:O	1.88	0.73
1:A:163:MET:HE2	1:A:171:LEU:HD21	1.70	0.73
1:D:3403:SER:OG	1:D:3406:GLN:HG3	1.88	0.73
1:A:419:LEU:O	1:A:423:VAL:HG23	1.87	0.73
1:D:3447:VAL:HG13	5:D:3601:HEM:CBA	2.16	0.73
3:B:1661:NAG:O7	3:B:1661:NAG:H3	1.89	0.73
1:A:131:ASN:C	1:A:131:ASN:HD22	1.96	0.73
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3464:ASN:HD21	1:D:3475:TYR:H	1.36	0.73
1:A:465:GLU:HA	1:A:465:GLU:OE1	1.88	0.72
1:C:2526:GLY:HA3	6:C:2701:DIF:C10	2.19	0.72
1:C:2419:LEU:O	1:C:2423:VAL:HG23	1.89	0.72
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.24	0.72
1:D:3090:HIS:CE1	1:D:3094:THR:HG21	2.24	0.72
1:D:3034:ASN:HD22	1:D:3036:CYS:H	1.36	0.72
1:A:74:PHE:CZ	1:A:78:ILE:HD11	2.25	0.71
1:A:447:VAL:HG13	5:A:704:HEM:HBA1	1.71	0.71
1:C:2033:ALA:HB3	1:C:2158:ASP:OD2	1.90	0.71
1:B:1152:LEU:HD12	1:B:1466:TYR:CD1	2.25	0.71
1:C:2322:GLU:HG2	1:D:3051:GLY:O	1.89	0.71
1:C:2051:GLY:C	1:D:3322:GLU:HG2	2.14	0.71
1:B:1464:ASN:HD21	1:B:1475:TYR:H	1.39	0.70
1:A:241:GLN:NE2	1:A:245:ARG:HH11	1.90	0.70
1:A:202:ALA:O	1:A:206:THR:HG23	1.90	0.70
1:D:3241:GLN:NE2	1:D:3245:ARG:HH11	1.89	0.70
1:D:3444:VAL:HG13	1:D:3444:VAL:O	1.90	0.70
1:C:2444:VAL:O	1:C:2444:VAL:HG13	1.91	0.70
3:C:2661:NAG:O7	3:C:2661:NAG:H3	1.90	0.70
1:A:34:ASN:ND2	1:A:36:CYS:H	1.89	0.70
1:B:1419:LEU:O	1:B:1423:VAL:HG23	1.91	0.70
1:B:1444:VAL:O	1:B:1444:VAL:HG13	1.90	0.70
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.27	0.70
1:B:1075:LEU:HD11	1:B:1079:LYS:HE3	1.73	0.69
1:D:3198:PHE:CZ	1:D:3352:LEU:HD13	2.26	0.69
1:D:3252:LEU:HD22	1:D:3309:HIS:CD2	2.27	0.69
1:B:1105(B):ILE:CG2	1:B:1108:LEU:HB2	2.22	0.69
1:C:2198:PHE:CE1	1:C:2352:LEU:HD13	2.28	0.69
1:C:2241:GLN:NE2	1:C:2245:ARG:HH11	1.90	0.69
1:C:2427:THR:HG22	1:C:2583:GLN:HE22	1.57	0.69
1:A:163:MET:CE	1:A:171:LEU:HD21	2.23	0.69
1:C:2504:TYR:HB3	1:C:2505:PRO:HD3	1.75	0.69
1:D:3179:GLU:HG2	4:D:3703:BOG:H1'1	1.73	0.69
1:A:247:PHE:C	1:A:248:LYS:HG2	2.17	0.69
1:C:2137:LYS:HE2	1:D:3543:GLN:O	1.93	0.69
1:B:1039:ASN:N	1:B:1040:PRO:HD3	2.08	0.68
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.58	0.68
3:D:3661:NAG:O7	3:D:3661:NAG:H3	1.93	0.68
4:D:3703:BOG:O1	4:D:3703:BOG:C2	2.41	0.68
1:B:1198:PHE:CZ	1:B:1352:LEU:HD13	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE2	1:B:1543:GLN:O	1.93	0.68
1:B:1082:LEU:CD1	1:B:1082:LEU:N	2.57	0.68
1:C:2142:PHE:O	1:C:2376:ARG:NH2	2.27	0.68
1:C:2403:SER:OG	1:C:2406:GLN:HG3	1.93	0.68
1:A:403:SER:OG	1:A:406:GLN:HG3	1.93	0.67
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.75	0.67
1:D:3340:THR:O	1:D:3344:VAL:HG23	1.95	0.67
1:C:2034:ASN:ND2	1:C:2036:CYS:H	1.92	0.67
1:C:2034:ASN:C	1:C:2034:ASN:HD22	2.01	0.67
1:C:2293:GLY:HA2	1:C:2299:MET:HE3	1.75	0.67
1:B:1107:PHE:CD1	1:B:1107:PHE:C	2.72	0.67
1:C:2113:MET:HG3	1:C:2117:LEU:HD22	1.75	0.67
1:D:3504:TYR:HB3	1:D:3505:PRO:HD3	1.77	0.67
1:B:1082:LEU:N	1:B:1082:LEU:HD13	2.09	0.67
1:A:246:LEU:HG	1:A:248:LYS:HG3	1.76	0.66
1:A:468:LYS:HD2	1:A:474:PRO:HG3	1.76	0.66
1:B:1252:LEU:HD22	1:B:1309:HIS:CD2	2.30	0.66
3:C:2661:NAG:O7	3:C:2661:NAG:C3	2.44	0.66
1:D:3577:PHE:C	1:D:3577:PHE:CD2	2.73	0.66
1:D:3152:LEU:HD12	1:D:3466:TYR:CD1	2.31	0.66
1:C:2247:PHE:C	1:C:2248:LYS:HG2	2.19	0.66
1:C:2464:ASN:HD21	1:C:2475:TYR:H	1.44	0.66
1:B:1251:LYS:HG2	1:B:1310:ASN:CG	2.21	0.66
1:D:3362:ASP:OD1	1:D:3364:GLU:HG3	1.95	0.66
1:A:340:THR:O	1:A:344:VAL:HG23	1.95	0.66
1:C:2113:MET:O	1:C:2117:LEU:HD22	1.96	0.66
1:B:1230:LEU:HG	1:B:1337:ILE:HG12	1.77	0.66
1:A:541:SER:HB2	7:B:5184:HOH:O	1.96	0.66
1:D:3163:MET:HE2	1:D:3171:LEU:HD21	1.78	0.65
1:A:447:VAL:HG13	5:A:704:HEM:CBA	2.26	0.65
1:B:1403:SER:OG	1:B:1406:GLN:HG3	1.96	0.65
1:A:51:GLY:C	1:B:1322:GLU:HG2	2.21	0.65
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.31	0.65
1:B:1163:MET:HE2	1:B:1171:LEU:HD21	1.78	0.65
1:B:1574:GLY:O	1:B:1575:CYS:C	2.39	0.65
1:D:3163:MET:CE	1:D:3171:LEU:HD21	2.26	0.65
1:B:1293:GLY:HA2	1:B:1299:MET:HE3	1.77	0.65
1:C:2526:GLY:HA3	6:C:2701:DIF:H10	1.78	0.65
4:D:3703:BOG:C2	4:D:3703:BOG:O5	2.45	0.65
1:B:1113:MET:HA	1:B:1116:VAL:HG13	1.78	0.65
1:C:2130:TYR:HB3	1:C:2134:TYR:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.78	0.65
1:C:2050:THR:HG21	1:C:2056:LYS:HB3	1.77	0.65
1:D:3041:CYS:SG	1:D:3047:CYS:HB2	2.37	0.65
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.77	0.64
1:B:1142:PHE:O	1:B:1376:ARG:NH2	2.30	0.64
1:B:1230:LEU:HD13	1:B:1233:ILE:HD12	1.79	0.64
3:B:1661:NAG:O7	3:B:1661:NAG:C3	2.46	0.64
1:A:198:PHE:CE1	1:A:352:LEU:HD13	2.31	0.64
1:B:1090:HIS:CE1	1:B:1094:THR:HG21	2.33	0.64
1:B:1113:MET:HG3	1:B:1117:LEU:HD22	1.78	0.64
1:D:3050:THR:HG21	1:D:3056:LYS:HB3	1.79	0.64
1:C:2068:ASN:ND2	3:C:2661:NAG:H61	2.13	0.64
1:A:526:GLY:HA3	6:A:701:DIF:C10	2.28	0.64
1:B:1040:PRO:HA	3:B:1661:NAG:H83	1.79	0.64
1:B:1043:ASN:O	1:B:1044:ARG:HB2	1.97	0.64
1:D:3247:PHE:C	1:D:3248:LYS:HG2	2.22	0.64
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.80	0.64
1:D:3427:THR:CG2	1:D:3583:GLN:HE22	2.11	0.64
1:A:251:LYS:HG2	1:A:310:ASN:CG	2.23	0.63
1:B:1193:GLY:O	1:B:1582:VAL:HG23	1.98	0.63
1:C:2482:THR:HG22	1:C:2509:VAL:HG13	1.79	0.63
1:D:3482:THR:HG22	1:D:3509:VAL:HG13	1.81	0.63
1:C:2043:ASN:O	1:C:2044:ARG:HB2	1.98	0.63
1:C:2251:LYS:HG2	1:C:2310:ASN:CG	2.23	0.63
1:D:3468:LYS:HD2	1:D:3474:PRO:HG3	1.81	0.63
1:C:2105(C):ILE:HG22	1:C:2108:LEU:H	1.63	0.63
1:C:2113:MET:HG3	1:C:2117:LEU:CD2	2.29	0.63
1:C:2173:ASP:HB3	1:C:2176:GLU:HB2	1.80	0.63
1:A:521:THR:HG23	7:A:5160:HOH:O	1.97	0.63
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.81	0.63
1:B:1247:PHE:C	1:B:1248:LYS:HG2	2.24	0.63
1:C:2300:MET:HE3	1:C:2423:VAL:HG22	1.81	0.63
1:C:2075:LEU:HD11	1:C:2079:LYS:HE3	1.80	0.62
1:C:2118:THR:HG21	1:C:2369:GLN:HG2	1.81	0.62
1:D:3090:HIS:HE1	1:D:3094:THR:HG21	1.62	0.62
1:B:1198:PHE:CE1	1:B:1352:LEU:HD13	2.34	0.62
1:A:362:ASP:OD1	1:A:364:GLU:HG3	1.98	0.62
1:D:3198:PHE:CE1	1:D:3352:LEU:HD13	2.35	0.62
1:B:1034:ASN:HD22	1:B:1034:ASN:C	2.06	0.62
1:C:2230:LEU:HD13	1:C:2233:ILE:HD12	1.81	0.62
1:D:3043:ASN:O	1:D:3044:ARG:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HB3	1:A:271:VAL:HG12	1.82	0.62
1:D:3113:MET:HE3	1:D:3116:VAL:CG2	2.29	0.62
1:A:543:GLN:OE1	1:A:543:GLN:HA	1.99	0.62
1:C:2131:ASN:ND2	1:C:2134:TYR:H	1.97	0.62
1:B:1430:ILE:HD12	1:B:1582:VAL:HG21	1.80	0.62
1:B:1482:THR:HG22	1:B:1509:VAL:HG13	1.79	0.62
1:B:1577:PHE:HE2	1:B:1583:GLN:HE21	1.46	0.62
1:A:510:GLU:OE1	1:A:519:GLY:HA3	2.00	0.62
1:B:1130:TYR:HB3	1:B:1134:TYR:O	2.00	0.62
1:A:322:GLU:HG2	1:B:1051:GLY:O	2.00	0.61
1:A:385:TYR:OH	6:A:701:DIF:H132	2.00	0.61
1:A:464:ASN:HD21	1:A:475:TYR:H	1.46	0.61
1:C:2112:ILE:HB	1:C:2357:PHE:CZ	2.35	0.61
1:C:2243:LYS:HB3	1:C:2271:VAL:HG12	1.81	0.61
1:D:3344:VAL:O	1:D:3349:VAL:HG23	2.00	0.61
1:C:2362:ASP:OD1	1:C:2364:GLU:HG3	2.01	0.61
3:A:661:NAG:O7	3:A:661:NAG:H3	2.01	0.61
1:B:1050:THR:HG21	1:B:1056:LYS:HB3	1.83	0.61
1:C:2468:LYS:HD2	1:C:2474:PRO:HG3	1.82	0.61
1:B:1300:MET:HE3	1:B:1423:VAL:HG22	1.81	0.61
1:C:2094:THR:O	1:C:2356:HIS:CE1	2.54	0.61
1:D:3076:THR:O	1:D:3080:LEU:HG	2.00	0.60
1:B:1152:LEU:HD12	1:B:1466:TYR:CE1	2.36	0.60
1:B:1173:ASP:HB3	1:B:1176:GLU:HB2	1.83	0.60
1:B:1184:ARG:NH1	1:B:1441:PRO:HG3	2.16	0.60
1:A:261:VAL:O	1:A:307:ARG:NH1	2.33	0.60
1:C:2198:PHE:CZ	1:C:2352:LEU:CD1	2.84	0.60
2:E:3:NAG:O7	2:E:3:NAG:H3	2.01	0.60
1:B:1468:LYS:HD2	1:B:1474:PRO:HG3	1.82	0.60
1:D:3130:TYR:HB3	1:D:3134:TYR:O	2.01	0.60
1:C:2543:GLN:OE1	1:C:2543:GLN:HA	1.99	0.60
1:C:2550:PHE:CD1	1:C:2556:PHE:CD1	2.89	0.60
1:D:3173:ASP:HB3	1:D:3176:GLU:HB2	1.82	0.60
1:D:3510:GLU:OE1	1:D:3519:GLY:HA3	2.01	0.60
1:B:1137:LYS:HA	7:B:5175:HOH:O	2.01	0.60
1:D:3075:LEU:HA	1:D:3078:ILE:HD13	1.83	0.60
2:E:2:NAG:H4	2:E:3:NAG:N2	2.15	0.60
1:D:3226:HIS:CE1	1:D:3376:ARG:HD2	2.37	0.60
1:C:2040:PRO:HA	3:C:2661:NAG:H83	1.84	0.59
1:D:3342:LYS:HG2	1:D:3562:ALA:HB3	1.84	0.59
1:A:185:ARG:NH1	4:A:703:BOG:H4'1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:GLU:O	1:B:1077:ARG:HG3	2.02	0.59
1:A:129:THR:HG22	1:A:137:LYS:HD3	1.84	0.59
1:B:1362:ASP:OD1	1:B:1364:GLU:HG3	2.02	0.59
1:C:2129:THR:HG22	1:C:2137:LYS:HD3	1.83	0.59
1:D:3230:LEU:HD13	1:D:3233:ILE:HD12	1.85	0.59
1:D:3056:LYS:HG3	1:D:3057:CYS:N	2.17	0.59
1:B:1117:LEU:HD12	1:B:1531:LEU:HD22	1.85	0.59
1:B:1381:PHE:O	1:B:1384:LEU:HG	2.02	0.59
1:A:68:ASN:ND2	3:A:661:NAG:H61	2.16	0.59
1:B:1400:GLN:HG3	1:B:1402:TYR:OH	2.03	0.59
1:C:2261:VAL:O	1:C:2307:ARG:NH1	2.35	0.59
3:D:3661:NAG:O7	3:D:3661:NAG:C3	2.51	0.59
1:D:3075:LEU:CD2	1:D:3079:LYS:HE3	2.32	0.59
1:D:3577:PHE:HE2	1:D:3583:GLN:HE21	1.51	0.59
1:C:2545:TRP:O	1:D:3061:ARG:NH2	2.36	0.59
1:A:100:TRP:O	1:A:104:ASN:HB2	2.03	0.58
1:A:322:GLU:HG2	1:B:1051:GLY:C	2.27	0.58
1:B:1117:LEU:CD1	1:B:1531:LEU:HD22	2.32	0.58
1:A:300:MET:HE3	1:A:423:VAL:HG22	1.85	0.58
1:A:131:ASN:ND2	1:A:134:TYR:H	2.00	0.58
1:A:197:MET:SD	1:A:300:MET:HE1	2.43	0.58
1:D:3543:GLN:OE1	1:D:3543:GLN:HA	2.03	0.58
1:A:198:PHE:CZ	1:A:352:LEU:CD1	2.86	0.58
1:C:2091:TYR:O	1:C:2095:HIS:HD2	1.86	0.58
1:B:1113:MET:CE	1:B:1116:VAL:HG21	2.33	0.58
1:B:1190:ASP:OD1	1:B:1517:ILE:HB	2.03	0.58
1:C:2075:LEU:CG	1:C:2079:LYS:HE3	2.34	0.58
1:C:2097:LYS:O	1:C:2097:LYS:HG3	2.02	0.58
1:D:3293:GLY:HA2	1:D:3299:MET:HE3	1.84	0.58
1:D:3550:PHE:CD1	1:D:3556:PHE:CD1	2.92	0.58
1:B:1050:THR:HG21	1:B:1056:LYS:CB	2.34	0.57
1:B:1344:VAL:O	1:B:1349:VAL:HG23	2.03	0.57
1:C:2344:VAL:O	1:C:2349:VAL:HG23	2.04	0.57
1:D:3243:LYS:HB3	1:D:3271:VAL:HG12	1.85	0.57
1:A:90:HIS:CD2	1:A:513:ARG:HG2	2.40	0.57
1:C:2333:ARG:O	1:C:2337:ILE:HG13	2.04	0.57
1:B:1050:THR:CG2	1:B:1056:LYS:HB3	2.34	0.57
1:D:3050:THR:CG2	1:D:3056:LYS:HB3	2.34	0.57
1:B:1430:ILE:HD12	1:B:1582:VAL:CG2	2.35	0.57
1:D:3034:ASN:ND2	1:D:3036:CYS:H	2.03	0.57
2:G:2:NAG:H4	2:G:3:NAG:N2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1210:PHE:HB3	5:B:1601:HEM:HBD1	1.87	0.57
1:B:1510:GLU:OE1	1:B:1519:GLY:HA3	2.03	0.57
1:D:3333:ARG:O	1:D:3337:ILE:HG13	2.05	0.57
1:A:73:GLU:O	1:A:77:ARG:HG3	2.04	0.57
1:B:1112:ILE:HB	1:B:1357:PHE:CZ	2.40	0.57
1:D:3391:LEU:HD21	5:D:3601:HEM:HHC	1.85	0.57
1:C:2105(C):ILE:HG21	1:C:2108:LEU:HB2	1.82	0.57
1:A:75:LEU:HD11	1:A:79:LYS:HE3	1.86	0.57
1:D:3252:LEU:HD22	1:D:3309:HIS:CG	2.40	0.57
1:D:3400:GLN:HG3	1:D:3402:TYR:OH	2.04	0.57
1:C:2089:VAL:HG12	1:C:2093:LEU:CD2	2.35	0.57
1:D:3090:HIS:CD2	1:D:3513:ARG:HG2	2.39	0.57
1:D:3116:VAL:CG2	1:D:3117:LEU:N	2.68	0.57
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.87	0.56
1:C:2061:ARG:NH1	1:D:3542:PRO:O	2.35	0.56
1:D:3173:ASP:O	1:D:3177:VAL:HG23	2.05	0.56
1:D:3184:ARG:HB2	1:D:3439:ASN:CA	2.32	0.56
1:A:444:VAL:O	1:A:444:VAL:CG1	2.52	0.56
1:B:1226:HIS:CE1	1:B:1376:ARG:HD2	2.39	0.56
1:B:1243:LYS:HB3	1:B:1271:VAL:HG12	1.86	0.56
1:C:2245:ARG:HH22	1:C:2326:GLU:HG2	1.70	0.56
1:C:2381:PHE:O	1:C:2384:LEU:HG	2.06	0.56
1:C:2543:GLN:O	1:D:3137:LYS:HE2	2.06	0.56
1:D:3387:TRP:O	1:D:3390:LEU:HB2	2.05	0.56
2:H:3:NAG:O7	2:H:3:NAG:H3	2.05	0.56
1:C:2447:VAL:HG13	5:C:2601:HEM:CBA	2.32	0.56
1:D:3203:GLN:NE2	1:D:3298:LEU:HD13	2.21	0.56
1:B:1387:TRP:O	1:B:1390:LEU:HB2	2.06	0.56
1:D:3142:PHE:O	1:D:3376:ARG:NH2	2.38	0.56
1:B:1118:THR:HG21	1:B:1369:GLN:HG2	1.88	0.56
1:D:3381:PHE:O	1:D:3384:LEU:HG	2.05	0.56
1:D:3269:THR:O	1:D:3270:GLN:HB2	2.06	0.56
1:A:387:TRP:O	1:A:390:LEU:HB2	2.06	0.56
1:B:1094:THR:O	1:B:1356:HIS:CE1	2.58	0.56
1:B:1116:VAL:CG2	1:B:1117:LEU:N	2.68	0.56
1:D:3152:LEU:HD12	1:D:3466:TYR:CE1	2.41	0.56
1:B:1388:HIS:N	1:B:1389:PRO:CD	2.68	0.56
1:C:2230:LEU:HG	1:C:2337:ILE:HG12	1.88	0.55
1:C:2090:HIS:CE1	1:C:2094:THR:HG21	2.41	0.55
1:C:2400:GLN:HG3	1:C:2402:TYR:OH	2.06	0.55
1:D:3251:LYS:HG2	1:D:3310:ASN:CG	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105(A):ILE:HD13	1:A:108:LEU:HD12	1.88	0.55
1:B:1543:GLN:OE1	1:B:1543:GLN:HA	2.07	0.55
1:C:2039:ASN:N	1:C:2040:PRO:HD3	2.21	0.55
1:C:2184:ARG:HB2	1:C:2439:ASN:CA	2.32	0.55
1:A:82:LEU:CD1	1:A:82:LEU:N	2.68	0.55
1:D:3238:LEU:HD22	1:D:3242:HIS:CE1	2.42	0.55
1:C:2398:GLU:HG3	1:C:2421:GLN:OE1	2.07	0.55
1:A:427:THR:CG2	1:A:583:GLN:HE22	2.18	0.55
1:C:2074:PHE:O	1:C:2077:ARG:HG3	2.06	0.55
1:C:2152:LEU:HD12	1:C:2466:TYR:CD1	2.42	0.55
1:B:1105(B):ILE:CD1	1:B:1108:LEU:HD12	2.32	0.55
1:B:1526:GLY:HA3	6:B:1701:DIF:C10	2.36	0.55
1:D:3145:LEU:HD13	7:D:5194:HOH:O	2.06	0.55
1:A:39:ASN:N	1:A:40:PRO:HD3	2.22	0.55
1:D:3100:TRP:HA	1:D:3100:TRP:CE3	2.42	0.55
1:D:3273:MET:SD	1:D:3290:GLU:HA	2.47	0.55
1:A:535:MET:HB2	7:A:5241:HOH:O	2.05	0.54
1:B:1203:GLN:NE2	1:B:1298:LEU:HD13	2.21	0.54
1:B:1252:LEU:HD22	1:B:1309:HIS:CG	2.41	0.54
1:C:2338:GLY:HA3	1:C:2559:ILE:HD13	1.89	0.54
1:D:3198:PHE:CZ	1:D:3352:LEU:CD1	2.89	0.54
1:C:2075:LEU:CD1	1:C:2079:LYS:HE3	2.38	0.54
1:A:532:LYS:HD3	1:A:532:LYS:C	2.33	0.54
1:B:1198:PHE:CZ	1:B:1352:LEU:CD1	2.90	0.54
1:B:1564:ILE:O	1:B:1568:ILE:HD13	2.08	0.54
1:C:2090:HIS:HE1	1:C:2094:THR:HG21	1.73	0.54
1:C:2226:HIS:CE1	1:C:2376:ARG:HD2	2.42	0.54
1:A:543:GLN:O	1:B:1137:LYS:HE2	2.07	0.54
1:D:3269:THR:OG1	1:D:3271:VAL:HG13	2.07	0.54
1:B:1516:ALA:HB1	7:B:5157:HOH:O	2.07	0.54
1:A:542:PRO:O	1:B:1061:ARG:NH1	2.33	0.54
1:B:1082:LEU:HD13	1:B:1082:LEU:H	1.72	0.54
1:D:3527:ALA:HB3	1:D:3528:PRO:HD3	1.88	0.54
1:A:568:ILE:HD13	1:A:578:THR:HG21	1.90	0.54
1:B:1105(B):ILE:HG22	1:B:1108:LEU:H	1.72	0.54
1:D:3034:ASN:HB3	1:D:3037:CYS:SG	2.48	0.54
1:A:34:ASN:HD21	1:A:36:CYS:HB2	1.71	0.54
1:C:2388:HIS:N	1:C:2389:PRO:CD	2.71	0.54
1:D:3300:MET:HE3	1:D:3423:VAL:HG22	1.89	0.54
1:B:1391:LEU:HD21	5:B:1601:HEM:HHC	1.90	0.53
1:A:196:MET:CE	1:A:392:PRO:HD3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:LEU:HB3	1:B:1355:TYR:CD1	2.43	0.53
1:C:2510:GLU:OE1	1:C:2519:GLY:HA3	2.08	0.53
1:B:1129:THR:HG22	1:B:1137:LYS:HD3	1.90	0.53
1:A:173:ASP:HB3	1:A:176:GLU:HB2	1.90	0.53
1:B:1068:ASN:ND2	3:B:1661:NAG:H61	2.21	0.53
1:B:1131:ASN:ND2	1:B:1133:HIS:H	2.06	0.53
1:C:2034:ASN:HD22	1:C:2036:CYS:H	1.56	0.53
1:C:2077:ARG:O	1:C:2081:LEU:HD13	2.08	0.53
1:D:3261:VAL:O	1:D:3307:ARG:NH1	2.41	0.53
2:F:2:NAG:H4	2:F:3:NAG:N2	2.22	0.53
1:B:1131:ASN:ND2	1:B:1134:TYR:H	2.07	0.53
1:B:1342:LYS:HG2	1:B:1562:ALA:HB3	1.89	0.53
1:C:2384:LEU:C	1:C:2384:LEU:HD12	2.33	0.53
1:C:2113:MET:CA	1:C:2116:VAL:HG13	2.39	0.53
1:D:3131:ASN:ND2	1:D:3134:TYR:H	2.07	0.53
1:D:3185:ARG:NH1	4:D:3703:BOG:H4'1	2.23	0.53
1:D:3320:HIS:HA	1:D:3322:GLU:OE2	2.09	0.53
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.08	0.53
1:C:2091:TYR:O	1:C:2095:HIS:CD2	2.62	0.53
1:B:1067:GLU:OE1	3:B:1661:NAG:H61	2.09	0.53
1:C:2197:MET:SD	1:C:2300:MET:HE1	2.49	0.53
1:A:82:LEU:N	1:A:82:LEU:HD13	2.24	0.53
1:A:142:PHE:O	1:A:376:ARG:NH2	2.41	0.53
1:B:1553:GLU:OE1	1:B:1553:GLU:HA	2.09	0.53
1:C:2398:GLU:HG3	1:C:2421:GLN:CG	2.39	0.52
1:C:2444:VAL:O	1:C:2444:VAL:CG1	2.57	0.52
1:D:3039:ASN:N	1:D:3040:PRO:CD	2.72	0.52
1:A:176:GLU:O	1:A:180:LYS:HG3	2.08	0.52
1:A:196:MET:HE1	1:A:392:PRO:HD3	1.90	0.52
1:B:1484:GLU:CD	1:B:1487:MET:HE2	2.35	0.52
1:D:3190:ASP:OD1	1:D:3517:ILE:HB	2.09	0.52
1:A:344:VAL:O	1:A:349:VAL:HG23	2.09	0.52
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.44	0.52
1:A:384:LEU:C	1:A:384:LEU:HD12	2.34	0.52
1:C:2387:TRP:O	1:C:2390:LEU:HB2	2.09	0.52
1:B:1398:GLU:HG3	1:B:1421:GLN:OE1	2.06	0.52
1:C:2059:CYS:HB3	1:C:2064:PHE:O	2.10	0.52
1:A:241:GLN:O	1:A:245:ARG:HG3	2.10	0.52
1:A:398:GLU:HG3	1:A:421:GLN:CG	2.39	0.52
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.10	0.52
1:D:3444:VAL:O	1:D:3444:VAL:CG1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2090:HIS:CD2	1:C:2513:ARG:NH1	2.77	0.52
1:D:3034:ASN:O	1:D:3037:CYS:HB2	2.10	0.52
1:C:2102:ILE:HG22	1:C:2105(C):ILE:HD12	1.92	0.52
1:C:2128:PRO:HD3	7:C:5118:HOH:O	2.09	0.52
1:C:2131:ASN:ND2	1:C:2133:HIS:H	2.08	0.52
1:C:2380:GLU:HG2	1:C:2466:TYR:CE1	2.45	0.52
1:C:2550:PHE:CD1	1:C:2556:PHE:HD1	2.28	0.52
1:D:3075:LEU:HD21	1:D:3079:LYS:HE3	1.90	0.52
1:A:532:LYS:HD3	1:A:532:LYS:O	2.10	0.51
1:B:1340:THR:O	1:B:1344:VAL:HG23	2.10	0.51
1:C:2340:THR:O	1:C:2344:VAL:HG23	2.10	0.51
1:A:413:ILE:O	1:A:416:GLU:HB3	2.11	0.51
1:B:1184:ARG:HB2	1:B:1439:ASN:CA	2.32	0.51
1:B:1398:GLU:HG3	1:B:1421:GLN:CG	2.40	0.51
1:B:1444:VAL:O	1:B:1444:VAL:CG1	2.58	0.51
1:D:3526:GLY:HA3	6:D:3701:DIF:C10	2.39	0.51
1:D:3058:ASP:OD1	1:D:3060:THR:OG1	2.18	0.51
1:D:3532:LYS:HD3	1:D:3532:LYS:C	2.35	0.51
1:A:90:HIS:HD2	1:A:513:ARG:HG2	1.76	0.51
1:A:577:PHE:C	1:A:577:PHE:CD2	2.88	0.51
1:B:1238:LEU:HD22	1:B:1242:HIS:CE1	2.46	0.51
1:D:3241:GLN:HE21	1:D:3245:ARG:HD3	1.75	0.51
1:D:3550:PHE:CD1	1:D:3556:PHE:HD1	2.28	0.51
1:A:75:LEU:CG	1:A:79:LYS:HE3	2.41	0.51
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.11	0.51
1:A:131:ASN:C	1:A:131:ASN:ND2	2.67	0.51
1:A:112:ILE:O	1:A:115:TYR:HB3	2.10	0.51
1:C:2442:ILE:O	1:C:2445:GLN:HG2	2.11	0.51
1:D:3137:LYS:HA	7:D:5223:HOH:O	2.10	0.51
1:D:3511:LYS:HG3	7:D:5134:HOH:O	2.10	0.51
1:A:333:ARG:O	1:A:337:ILE:HG13	2.11	0.51
1:B:1532:LYS:HD3	1:B:1532:LYS:C	2.36	0.51
1:B:1550:PHE:CD1	1:B:1556:PHE:CD1	2.99	0.51
1:A:122:TYR:CZ	1:A:123:LEU:HD22	2.46	0.51
1:A:400:GLN:HG3	1:A:402:TYR:OH	2.11	0.51
1:C:2203:GLN:NE2	1:C:2298:LEU:HD13	2.26	0.51
1:A:464:ASN:HD22	1:A:467:ARG:HD3	1.76	0.50
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.92	0.50
1:B:1034:ASN:HD21	1:B:1036:CYS:HB2	1.74	0.50
1:B:1307:ARG:HB3	1:B:1571:ASN:OD1	2.10	0.50
1:B:1495:TYR:O	1:B:1496:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2433:ARG:HD3	7:C:5051:HOH:O	2.11	0.50
1:D:3197:MET:SD	1:D:3300:MET:HE1	2.50	0.50
1:A:269:THR:O	1:A:270:GLN:HB2	2.09	0.50
1:B:1382:ASN:O	1:B:1386:HIS:HD2	1.93	0.50
1:C:2391:LEU:HD21	5:C:2601:HEM:HHC	1.92	0.50
1:C:2532:LYS:HD3	1:C:2532:LYS:C	2.36	0.50
1:D:3241:GLN:O	1:D:3245:ARG:HG3	2.11	0.50
1:C:2320:HIS:HA	1:C:2322:GLU:OE2	2.11	0.50
1:D:3113:MET:C	1:D:3116:VAL:HG22	2.35	0.50
1:A:382:ASN:O	1:A:386:HIS:HD2	1.95	0.50
2:G:3:NAG:O7	2:G:3:NAG:H3	2.11	0.50
1:A:417:HIS:HB3	1:A:421:GLN:HG2	1.94	0.50
1:B:1181:VAL:CG1	1:B:1487:MET:HG2	2.35	0.50
1:C:2382:ASN:O	1:C:2386:HIS:HD2	1.94	0.50
1:D:3388:HIS:N	1:D:3389:PRO:CD	2.75	0.50
1:A:398:GLU:HG3	1:A:421:GLN:OE1	2.12	0.50
1:C:2500:VAL:HG12	1:C:2500:VAL:O	2.12	0.50
1:D:3116:VAL:HG23	1:D:3117:LEU:N	2.25	0.50
1:B:1241:GLN:HE21	1:B:1245:ARG:HH11	1.60	0.50
1:D:3126:SER:HA	1:D:3127:PRO:C	2.36	0.50
1:A:118:THR:HG21	1:A:369:GLN:HG2	1.94	0.50
1:B:1067:GLU:OE1	3:B:1661:NAG:C6	2.59	0.50
1:B:1338:GLY:HA3	1:B:1559:ILE:HD13	1.94	0.50
1:B:1495:TYR:O	1:B:1496:SER:CB	2.59	0.50
1:C:2550:PHE:CE1	1:C:2556:PHE:CE1	3.00	0.50
1:D:3118:THR:HG21	1:D:3369:GLN:HG2	1.94	0.50
1:D:3495:TYR:O	1:D:3496:SER:HB2	2.12	0.50
1:D:3532:LYS:HD3	1:D:3532:LYS:O	2.11	0.50
1:A:105(A):ILE:HG21	1:A:108:LEU:HB2	1.89	0.50
1:A:543:GLN:HB2	7:B:5259:HOH:O	2.11	0.50
1:B:1116:VAL:HG22	1:B:1117:LEU:N	2.27	0.50
1:B:1163:MET:HE3	1:B:1171:LEU:HD21	1.89	0.49
1:C:2034:ASN:ND2	1:C:2034:ASN:C	2.69	0.49
1:C:2269:THR:O	1:C:2270:GLN:HB2	2.11	0.49
1:D:3033:ALA:O	1:D:3035:PRO:HD3	2.12	0.49
1:A:388:HIS:N	1:A:389:PRO:CD	2.74	0.49
1:B:1308:GLU:OE1	1:B:1311:ARG:NH1	2.44	0.49
1:D:3091:TYR:CD1	1:D:3095:HIS:CD2	3.00	0.49
1:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.94	0.49
1:D:3464:ASN:ND2	1:D:3475:TYR:H	2.09	0.49
1:B:1273:MET:SD	1:B:1290:GLU:HA	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1320:HIS:HA	1:B:1322:GLU:OE2	2.12	0.49
1:B:1532:LYS:HD3	1:B:1532:LYS:O	2.12	0.49
1:D:3577:PHE:HE2	1:D:3583:GLN:NE2	2.09	0.49
1:C:2061:ARG:NH2	1:D:3545:TRP:O	2.43	0.49
1:C:2082:LEU:N	1:C:2082:LEU:CD1	2.75	0.49
1:C:2113:MET:HA	1:C:2116:VAL:CG1	2.41	0.49
1:C:2252:LEU:HD22	1:C:2309:HIS:CD2	2.47	0.49
1:D:3082:LEU:N	1:D:3082:LEU:CD1	2.75	0.49
1:D:3398:GLU:HG3	1:D:3421:GLN:OE1	2.12	0.49
1:A:34:ASN:ND2	1:A:36:CYS:HB2	2.27	0.49
1:A:68:ASN:ND2	3:A:661:NAG:C6	2.75	0.49
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.36	0.49
1:B:1114:LYS:HE2	1:B:1365:LEU:O	2.13	0.49
1:B:1112:ILE:O	1:B:1116:VAL:HG13	2.12	0.49
1:B:1246:LEU:O	1:B:1247:PHE:HB2	2.11	0.49
1:B:1269:THR:O	1:B:1270:GLN:HB2	2.12	0.49
1:C:2088:THR:O	1:C:2091:TYR:HB3	2.13	0.49
1:D:3131:ASN:ND2	1:D:3133:HIS:H	2.11	0.49
1:D:3495:TYR:O	1:D:3496:SER:CB	2.60	0.49
1:A:550:PHE:CD1	1:A:556:PHE:CD1	3.00	0.49
1:B:1033:ALA:HB3	1:B:1158:ASP:OD2	2.12	0.49
1:B:1113:MET:HE3	1:B:1116:VAL:HG22	1.89	0.49
1:B:1261:VAL:O	1:B:1307:ARG:NH1	2.43	0.49
1:C:2056:LYS:HG3	1:C:2057:CYS:N	2.27	0.49
1:D:3034:ASN:HD22	1:D:3034:ASN:C	2.21	0.49
1:D:3246:LEU:O	1:D:3247:PHE:HB2	2.12	0.49
1:D:3417:HIS:HB3	1:D:3421:GLN:HG2	1.95	0.49
1:D:3442:ILE:HD11	4:D:3703:BOG:H5'1	1.95	0.49
1:A:122:TYR:CD1	1:A:122:TYR:C	2.90	0.49
1:B:1108:LEU:O	1:B:1112:ILE:HG12	2.13	0.49
1:C:2060:THR:HG21	1:D:3546:LYS:HB3	1.95	0.49
1:A:131:ASN:HD22	1:A:134:TYR:H	1.60	0.49
1:D:3553:GLU:OE1	1:D:3553:GLU:HA	2.12	0.49
1:A:468:LYS:HD2	1:A:474:PRO:CG	2.41	0.49
1:A:525:LEU:O	1:A:528:PRO:HD2	2.13	0.49
1:B:1583:GLN:CD	1:B:1583:GLN:H	2.21	0.49
1:A:338:GLY:HA3	1:A:559:ILE:HD13	1.95	0.48
2:H:2:NAG:H4	2:H:3:NAG:N2	2.28	0.48
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.48	0.48
1:B:1068:ASN:O	1:B:1069:CYS:HB2	2.13	0.48
1:B:1298:LEU:HD13	7:B:5268:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1414:LEU:HD11	1:B:1419:LEU:HD22	1.95	0.48
1:C:2067:GLU:OE1	3:C:2661:NAG:H61	2.12	0.48
1:C:2484:GLU:OE2	1:C:2487:MET:HE2	2.13	0.48
1:D:3181:VAL:HG21	1:D:3491:LEU:HD21	1.94	0.48
1:A:48:MET:HE3	1:A:50:THR:HG22	1.94	0.48
1:A:545:TRP:O	1:B:1061:ARG:NH2	2.41	0.48
1:B:1468:LYS:HD2	1:B:1474:PRO:CG	2.44	0.48
1:B:1564:ILE:HD12	1:B:1567:LEU:HD23	1.96	0.48
1:C:2413:ILE:O	1:C:2416:GLU:HB3	2.13	0.48
1:A:75:LEU:CD1	1:A:79:LYS:HE3	2.43	0.48
1:A:433:ARG:NH2	1:A:516:ALA:O	2.45	0.48
1:B:1122:TYR:CD1	1:B:1122:TYR:C	2.91	0.48
1:D:3131:ASN:C	1:D:3131:ASN:ND2	2.65	0.48
1:D:3338:GLY:HA3	1:D:3559:ILE:HD13	1.96	0.48
1:D:3413:ILE:O	1:D:3416:GLU:HB3	2.13	0.48
1:B:1417:HIS:HB3	1:B:1421:GLN:HG2	1.95	0.48
1:C:2246:LEU:O	1:C:2247:PHE:HB2	2.13	0.48
1:C:2308:GLU:OE1	1:C:2311:ARG:NH1	2.47	0.48
1:C:2417:HIS:HB3	1:C:2421:GLN:HG2	1.94	0.48
1:B:1070:THR:O	1:B:1072:PRO:HD3	2.14	0.48
1:C:2190:ASP:OD1	1:C:2517:ILE:HB	2.13	0.48
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.47	0.48
1:B:1034:ASN:O	1:B:1037:CYS:HB2	2.14	0.48
1:B:1064:PHE:CD1	1:B:1064:PHE:N	2.81	0.48
1:C:2484:GLU:CD	1:C:2487:MET:HE2	2.39	0.48
1:D:3532:LYS:HE3	7:D:5260:HOH:O	2.14	0.48
1:B:1173:ASP:O	1:B:1177:VAL:HG23	2.14	0.48
1:A:387:TRP:C	1:A:389:PRO:HD2	2.39	0.48
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.96	0.48
1:C:2193:GLY:O	1:C:2582:VAL:HG23	2.14	0.48
1:C:2238:LEU:HD22	1:C:2242:HIS:CE1	2.49	0.48
1:A:238:LEU:HD22	1:A:242:HIS:CE1	2.49	0.47
1:A:423:VAL:HG11	1:A:568:ILE:HG21	1.96	0.47
1:C:2430:ILE:HG13	1:C:2431:ALA:N	2.29	0.47
1:B:1126:SER:HA	1:B:1127:PRO:C	2.39	0.47
1:B:1333:ARG:O	1:B:1337:ILE:HG13	2.14	0.47
1:C:2252:LEU:HD22	1:C:2309:HIS:CG	2.49	0.47
1:A:190:ASP:OD2	1:A:192:GLN:HB2	2.14	0.47
1:D:3100:TRP:CD1	1:D:3356:HIS:HB2	2.49	0.47
1:A:566:SER:O	1:A:570:ASN:ND2	2.48	0.47
1:B:1197:MET:SD	1:B:1300:MET:HE1	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:THR:HG21	1:B:1385:TYR:CD2	2.49	0.47
1:B:1427:THR:CG2	1:B:1583:GLN:HE22	2.21	0.47
1:D:3382:ASN:O	1:D:3386:HIS:HD2	1.97	0.47
1:D:3583:GLN:CD	1:D:3583:GLN:H	2.21	0.47
1:B:1241:GLN:HE21	1:B:1245:ARG:CD	2.28	0.47
1:A:131:ASN:ND2	1:A:134:TYR:N	2.62	0.47
1:C:2126:SER:HA	1:C:2127:PRO:C	2.39	0.47
1:C:2322:GLU:CG	1:D:3051:GLY:C	2.82	0.47
1:D:3043:ASN:O	1:D:3044:ARG:CB	2.63	0.47
1:D:3075:LEU:CD1	1:D:3079:LYS:HE3	2.45	0.47
1:D:3156:ALA:HB3	1:D:3159:CYS:SG	2.55	0.47
1:D:3176:GLU:O	1:D:3180:LYS:HG3	2.13	0.47
1:D:3184:ARG:NH1	1:D:3441:PRO:HG3	2.28	0.47
1:A:43:ASN:O	1:A:44:ARG:HB2	2.14	0.47
1:B:1294:LEU:CD2	1:B:1409:TYR:CD2	2.80	0.47
1:C:2102:ILE:O	1:C:2103:VAL:C	2.58	0.47
1:C:2108:LEU:HD23	1:C:2108:LEU:HA	1.63	0.47
1:C:2122:TYR:CZ	1:C:2123:LEU:HD22	2.49	0.47
1:D:3468:LYS:HD2	1:D:3474:PRO:CG	2.45	0.47
1:A:33:ALA:C	1:A:34:ASN:C	2.82	0.47
1:A:526:GLY:HA3	6:A:701:DIF:H10	1.97	0.47
1:B:1190:ASP:OD2	1:B:1192:GLN:HB2	2.14	0.47
1:A:126:SER:HA	1:A:127:PRO:C	2.39	0.47
1:B:1202:ALA:HB2	1:B:1348:TYR:CE1	2.49	0.47
1:C:2436:GLY:HA3	7:C:5051:HOH:O	2.15	0.47
1:D:3550:PHE:CE1	1:D:3556:PHE:CE1	3.03	0.47
1:B:1241:GLN:HE21	1:B:1245:ARG:HD3	1.79	0.46
1:C:2050:THR:CG2	1:C:2056:LYS:HB3	2.43	0.46
1:A:500:VAL:O	1:A:500:VAL:HG12	2.15	0.46
1:C:2124:ILE:HG21	1:C:2532:LYS:HG3	1.97	0.46
1:B:1298:LEU:HD12	1:B:1298:LEU:HA	1.78	0.46
1:B:1525:LEU:N	1:B:1525:LEU:HD23	2.30	0.46
1:D:3040:PRO:HA	3:D:3661:NAG:H83	1.96	0.46
1:D:3068:ASN:ND2	3:D:3661:NAG:H61	2.31	0.46
1:A:401:GLU:HG3	7:A:5314:HOH:O	2.15	0.46
1:B:1089:VAL:HG12	1:B:1093:LEU:CD2	2.45	0.46
1:B:1202:ALA:CB	1:B:1348:TYR:OH	2.63	0.46
1:C:2093:LEU:HB3	1:C:2355:TYR:CD1	2.50	0.46
1:C:2525:LEU:O	1:C:2528:PRO:HD2	2.16	0.46
1:D:3129:THR:HG22	1:D:3137:LYS:HD3	1.97	0.46
2:E:2:NAG:H4	2:E:3:NAG:HN2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:O	1:A:95:HIS:HD2	1.98	0.46
1:A:113:MET:HA	1:A:116:VAL:HG13	1.97	0.46
1:C:2073:GLU:O	1:C:2076:THR:HB	2.16	0.46
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.56	0.46
1:B:1184:ARG:HH12	1:B:1441:PRO:HG3	1.81	0.46
1:C:2202:ALA:CB	1:C:2348:TYR:OH	2.63	0.46
1:D:3211:LYS:HE2	1:D:3223:GLY:CA	2.46	0.46
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.77	0.46
1:A:252:LEU:HD22	1:A:309:HIS:CG	2.50	0.46
1:A:428:ARG:HG3	7:A:5286:HOH:O	2.15	0.46
1:C:2577:PHE:C	1:C:2577:PHE:CD2	2.93	0.46
1:A:320:HIS:HA	1:A:322:GLU:OE2	2.15	0.46
1:B:1075:LEU:HD11	1:B:1079:LYS:CE	2.44	0.46
1:C:2090:HIS:HD2	1:C:2513:ARG:NH1	2.13	0.46
1:C:2387:TRP:HB2	5:C:2601:HEM:HAC	1.98	0.46
1:C:2464:ASN:HD22	1:C:2467:ARG:HD3	1.81	0.46
1:C:2532:LYS:HD3	1:C:2532:LYS:O	2.15	0.46
1:D:3185:ARG:HH11	4:D:3703:BOG:H4'1	1.81	0.46
1:D:3442:ILE:O	1:D:3445:GLN:HG2	2.15	0.46
1:D:3500:VAL:O	1:D:3500:VAL:HG12	2.16	0.46
1:A:75:LEU:HG	1:A:79:LYS:HE3	1.98	0.46
1:A:77:ARG:O	1:A:81:LEU:HD13	2.16	0.46
1:D:3093:LEU:HB3	1:D:3355:TYR:CD1	2.50	0.46
1:D:3241:GLN:HE21	1:D:3245:ARG:CD	2.29	0.46
1:D:3280:PRO:HG2	1:D:3283:LEU:HB2	1.97	0.46
1:D:3308:GLU:OE1	1:D:3311:ARG:NH1	2.49	0.46
1:A:34:ASN:HD22	1:A:34:ASN:C	2.23	0.46
1:A:118:THR:CG2	1:A:369:GLN:HG2	2.46	0.46
1:B:1550:PHE:O	1:B:1555:GLY:HA3	2.16	0.46
1:D:3073:GLU:O	1:D:3076:THR:HB	2.15	0.46
1:D:3550:PHE:O	1:D:3555:GLY:HA3	2.16	0.46
1:A:142:PHE:C	1:A:142:PHE:CD2	2.90	0.45
1:C:2066:GLY:O	1:C:2067:GLU:C	2.56	0.45
1:C:2468:LYS:HD2	1:C:2474:PRO:CG	2.46	0.45
1:D:3122:TYR:CD1	1:D:3122:TYR:C	2.94	0.45
1:D:3435:ALA:O	1:D:3510:GLU:O	2.33	0.45
1:A:64:PHE:CB	1:A:69:CYS:O	2.64	0.45
1:A:442:ILE:HG23	4:A:703:BOG:H61	1.98	0.45
1:B:1447:VAL:HG13	5:B:1601:HEM:CBA	2.37	0.45
1:D:3202:ALA:HB2	1:D:3348:TYR:CE1	2.52	0.45
1:B:1074:PHE:O	1:B:1077:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1419:LEU:HB2	7:B:5247:HOH:O	2.16	0.45
1:B:1454:GLN:O	1:B:1458:MET:HG3	2.15	0.45
1:C:2527:ALA:HB3	1:C:2528:PRO:HD3	1.96	0.45
1:A:173:ASP:O	1:A:177:VAL:HG23	2.16	0.45
1:B:1105(B):ILE:HG22	1:B:1108:LEU:HB2	1.94	0.45
1:B:1442:ILE:O	1:B:1445:GLN:HG2	2.15	0.45
1:C:2068:ASN:ND2	3:C:2661:NAG:C6	2.79	0.45
1:C:2202:ALA:HB2	1:C:2348:TYR:CE1	2.52	0.45
1:C:2433:ARG:NH2	1:C:2516:ALA:O	2.49	0.45
1:D:3113:MET:CE	1:D:3116:VAL:HG21	2.44	0.45
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.98	0.45
1:C:2122:TYR:CD1	1:C:2122:TYR:C	2.94	0.45
1:C:2232:HIS:CE1	7:C:5038:HOH:O	2.69	0.45
1:D:3094:THR:O	1:D:3356:HIS:CE1	2.70	0.45
1:D:3132:VAL:HG13	1:D:3133:HIS:CD2	2.51	0.45
1:D:3387:TRP:C	1:D:3389:PRO:HD2	2.41	0.45
1:D:3501:MET:HE3	1:D:3506:ALA:HB2	1.98	0.45
1:B:1196:MET:HG2	1:B:1429:GLN:HG2	1.98	0.45
1:B:1413:ILE:O	1:B:1416:GLU:HB3	2.17	0.45
1:C:2197:MET:O	1:C:2201:PHE:HB2	2.17	0.45
1:B:1444:VAL:HG22	1:B:1447:VAL:HG21	1.98	0.45
1:C:2142:PHE:CD2	1:C:2142:PHE:C	2.94	0.45
1:D:3064:PHE:N	1:D:3064:PHE:CD1	2.85	0.45
1:D:3267:LYS:O	1:D:3267:LYS:HG3	2.17	0.45
1:C:2075:LEU:HG	1:C:2079:LYS:HE3	1.98	0.45
1:C:2198:PHE:HZ	1:C:2352:LEU:CD1	2.28	0.45
1:D:3241:GLN:HE21	1:D:3245:ARG:HH11	1.64	0.45
1:A:294:LEU:CD2	1:A:409:TYR:CD2	2.71	0.45
1:A:391:LEU:HD21	5:A:704:HEM:HHC	1.99	0.45
1:A:553:GLU:HA	1:A:553:GLU:OE1	2.17	0.45
1:B:1131:ASN:C	1:B:1131:ASN:ND2	2.63	0.45
1:B:1501:MET:HE3	1:B:1506:ALA:HB2	1.98	0.45
1:C:2067:GLU:OE1	3:C:2661:NAG:C6	2.64	0.45
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.82	0.45
1:A:252:LEU:HD22	1:A:309:HIS:CD2	2.51	0.45
1:A:381:PHE:O	1:A:384:LEU:HG	2.16	0.45
1:A:542:PRO:HD2	7:B:5184:HOH:O	2.16	0.45
1:B:1066:GLY:O	1:B:1067:GLU:C	2.60	0.45
1:B:1142:PHE:CD2	1:B:1142:PHE:C	2.91	0.45
1:C:2387:TRP:C	1:C:2389:PRO:HD2	2.42	0.45
1:D:3091:TYR:CE1	1:D:3095:HIS:CD2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:LEU:N	1:B:1408:LEU:HD23	2.32	0.44
1:C:2574:GLY:O	1:C:2575:CYS:C	2.59	0.44
1:A:65:TYR:O	1:A:71:THR:HB	2.17	0.44
1:A:197:MET:O	1:A:201:PHE:HB2	2.16	0.44
1:B:1075:LEU:HD21	1:B:1079:LYS:HE3	2.00	0.44
1:D:3433:ARG:NH2	1:D:3516:ALA:O	2.50	0.44
1:C:2181:VAL:CG1	1:C:2487:MET:HG2	2.39	0.44
1:C:2273:MET:SD	1:C:2290:GLU:HA	2.58	0.44
1:C:2315:ILE:O	1:C:2318:GLN:HB3	2.17	0.44
1:B:1114:LYS:O	1:B:1118:THR:OG1	2.34	0.44
1:C:2090:HIS:HD2	1:C:2513:ARG:CZ	2.30	0.44
1:C:2553:GLU:OE1	1:C:2553:GLU:HA	2.17	0.44
1:D:3415:LEU:HD23	1:D:3415:LEU:HA	1.83	0.44
1:A:246:LEU:O	1:A:247:PHE:HB2	2.18	0.44
1:C:2046:GLU:O	1:C:2057:CYS:HA	2.16	0.44
1:A:102:ILE:HG22	1:A:105(A):ILE:CD1	2.47	0.44
1:B:1156:ALA:HB3	1:B:1159:CYS:SG	2.57	0.44
1:C:2118:THR:CG2	1:C:2369:GLN:HG2	2.46	0.44
1:D:3089:VAL:O	1:D:3090:HIS:C	2.60	0.44
1:B:1280:PRO:HG2	1:B:1283:LEU:HB2	1.99	0.44
1:C:2211:LYS:HE2	1:C:2223:GLY:CA	2.48	0.44
1:C:2477:SER:HB2	7:C:5245:HOH:O	2.18	0.44
1:D:3048:MET:HE3	1:D:3050:THR:HG22	2.00	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.51	0.44
1:C:2525:LEU:N	1:C:2525:LEU:HD23	2.33	0.44
1:D:3122:TYR:CZ	1:D:3123:LEU:HD22	2.52	0.44
1:D:3203:GLN:HB2	5:D:3601:HEM:HMC3	2.00	0.44
1:B:1464:ASN:HD22	1:B:1467:ARG:HD3	1.82	0.44
6:B:1701:DIF:CL2	6:B:1701:DIF:C9	3.03	0.44
1:C:2076:THR:O	1:C:2080:LEU:HG	2.17	0.44
1:C:2385:TYR:CE1	6:C:2701:DIF:H12	2.53	0.44
1:D:3172:PRO:CG	1:D:3495:TYR:CE2	3.01	0.44
1:D:3211:LYS:HZ1	1:D:3236:GLU:HG3	1.83	0.44
1:D:3454:GLN:O	1:D:3458:MET:HG3	2.18	0.44
1:A:198:PHE:HZ	1:A:352:LEU:CD1	2.29	0.43
1:A:211:LYS:HE2	1:A:223:GLY:CA	2.48	0.43
1:A:500:VAL:O	1:A:500:VAL:CG1	2.66	0.43
1:C:2033:ALA:O	1:C:2035:PRO:HD3	2.18	0.43
1:C:2180:LYS:HD3	1:C:2490:GLU:OE1	2.18	0.43
1:D:3202:ALA:HB2	1:D:3348:TYR:HE1	1.83	0.43
1:C:2196:MET:CE	1:C:2392:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2435:ALA:O	1:C:2510:GLU:O	2.36	0.43
1:D:3196:MET:CE	1:D:3392:PRO:HD3	2.48	0.43
1:A:400:GLN:HB2	1:A:402:TYR:CE2	2.53	0.43
1:A:464:ASN:ND2	1:A:467:ARG:HD3	2.33	0.43
1:B:1283:LEU:HD23	1:B:1283:LEU:HA	1.88	0.43
1:C:2112:ILE:O	1:C:2116:VAL:HG13	2.18	0.43
1:C:2400:GLN:HB2	1:C:2402:TYR:CE2	2.52	0.43
1:D:3190:ASP:OD2	1:D:3192:GLN:HB2	2.18	0.43
1:B:1203:GLN:HB2	5:B:1601:HEM:CMC	2.49	0.43
1:B:1450:ALA:O	1:B:1451:SER:C	2.58	0.43
1:C:2131:ASN:HD22	1:C:2134:TYR:H	1.64	0.43
1:C:2255:GLN:NE2	1:C:2263:PRO:O	2.42	0.43
1:C:2398:GLU:HB3	1:C:2399:ASP:H	1.44	0.43
1:A:430:ILE:HG13	1:A:431:ALA:N	2.34	0.43
1:A:435:ALA:O	1:A:510:GLU:O	2.36	0.43
1:A:444:VAL:HG22	1:A:447:VAL:HG21	1.99	0.43
1:B:1387:TRP:C	1:B:1389:PRO:HD2	2.43	0.43
1:B:1400:GLN:HB2	1:B:1402:TYR:CE2	2.54	0.43
1:B:1464:ASN:HD22	1:B:1464:ASN:HA	1.58	0.43
1:C:2152:LEU:HD12	1:C:2466:TYR:CE1	2.53	0.43
1:A:185:ARG:HD3	4:A:703:BOG:H5'2	2.00	0.43
1:A:280:PRO:HG2	1:A:283:LEU:HB2	2.00	0.43
1:B:1245:ARG:HH22	1:B:1326:GLU:HG2	1.83	0.43
1:C:2082:LEU:N	1:C:2082:LEU:HD13	2.33	0.43
1:D:3206:THR:CG2	1:D:3385:TYR:CE2	2.97	0.43
1:A:280:PRO:HG2	1:A:283:LEU:HD12	2.00	0.43
1:A:495:TYR:O	1:A:496:SER:CB	2.67	0.43
1:B:1398:GLU:HB3	1:B:1399:ASP:H	1.46	0.43
1:C:2172:PRO:CG	1:C:2495:TYR:CE2	3.01	0.43
1:D:3090:HIS:HD2	1:D:3513:ARG:HG2	1.80	0.43
1:D:3444:VAL:HG22	1:D:3447:VAL:HG21	2.00	0.43
1:A:91:TYR:CE1	1:A:95:HIS:CD2	3.07	0.43
1:A:132:VAL:HG13	1:A:133:HIS:CD2	2.54	0.43
1:A:273:MET:SD	1:A:290:GLU:HA	2.58	0.43
1:A:564:ILE:HG22	7:A:5064:HOH:O	2.18	0.43
1:B:1181:VAL:HG21	1:B:1491:LEU:HD21	2.00	0.43
1:B:1435:ALA:O	1:B:1510:GLU:O	2.36	0.43
1:C:2034:ASN:HA	1:C:2035:PRO:HD2	1.89	0.43
1:C:2181:VAL:HG21	1:C:2491:LEU:HD21	2.00	0.43
1:D:3390:LEU:HB2	7:D:5235:HOH:O	2.18	0.43
1:D:3492:LYS:O	1:D:3492:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105(A):ILE:CB	1:A:108:LEU:HB2	2.47	0.43
1:A:131:ASN:ND2	1:A:133:HIS:H	2.16	0.43
1:A:276:PRO:HG2	1:A:279:ILE:HG12	2.01	0.43
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.43
1:B:1047:CYS:HB2	7:B:5007:HOH:O	2.19	0.43
1:B:1113:MET:HE1	1:B:1359:LEU:HD22	2.00	0.43
1:C:2131:ASN:ND2	1:C:2134:TYR:N	2.64	0.43
1:C:2415:LEU:HD23	1:C:2415:LEU:HA	1.82	0.43
1:C:2500:VAL:O	1:C:2500:VAL:CG1	2.66	0.43
1:D:3112:ILE:O	1:D:3115:TYR:N	2.52	0.43
1:D:3113:MET:HG3	1:D:3117:LEU:HD22	2.00	0.43
1:D:3198:PHE:HZ	1:D:3352:LEU:CD1	2.31	0.43
1:C:2039:ASN:N	1:C:2040:PRO:CD	2.81	0.43
1:C:2495:TYR:O	1:C:2496:SER:HB2	2.19	0.43
1:D:3464:ASN:HD22	1:D:3467:ARG:HD3	1.84	0.43
4:D:3703:BOG:O1	4:D:3703:BOG:O5	2.36	0.43
1:B:1090:HIS:HE1	1:B:1094:THR:HG21	1.81	0.42
1:B:1241:GLN:O	1:B:1245:ARG:HG3	2.19	0.42
1:C:2202:ALA:HB2	1:C:2348:TYR:HE1	1.84	0.42
1:C:2414:LEU:HD11	1:C:2419:LEU:HD22	2.01	0.42
1:D:3238:LEU:HD23	1:D:3238:LEU:HA	1.85	0.42
1:D:3537:ASN:CG	1:D:3538:PRO:HD2	2.44	0.42
2:H:1:NAG:H61	2:H:2:NAG:O7	2.18	0.42
1:A:91:TYR:CD1	1:A:95:HIS:CD2	3.07	0.42
1:A:565:GLN:O	1:A:569:CYS:HB2	2.19	0.42
1:B:1079:LYS:O	1:B:1083:LYS:HB2	2.19	0.42
1:B:1430:ILE:HG13	1:B:1431:ALA:N	2.34	0.42
1:D:3050:THR:HG21	1:D:3056:LYS:CB	2.48	0.42
1:A:77:ARG:HG3	1:A:77:ARG:H	1.62	0.42
1:B:1320:HIS:HB3	1:B:1323:TRP:CG	2.55	0.42
1:B:1484:GLU:OE2	1:B:1487:MET:HE2	2.19	0.42
1:C:2105(C):ILE:CG2	1:C:2108:LEU:CB	2.77	0.42
1:C:2509:VAL:HG13	1:C:2509:VAL:O	2.19	0.42
1:D:3384:LEU:C	1:D:3384:LEU:HD12	2.44	0.42
1:D:3398:GLU:HG3	1:D:3421:GLN:CG	2.47	0.42
1:A:105(A):ILE:O	1:A:108:LEU:N	2.51	0.42
1:A:398:GLU:CG	1:A:421:GLN:CD	2.78	0.42
1:C:2450:ALA:O	1:C:2451:SER:C	2.62	0.42
1:A:105(A):ILE:O	1:A:106:PRO:C	2.63	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE2	1.98	0.42
1:B:1248:LYS:O	1:B:1249:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:HB2	1:A:69:CYS:O	2.20	0.42
1:A:132:VAL:HB	7:A:5078:HOH:O	2.20	0.42
1:A:525:LEU:N	1:A:525:LEU:HD23	2.34	0.42
1:B:1176:GLU:O	1:B:1180:LYS:HG3	2.20	0.42
1:C:2316:LEU:HD23	1:C:2316:LEU:HA	1.91	0.42
1:D:3298:LEU:HD12	1:D:3298:LEU:HA	1.74	0.42
1:A:61:ARG:NH2	1:B:1545:TRP:O	2.46	0.42
1:A:408:LEU:N	1:A:408:LEU:HD23	2.34	0.42
1:B:1078:ILE:HD12	1:B:1078:ILE:N	2.35	0.42
1:B:1197:MET:O	1:B:1201:PHE:HB2	2.19	0.42
1:C:2454:GLN:HE21	1:C:2454:GLN:HB2	1.64	0.42
1:A:95:HIS:O	1:A:100:TRP:CD1	2.73	0.42
1:A:181:VAL:HG21	1:A:491:LEU:HD21	2.00	0.42
1:A:312:VAL:HA	1:A:315:ILE:HD12	2.02	0.42
1:B:1359:LEU:HD23	1:B:1359:LEU:HA	1.83	0.42
1:D:3113:MET:O	1:D:3117:LEU:HD22	2.20	0.42
1:D:3579:SER:OG	1:D:3580:PHE:N	2.53	0.42
1:A:47:CYS:HB2	7:A:5294:HOH:O	2.19	0.42
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.87	0.42
3:A:661:NAG:O7	3:A:661:NAG:C3	2.66	0.42
1:B:1300:MET:HG2	1:B:1419:LEU:HD11	2.02	0.42
1:C:2073:GLU:O	1:C:2074:PHE:C	2.63	0.42
1:C:2113:MET:O	1:C:2117:LEU:CD2	2.67	0.42
1:C:2190:ASP:OD2	1:C:2192:GLN:HB2	2.20	0.42
1:C:2312:VAL:HA	1:C:2315:ILE:HD12	2.01	0.42
1:C:2368:ASN:ND2	7:C:5124:HOH:O	2.52	0.42
1:D:3034:ASN:HA	1:D:3035:PRO:HD2	1.85	0.42
1:A:46:GLU:O	1:A:57:CYS:HA	2.20	0.41
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.34	0.41
1:A:467:ARG:HA	7:A:5160:HOH:O	2.19	0.41
1:B:1295:VAL:HG11	5:B:1601:HEM:HBB2	2.02	0.41
1:B:1329:PHE:CD2	1:B:1329:PHE:C	2.98	0.41
1:B:1500:VAL:O	1:B:1500:VAL:HG12	2.18	0.41
1:C:2176:GLU:O	1:C:2180:LYS:HG3	2.20	0.41
1:C:2385:TYR:OH	6:C:2701:DIF:H132	2.20	0.41
1:D:3500:VAL:O	1:D:3500:VAL:CG1	2.67	0.41
1:A:73:GLU:O	1:A:76:THR:HB	2.19	0.41
1:A:202:ALA:HB2	1:A:348:TYR:CE1	2.56	0.41
1:A:495:TYR:O	1:A:496:SER:HB2	2.19	0.41
1:B:1048:MET:HE3	1:B:1050:THR:HG22	2.01	0.41
1:B:1464:ASN:ND2	1:B:1467:ARG:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2105(C):ILE:HG22	1:C:2108:LEU:CB	2.23	0.41
1:C:2464:ASN:HD22	1:C:2464:ASN:HA	1.57	0.41
1:C:2575:CYS:O	1:C:2575:CYS:SG	2.78	0.41
1:D:3142:PHE:CD2	1:D:3142:PHE:C	2.95	0.41
1:D:3161:THR:HB	1:D:3162:PRO:HD2	2.02	0.41
1:D:3450:ALA:O	1:D:3451:SER:C	2.61	0.41
1:A:97:LYS:HD2	1:A:356:HIS:CD2	2.54	0.41
1:B:1105(B):ILE:HB	1:B:1108:LEU:HB2	2.02	0.41
1:C:2464:ASN:ND2	1:C:2467:ARG:HD3	2.35	0.41
1:D:3091:TYR:O	1:D:3095:HIS:HD2	2.03	0.41
1:A:124:ILE:HG21	1:A:532:LYS:HG3	2.02	0.41
1:A:309:HIS:HD2	1:A:310:ASN:OD1	2.03	0.41
1:A:447:VAL:HG13	5:A:704:HEM:HBA2	2.02	0.41
1:B:1132:VAL:HG13	1:B:1133:HIS:CD2	2.56	0.41
1:D:3442:ILE:HG23	4:D:3703:BOG:H61	2.03	0.41
1:D:3484:GLU:CD	1:D:3487:MET:HE2	2.45	0.41
1:B:1251:LYS:HG2	1:B:1310:ASN:CB	2.50	0.41
1:B:1537:ASN:CG	1:B:1538:PRO:HD2	2.45	0.41
1:A:44:ARG:HD3	1:A:469:ARG:NE	2.36	0.41
1:A:102:ILE:HG22	1:A:105(A):ILE:HD12	2.03	0.41
1:B:1202:ALA:HB2	1:B:1348:TYR:HE1	1.84	0.41
1:C:2089:VAL:HG12	1:C:2093:LEU:HD22	2.01	0.41
1:C:2114:LYS:HE2	1:C:2365:LEU:O	2.20	0.41
1:A:243:LYS:HE2	1:A:270:GLN:HB3	2.02	0.41
1:A:450:ALA:O	1:A:451:SER:C	2.63	0.41
1:A:550:PHE:O	1:A:555:GLY:HA3	2.21	0.41
1:B:1487:MET:HE2	1:B:1487:MET:HB2	1.93	0.41
1:C:2538:PRO:HG3	1:D:3142:PHE:CE2	2.56	0.41
1:D:3197:MET:O	1:D:3201:PHE:HB2	2.20	0.41
1:D:3398:GLU:HB3	1:D:3399:ASP:H	1.44	0.41
1:D:3470:PHE:CG	1:D:3525:LEU:HD22	2.55	0.41
1:B:1034:ASN:HD22	1:B:1035:PRO:N	2.19	0.41
1:B:1113:MET:O	1:B:1116:VAL:HG22	2.21	0.41
1:C:2300:MET:CE	1:C:2423:VAL:HG22	2.50	0.41
1:A:50:THR:CG2	1:A:56:LYS:HB3	2.51	0.41
1:A:76:THR:O	1:A:80:LEU:HG	2.20	0.41
1:A:414:LEU:HD11	1:A:419:LEU:HD22	2.01	0.41
1:A:464:ASN:ND2	1:A:475:TYR:H	2.16	0.41
1:B:1058:ASP:OD1	1:B:1060:THR:OG1	2.33	0.41
1:B:1352:LEU:HA	1:B:1352:LEU:HD12	1.82	0.41
1:B:1433:ARG:NH2	1:B:1516:ALA:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2047:CYS:HB2	7:C:5307:HOH:O	2.21	0.41
1:C:2248:LYS:O	1:C:2249:ASP:HB2	2.21	0.41
1:C:2298:LEU:HD12	1:C:2298:LEU:HA	1.74	0.41
1:C:2414:LEU:HA	1:C:2422:PHE:CE1	2.56	0.41
1:D:3048:MET:O	1:D:3050:THR:HG23	2.21	0.41
1:D:3316:LEU:HD23	1:D:3316:LEU:HA	1.82	0.41
1:B:1316:LEU:HD23	1:B:1316:LEU:HA	1.83	0.41
1:D:3112:ILE:HB	1:D:3357:PHE:CZ	2.56	0.41
1:D:3574:GLY:O	1:D:3575:CYS:C	2.62	0.41
1:A:52:PHE:N	1:B:1322:GLU:HG2	2.36	0.40
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.85	0.40
1:B:1384:LEU:HD12	1:B:1384:LEU:C	2.46	0.40
1:C:2185:ARG:H	1:C:2185:ARG:HG2	1.68	0.40
1:C:2320:HIS:HB3	1:C:2323:TRP:CG	2.56	0.40
1:C:2537:ASN:OD1	1:C:2539:ILE:HG12	2.20	0.40
1:D:3464:ASN:HD22	1:D:3464:ASN:HA	1.67	0.40
1:A:577:PHE:HE2	1:A:583:GLN:HE21	1.69	0.40
1:B:1075:LEU:CD1	1:B:1079:LYS:HE3	2.46	0.40
1:D:3090:HIS:CE1	1:D:3094:THR:CG2	3.00	0.40
1:A:94:THR:O	1:A:356:HIS:CE1	2.74	0.40
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.37	0.40
1:B:1050:THR:HG21	1:B:1056:LYS:HB2	2.02	0.40
1:C:2451:SER:HB2	1:C:2504:TYR:CE2	2.56	0.40
1:D:3204:HIS:CE1	1:D:3232:HIS:CD2	3.09	0.40
1:D:3250:GLY:HA2	1:D:3329:PHE:HB2	2.04	0.40
1:D:3276:PRO:HG2	1:D:3279:ILE:HG12	2.02	0.40
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.22	0.40
1:B:1113:MET:CA	1:B:1116:VAL:HG13	2.47	0.40
1:B:1198:PHE:HZ	1:B:1352:LEU:CD1	2.33	0.40
1:B:1298:LEU:N	7:B:5268:HOH:O	2.54	0.40
1:C:2064:PHE:CD1	1:C:2064:PHE:N	2.89	0.40
1:D:3253:LYS:O	1:D:3264:PRO:HD3	2.21	0.40
1:D:3525:LEU:HD23	1:D:3525:LEU:N	2.36	0.40
1:B:1100:TRP:HA	1:B:1100:TRP:CE3	2.57	0.40
1:B:1197:MET:HE1	1:B:1300:MET:HE1	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1490:GLU:OE1	4:A:703:BOG:O2[4_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2490:GLU:OE1	4:D:3703:BOG:O2[4_456]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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	549/604 (91%)	516 (94%)	31 (6%)	2 (0%)	30	59
1	B	550/604 (91%)	513 (93%)	36 (6%)	1 (0%)	43	72
1	C	550/604 (91%)	510 (93%)	37 (7%)	3 (0%)	24	54
1	D	550/604 (91%)	510 (93%)	40 (7%)	0	100	100
All	All	2199/2416 (91%)	2049 (93%)	144 (6%)	6 (0%)	36	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	C	2106	PRO
1	C	2074	PHE
1	C	2438	ARG
1	A	106	PRO
1	B	1582	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 X-ray entries followed by that with respect to entries of similar resolution.

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	492/537 (92%)	422 (86%)	70 (14%)	3	11
1	B	493/537 (92%)	422 (86%)	71 (14%)	3	11
1	C	493/537 (92%)	420 (85%)	73 (15%)	3	10
1	D	493/537 (92%)	423 (86%)	70 (14%)	3	11
All	All	1971/2148 (92%)	1687 (86%)	284 (14%)	3	11

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	56	LYS
1	A	70	THR
1	A	78	ILE
1	A	82	LEU
1	A	83	LYS
1	A	85	THR
1	A	93	LEU
1	A	101	ASN
1	A	107	PHE
1	A	108	LEU
1	A	111	LEU
1	A	112	ILE
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	123	LEU
1	A	131	ASN
1	A	171	LEU
1	A	178	LEU
1	A	185	ARG
1	A	215	LYS
1	A	230	LEU
1	A	238	LEU
1	A	248	LYS
1	A	252	LEU
1	A	267	LYS
1	A	270	GLN
1	A	271	VAL
1	A	272	GLU
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	306	LEU
1	A	307	ARG
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	341	ILE
1	A	376	ARG
1	A	385	TYR
1	A	405	LYS
1	A	406	GLN
1	A	408	LEU
1	A	409	TYR
1	A	412	SER
1	A	428	ARG
1	A	430	ILE
1	A	444	VAL
1	A	463	LEU
1	A	465	GLU
1	A	468	LYS
1	A	469	ARG
1	A	484	GLU
1	A	487	MET
1	A	492	LYS
1	A	509	VAL
1	A	513	ARG
1	A	525	LEU
1	A	532	LYS
1	A	534	LEU
1	A	535	MET
1	A	539	ILE
1	A	543	GLN
1	A	556	PHE
1	A	557	LYS
1	A	568	ILE
1	A	578	THR
1	A	583	GLN
1	B	1034	ASN
1	B	1038	SER
1	B	1046	GLU
1	B	1064	PHE
1	B	1065	TYR

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Mol	Chain	Res	Type
1	B	1081	LEU
1	B	1082	LEU
1	B	1085	THR
1	B	1093	LEU
1	B	1097	LYS
1	B	1101	ASN
1	B	1107	PHE
1	B	1111	LEU
1	B	1112	ILE
1	B	1116	VAL
1	B	1117	LEU
1	B	1118	THR
1	B	1120	ARG
1	B	1123	LEU
1	B	1131	ASN
1	B	1171	LEU
1	B	1176	GLU
1	B	1178	LEU
1	B	1185	ARG
1	B	1215	LYS
1	B	1230	LEU
1	B	1238	LEU
1	B	1248	LYS
1	B	1252	LEU
1	B	1267	LYS
1	B	1270	GLN
1	B	1271	VAL
1	B	1272	GLU
1	B	1289	GLN
1	B	1290	GLU
1	B	1291	VAL
1	B	1298	LEU
1	B	1306	LEU
1	B	1307	ARG
1	B	1318	GLN
1	B	1322	GLU
1	B	1341	ILE
1	B	1369	GLN
1	B	1376	ARG
1	B	1385	TYR
1	B	1405	LYS
1	B	1406	GLN

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Mol	Chain	Res	Type
1	B	1408	LEU
1	B	1409	TYR
1	B	1412	SER
1	B	1428	ARG
1	B	1430	ILE
1	B	1444	VAL
1	B	1463	LEU
1	B	1464	ASN
1	B	1465	GLU
1	B	1468	LYS
1	B	1469	ARG
1	B	1484	GLU
1	B	1487	MET
1	B	1492	LYS
1	B	1509	VAL
1	B	1513	ARG
1	B	1525	LEU
1	B	1532	LYS
1	B	1534	LEU
1	B	1535	MET
1	B	1557	LYS
1	B	1578	THR
1	B	1579	SER
1	B	1583	GLN
1	C	2034	ASN
1	C	2038	SER
1	C	2041	CYS
1	C	2056	LYS
1	C	2077	ARG
1	C	2081	LEU
1	C	2082	LEU
1	C	2083	LYS
1	C	2093	LEU
1	C	2097	LYS
1	C	2101	ASN
1	C	2107	PHE
1	C	2108	LEU
1	C	2116	VAL
1	C	2117	LEU
1	C	2120	ARG
1	C	2123	LEU
1	C	2131	ASN

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Mol	Chain	Res	Type
1	C	2171	LEU
1	C	2176	GLU
1	C	2178	LEU
1	C	2185	ARG
1	C	2215	LYS
1	C	2230	LEU
1	C	2238	LEU
1	C	2248	LYS
1	C	2252	LEU
1	C	2267	LYS
1	C	2270	GLN
1	C	2271	VAL
1	C	2272	GLU
1	C	2289	GLN
1	C	2290	GLU
1	C	2291	VAL
1	C	2298	LEU
1	C	2306	LEU
1	C	2307	ARG
1	C	2318	GLN
1	C	2322	GLU
1	C	2326	GLU
1	C	2341	ILE
1	C	2369	GLN
1	C	2376	ARG
1	C	2385	TYR
1	C	2405	LYS
1	C	2406	GLN
1	C	2408	LEU
1	C	2409	TYR
1	C	2412	SER
1	C	2428	ARG
1	C	2430	ILE
1	C	2438	ARG
1	C	2444	VAL
1	C	2463	LEU
1	C	2464	ASN
1	C	2465	GLU
1	C	2468	LYS
1	C	2469	ARG
1	C	2484	GLU
1	C	2487	MET

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Mol	Chain	Res	Type
1	C	2492	LYS
1	C	2509	VAL
1	C	2513	ARG
1	C	2525	LEU
1	C	2532	LYS
1	C	2534	LEU
1	C	2535	MET
1	C	2539	ILE
1	C	2557	LYS
1	C	2568	ILE
1	C	2578	THR
1	C	2582	VAL
1	C	2583	GLN
1	D	3034	ASN
1	D	3038	SER
1	D	3046	GLU
1	D	3056	LYS
1	D	3081	LEU
1	D	3082	LEU
1	D	3083	LYS
1	D	3085	THR
1	D	3093	LEU
1	D	3101	ASN
1	D	3107	PHE
1	D	3108	LEU
1	D	3111	LEU
1	D	3112	ILE
1	D	3116	VAL
1	D	3117	LEU
1	D	3120	ARG
1	D	3123	LEU
1	D	3131	ASN
1	D	3171	LEU
1	D	3176	GLU
1	D	3178	LEU
1	D	3185	ARG
1	D	3215	LYS
1	D	3230	LEU
1	D	3238	LEU
1	D	3248	LYS
1	D	3252	LEU
1	D	3267	LYS

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Mol	Chain	Res	Type
1	D	3270	GLN
1	D	3271	VAL
1	D	3272	GLU
1	D	3289	GLN
1	D	3290	GLU
1	D	3291	VAL
1	D	3298	LEU
1	D	3306	LEU
1	D	3307	ARG
1	D	3318	GLN
1	D	3322	GLU
1	D	3326	GLU
1	D	3341	ILE
1	D	3369	GLN
1	D	3376	ARG
1	D	3385	TYR
1	D	3405	LYS
1	D	3406	GLN
1	D	3408	LEU
1	D	3409	TYR
1	D	3412	SER
1	D	3430	ILE
1	D	3438	ARG
1	D	3444	VAL
1	D	3463	LEU
1	D	3465	GLU
1	D	3468	LYS
1	D	3469	ARG
1	D	3484	GLU
1	D	3487	MET
1	D	3492	LYS
1	D	3509	VAL
1	D	3513	ARG
1	D	3525	LEU
1	D	3532	LYS
1	D	3534	LEU
1	D	3535	MET
1	D	3539	ILE
1	D	3557	LYS
1	D	3568	ILE
1	D	3583	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	95	HIS
1	A	131	ASN
1	A	203	GLN
1	A	204	HIS
1	A	214	HIS
1	A	241	GLN
1	A	242	HIS
1	A	327	GLN
1	A	356	HIS
1	A	386	HIS
1	A	454	GLN
1	A	464	ASN
1	A	560	ASN
1	A	570	ASN
1	A	583	GLN
1	B	1034	ASN
1	B	1090	HIS
1	B	1131	ASN
1	B	1203	GLN
1	B	1204	HIS
1	B	1241	GLN
1	B	1242	HIS
1	B	1284	GLN
1	B	1356	HIS
1	B	1369	GLN
1	B	1454	GLN
1	B	1464	ASN
1	B	1583	GLN
1	C	2034	ASN
1	C	2090	HIS
1	C	2095	HIS
1	C	2131	ASN
1	C	2203	GLN
1	C	2204	HIS
1	C	2214	HIS
1	C	2241	GLN
1	C	2242	HIS
1	C	2284	GLN
1	C	2454	GLN
1	C	2464	ASN
1	C	2583	GLN

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Mol	Chain	Res	Type
1	D	3034	ASN
1	D	3042	GLN
1	D	3090	HIS
1	D	3095	HIS
1	D	3131	ASN
1	D	3203	GLN
1	D	3204	HIS
1	D	3214	HIS
1	D	3241	GLN
1	D	3242	HIS
1	D	3356	HIS
1	D	3386	HIS
1	D	3454	GLN
1	D	3464	ASN
1	D	3571	ASN
1	D	3583	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 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	2,1	14,14,15	0.47	0	17,19,21	0.67	0
2	NAG	E	2	2	14,14,15	0.80	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	3	2	14,14,15	0.86	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.52	0	17,19,21	0.72	1 (5%)
2	NAG	F	2	2	14,14,15	0.77	0	17,19,21	0.82	1 (5%)
2	NAG	F	3	2	14,14,15	1.00	1 (7%)	17,19,21	0.80	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.46	0	17,19,21	0.70	0
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.79	1 (5%)
2	NAG	G	3	2	14,14,15	0.96	1 (7%)	17,19,21	0.67	0
2	NAG	H	1	2,1	14,14,15	0.60	0	17,19,21	0.68	0
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	0.84	1 (5%)
2	NAG	H	3	2	14,14,15	0.96	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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	3	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	3	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	3	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	3	2	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	NAG	C1-C2	2.78	1.56	1.52
2	G	3	NAG	C1-C2	2.75	1.56	1.52
2	H	3	NAG	C1-C2	2.43	1.55	1.52
2	E	3	NAG	C1-C2	2.05	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	NAG	C1-O5-C5	2.63	115.72	112.19
2	G	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
2	H	2	NAG	O5-C1-C2	-2.17	107.93	111.29
2	H	3	NAG	C1-O5-C5	2.17	115.10	112.19
2	E	2	NAG	O5-C1-C2	-2.14	107.98	111.29
2	F	1	NAG	C2-N2-C7	-2.13	120.05	122.90
2	E	3	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	E	3	NAG	C3-C2-N2-C7
2	G	3	NAG	C3-C2-N2-C7
2	H	3	NAG	C3-C2-N2-C7
2	F	3	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	F	3	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7

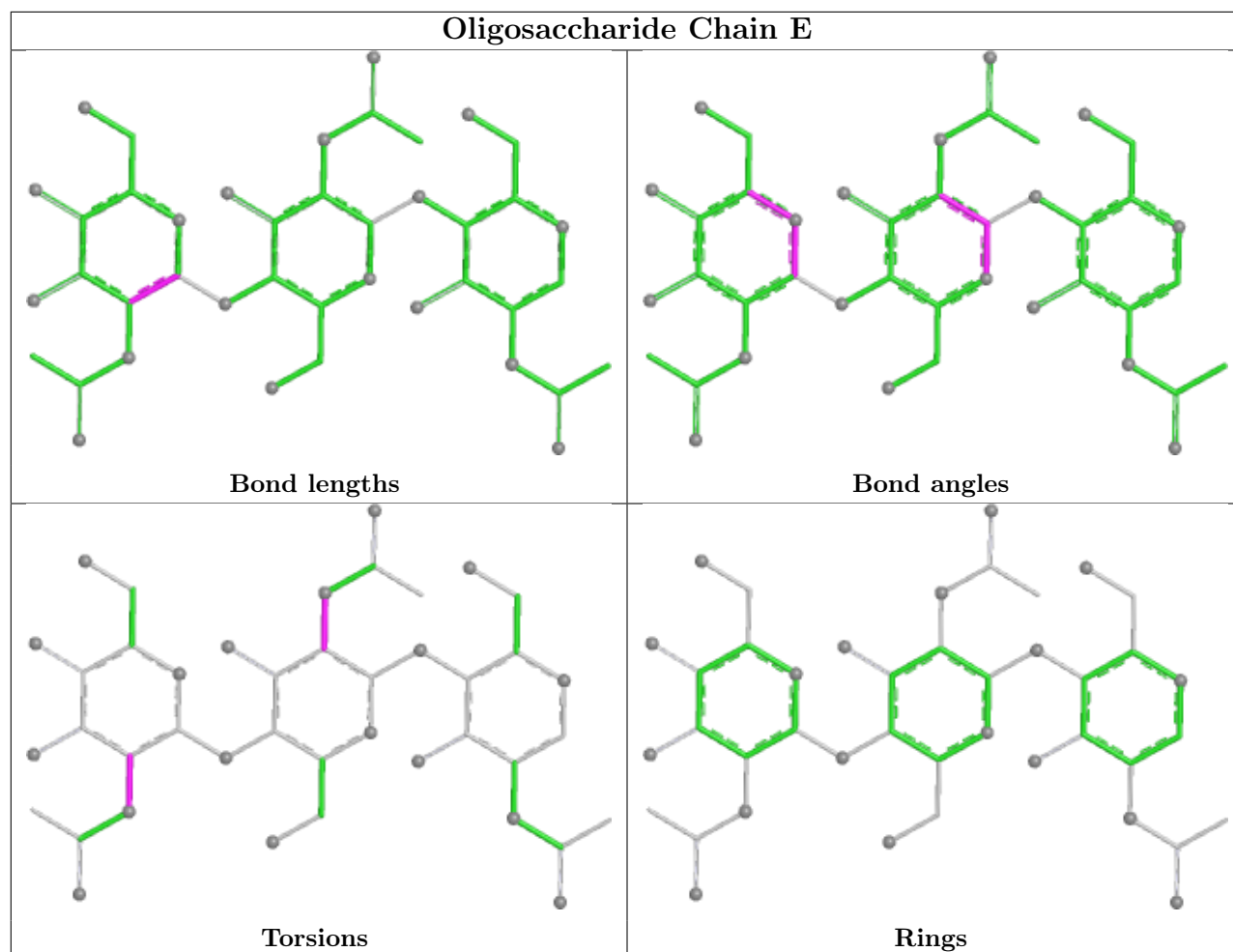
There are no ring outliers.

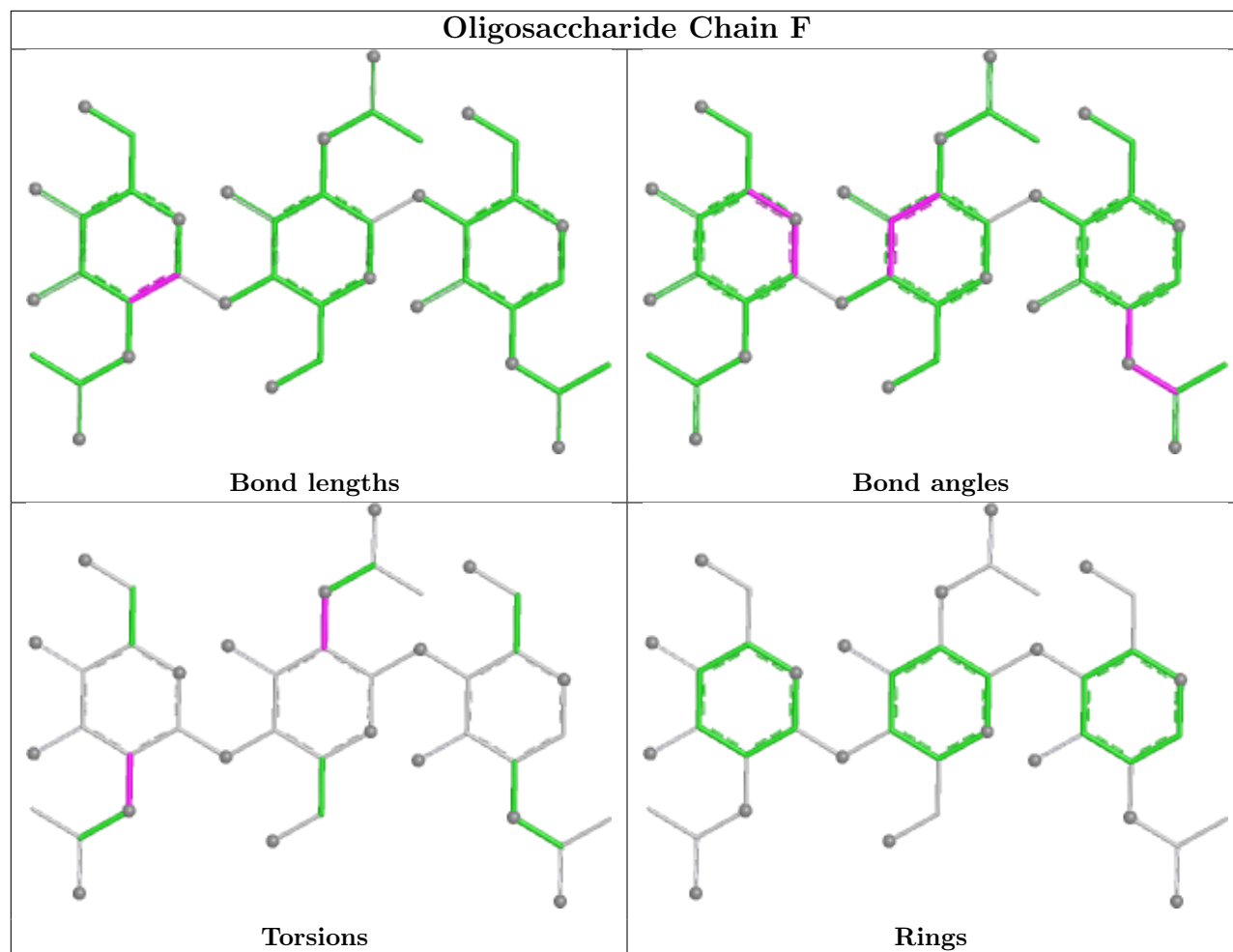
9 monomers are involved in 9 short contacts:

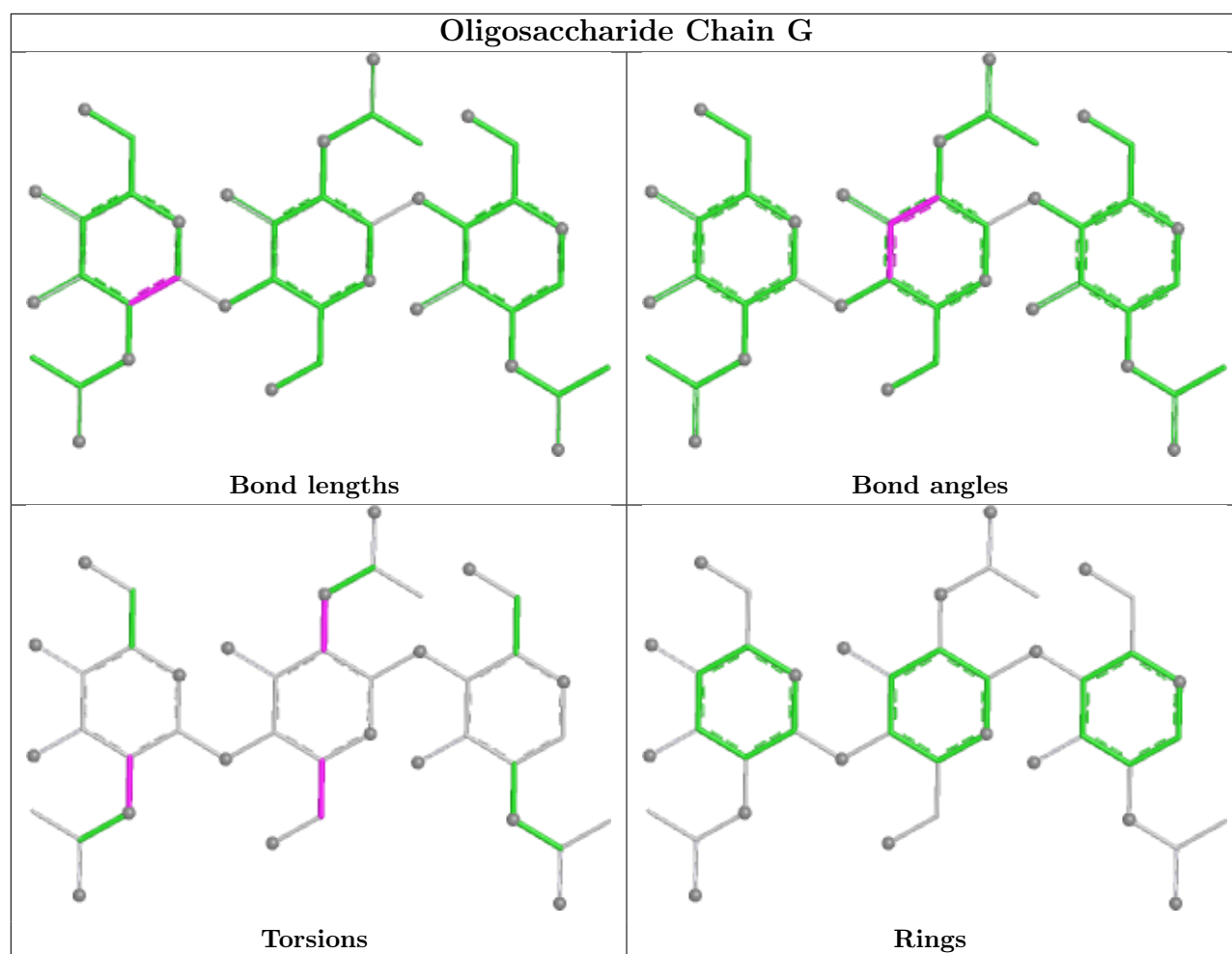
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	F	3	NAG	1	0
2	E	3	NAG	3	0
2	H	1	NAG	1	0
2	H	3	NAG	2	0
2	E	2	NAG	2	0
2	F	2	NAG	1	0
2	H	2	NAG	2	0
2	G	3	NAG	2	0

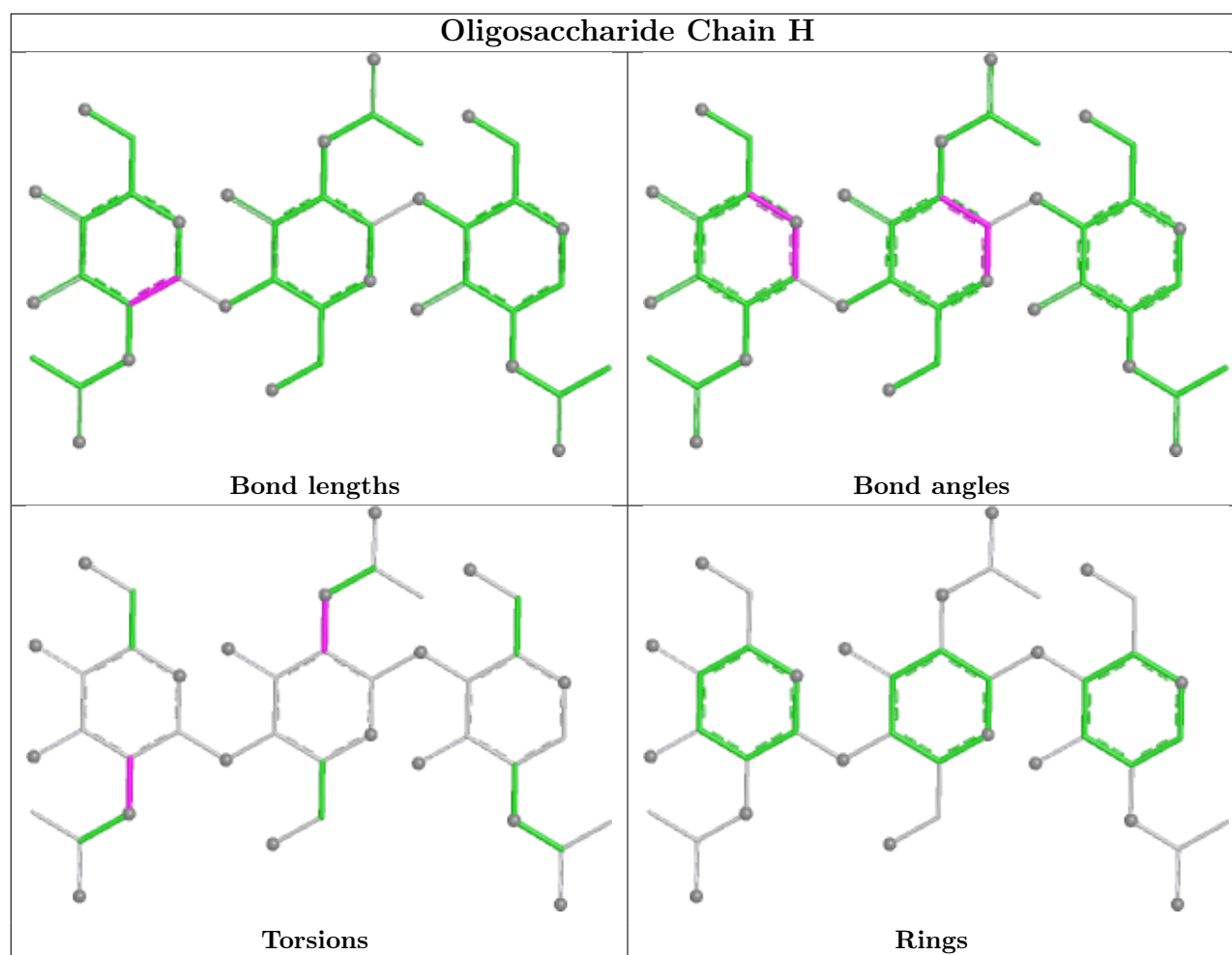
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DIF	C	2701	-	20,20,20	1.54	3 (15%)	27,27,27	1.75	7 (25%)
4	BOG	D	3703	-	17,17,20	0.38	0	18,18,25	0.91	2 (11%)
5	HEM	D	3601	1	50,50,50	1.20	5 (10%)	67,82,82	0.93	1 (1%)
3	NAG	C	2681	1	14,14,15	0.48	0	17,19,21	1.00	1 (5%)
6	DIF	D	3701	-	20,20,20	1.48	3 (15%)	27,27,27	2.02	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1681	1	14,14,15	0.47	0	17,19,21	0.81	0
3	NAG	D	3661	1	14,14,15	0.74	0	17,19,21	0.80	1 (5%)
5	HEM	B	1601	1	50,50,50	1.12	4 (8%)	67,82,82	0.89	1 (1%)
6	DIF	B	1701	-	20,20,20	1.41	3 (15%)	27,27,27	1.95	6 (22%)
5	HEM	C	2601	1	50,50,50	1.26	4 (8%)	67,82,82	0.93	1 (1%)
4	BOG	A	703	-	20,20,20	0.72	1 (5%)	25,25,25	0.65	0
6	DIF	A	701	-	20,20,20	1.50	3 (15%)	27,27,27	2.28	7 (25%)
5	HEM	A	704	1	50,50,50	1.26	5 (10%)	67,82,82	0.96	2 (2%)
3	NAG	B	1661	1	14,14,15	0.49	0	17,19,21	0.68	0
3	NAG	A	661	1	14,14,15	0.56	0	17,19,21	0.64	0
3	NAG	A	681	1	14,14,15	0.60	0	17,19,21	0.75	0
3	NAG	D	3681	1	14,14,15	0.48	0	17,19,21	0.86	0
3	NAG	C	2661	1	14,14,15	0.61	0	17,19,21	0.63	0

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
6	DIF	C	2701	-	-	0/8/8/8	0/2/2/2
4	BOG	D	3703	-	-	5/18/18/31	-
5	HEM	D	3601	1	-	4/14/54/54	-
3	NAG	C	2681	1	-	1/6/23/26	0/1/1/1
6	DIF	D	3701	-	-	0/8/8/8	0/2/2/2
3	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
3	NAG	D	3661	1	-	1/6/23/26	0/1/1/1
5	HEM	B	1601	1	-	8/14/54/54	-
6	DIF	B	1701	-	-	0/8/8/8	0/2/2/2
5	HEM	C	2601	1	-	6/14/54/54	-
4	BOG	A	703	-	-	6/11/31/31	0/1/1/1
6	DIF	A	701	-	-	0/8/8/8	0/2/2/2
5	HEM	A	704	1	-	5/14/54/54	-
3	NAG	B	1661	1	-	1/6/23/26	0/1/1/1
3	NAG	A	661	1	-	1/6/23/26	0/1/1/1
3	NAG	A	681	1	-	2/6/23/26	0/1/1/1
3	NAG	D	3681	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2661	1	-	1/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	DIF	O2-C14	4.22	1.35	1.22
6	C	2701	DIF	O2-C14	4.08	1.35	1.22
5	C	2601	HEM	CBB-CAB	4.03	1.49	1.30
6	A	701	DIF	O2-C14	3.97	1.35	1.22
5	A	704	HEM	CBC-CAC	3.93	1.49	1.30
6	D	3701	DIF	O2-C14	3.84	1.34	1.22
5	D	3601	HEM	CBB-CAB	3.74	1.48	1.30
5	A	704	HEM	CBB-CAB	3.48	1.47	1.30
5	B	1601	HEM	CBB-CAB	3.46	1.47	1.30
5	C	2601	HEM	CBC-CAC	3.41	1.46	1.30
5	C	2601	HEM	CAB-C3B	-3.34	1.38	1.47
5	B	1601	HEM	CAB-C3B	-3.28	1.38	1.47
6	C	2701	DIF	C3-C4	3.24	1.44	1.40
5	C	2601	HEM	CAC-C3C	-3.12	1.39	1.47
6	D	3701	DIF	C3-C4	3.07	1.44	1.40
5	B	1601	HEM	CAC-C3C	-3.04	1.39	1.47
5	D	3601	HEM	CAB-C3B	-2.99	1.39	1.47
5	D	3601	HEM	CAC-C3C	-2.99	1.39	1.47
5	D	3601	HEM	CBC-CAC	2.98	1.44	1.30
5	A	704	HEM	CAC-C3C	-2.97	1.39	1.47
6	A	701	DIF	C3-C4	2.70	1.44	1.40
5	A	704	HEM	CAB-C3B	-2.69	1.40	1.47
6	B	1701	DIF	C3-C4	2.44	1.43	1.40
6	C	2701	DIF	O1-C14	-2.44	1.22	1.30
6	B	1701	DIF	O1-C14	-2.39	1.22	1.30
4	A	703	BOG	O1-C1	2.32	1.44	1.40
6	A	701	DIF	O1-C14	-2.29	1.23	1.30
5	B	1601	HEM	CBC-CAC	2.27	1.41	1.30
6	D	3701	DIF	O1-C14	-2.20	1.23	1.30
5	A	704	HEM	CBD-CGD	2.08	1.55	1.50
5	D	3601	HEM	CBD-CGD	2.03	1.55	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	DIF	C7-C8-N1	5.39	122.98	118.59
6	A	701	DIF	C4-C3-N1	-5.23	115.08	121.97
6	A	701	DIF	C2-C3-N1	5.07	128.64	121.97
6	D	3701	DIF	C4-C3-N1	-5.03	115.33	121.97
6	B	1701	DIF	C7-C8-N1	4.88	122.57	118.59
6	B	1701	DIF	C4-C3-N1	-4.52	116.01	121.97
6	D	3701	DIF	C2-C3-N1	4.47	127.85	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	DIF	C3-C2-CL2	4.29	124.15	119.28
6	D	3701	DIF	C3-C2-CL2	4.10	123.94	119.28
6	C	2701	DIF	C4-C3-N1	-3.76	117.02	121.97
6	D	3701	DIF	C7-C8-N1	3.75	121.64	118.59
6	C	2701	DIF	C7-C8-N1	3.53	121.47	118.59
6	B	1701	DIF	C2-C3-N1	3.42	126.47	121.97
6	B	1701	DIF	C3-C2-CL2	3.36	123.10	119.28
6	C	2701	DIF	C2-C3-N1	3.27	126.27	121.97
6	A	701	DIF	O2-C14-C13	-3.24	113.16	122.94
5	A	704	HEM	C3B-C4B-NB	3.15	111.73	109.47
6	D	3701	DIF	O2-C14-C13	-3.13	113.51	122.94
6	C	2701	DIF	C3-C2-CL2	3.08	122.78	119.28
6	C	2701	DIF	O2-C14-C13	-2.93	114.09	122.94
6	B	1701	DIF	O2-C14-C13	-2.89	114.23	122.94
6	C	2701	DIF	C3-C4-CL4	2.82	122.49	119.28
6	D	3701	DIF	O1-C14-C13	2.67	124.15	113.98
6	A	701	DIF	O1-C14-C13	2.64	124.04	113.98
6	B	1701	DIF	O1-C14-C13	2.55	123.69	113.98
6	C	2701	DIF	O1-C14-C13	2.47	123.40	113.98
3	D	3661	NAG	C1-O5-C5	2.39	115.39	112.19
3	C	2681	NAG	C2-N2-C7	-2.34	119.77	122.90
4	D	3703	BOG	C5-C4-C3	-2.28	109.77	113.57
4	D	3703	BOG	C2-C3-C4	-2.26	107.56	112.17
6	A	701	DIF	C1-C2-CL2	-2.21	114.08	118.42
5	C	2601	HEM	C3B-C4B-NB	2.19	111.04	109.47
6	D	3701	DIF	C3-C4-CL4	2.18	121.76	119.28
5	A	704	HEM	CBA-CAA-C2A	-2.17	106.55	112.53
5	D	3601	HEM	C3B-C4B-NB	2.10	110.97	109.47
5	B	1601	HEM	CBA-CAA-C2A	-2.06	106.83	112.53

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1661	NAG	C3-C2-N2-C7
3	C	2661	NAG	C3-C2-N2-C7
3	D	3661	NAG	C3-C2-N2-C7
5	B	1601	HEM	C2B-C3B-CAB-CBB
5	B	1601	HEM	C4B-C3B-CAB-CBB
5	B	1601	HEM	C2C-C3C-CAC-CBC
4	D	3703	BOG	O5-C5-C6-O6
4	D	3703	BOG	C4-C5-C6-O6

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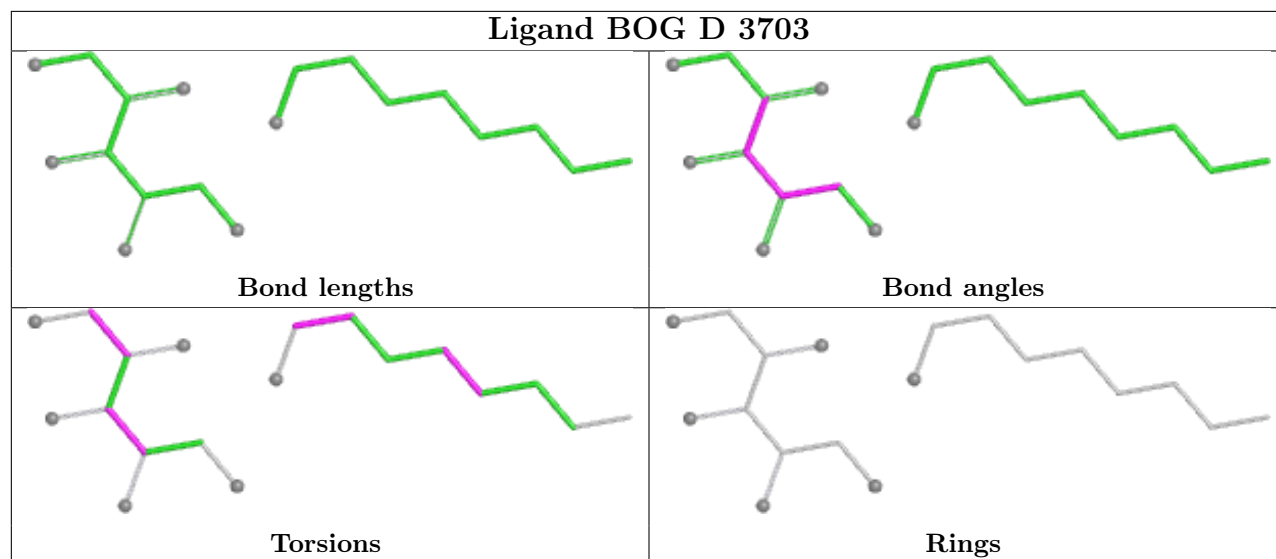
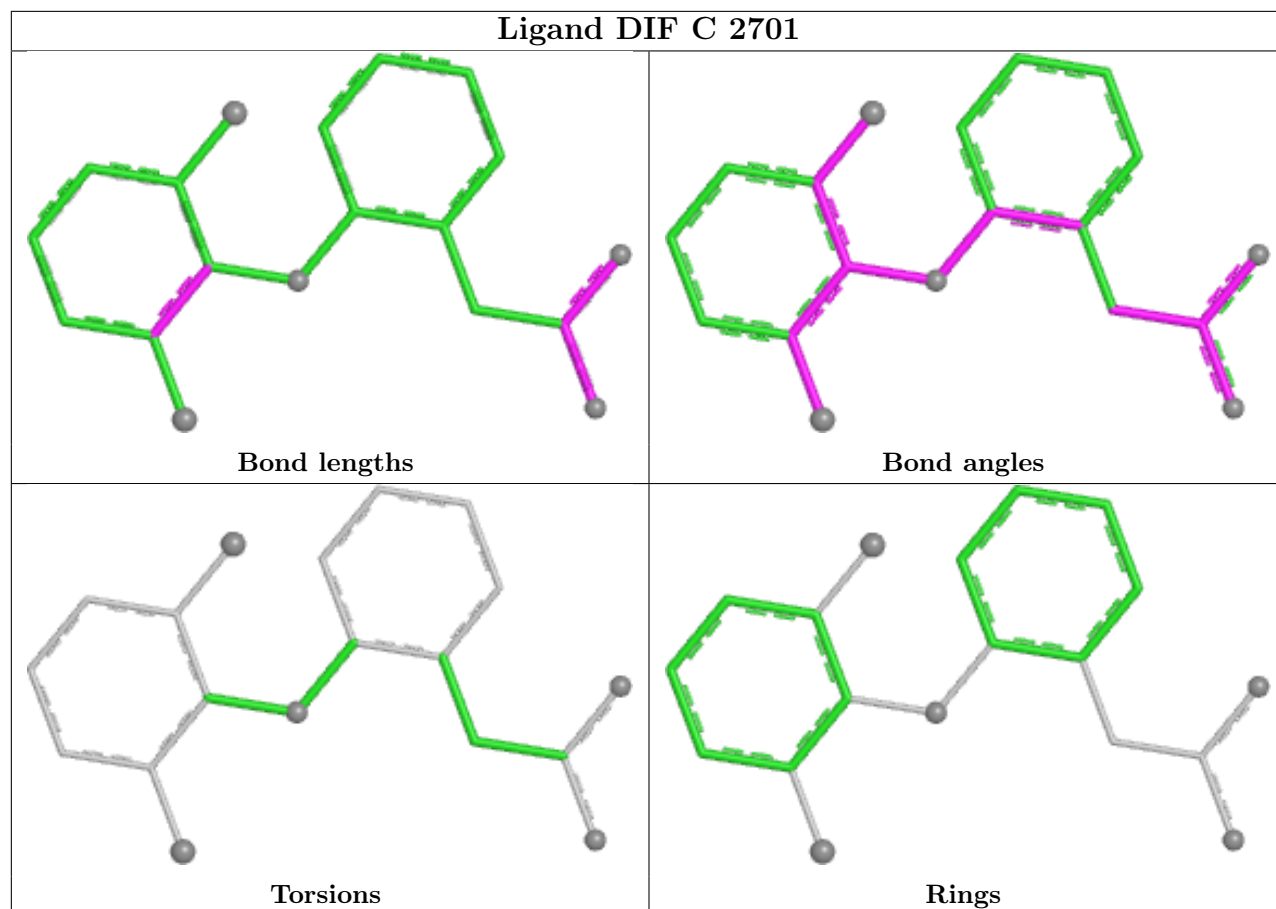
Mol	Chain	Res	Type	Atoms
4	A	703	BOG	C4-C5-C6-O6
4	A	703	BOG	O5-C1-O1-C1'
4	A	703	BOG	C2-C1-O1-C1'
4	A	703	BOG	C3'-C4'-C5'-C6'
4	D	3703	BOG	C3'-C4'-C5'-C6'
4	A	703	BOG	O5-C5-C6-O6
5	A	704	HEM	C2B-C3B-CAB-CBB
5	C	2601	HEM	C2B-C3B-CAB-CBB
5	C	2601	HEM	C2C-C3C-CAC-CBC
5	B	1601	HEM	C4C-C3C-CAC-CBC
3	D	3681	NAG	C4-C5-C6-O6
3	A	661	NAG	C3-C2-N2-C7
3	D	3681	NAG	O5-C5-C6-O6
5	A	704	HEM	C4B-C3B-CAB-CBB
5	C	2601	HEM	C4B-C3B-CAB-CBB
3	B	1681	NAG	C4-C5-C6-O6
3	A	681	NAG	C4-C5-C6-O6
4	A	703	BOG	C2'-C1'-O1-C1
4	D	3703	BOG	C2-C3-C4-O4
5	A	704	HEM	C4C-C3C-CAC-CBC
5	C	2601	HEM	C4C-C3C-CAC-CBC
5	C	2601	HEM	CAA-CBA-CGA-O1A
5	D	3601	HEM	CAD-CBD-CGD-O2D
5	A	704	HEM	CAA-CBA-CGA-O1A
5	D	3601	HEM	CAD-CBD-CGD-O1D
5	D	3601	HEM	CAA-CBA-CGA-O1A
5	A	704	HEM	CAA-CBA-CGA-O2A
5	C	2601	HEM	CAA-CBA-CGA-O2A
5	B	1601	HEM	CAA-CBA-CGA-O1A
3	B	1681	NAG	O5-C5-C6-O6
5	B	1601	HEM	CAD-CBD-CGD-O2D
5	D	3601	HEM	CAA-CBA-CGA-O2A
5	B	1601	HEM	CAA-CBA-CGA-O2A
3	C	2681	NAG	C4-C5-C6-O6
5	B	1601	HEM	CAD-CBD-CGD-O1D
3	A	681	NAG	O5-C5-C6-O6
4	D	3703	BOG	O1-C1'-C2'-C3'

There are no ring outliers.

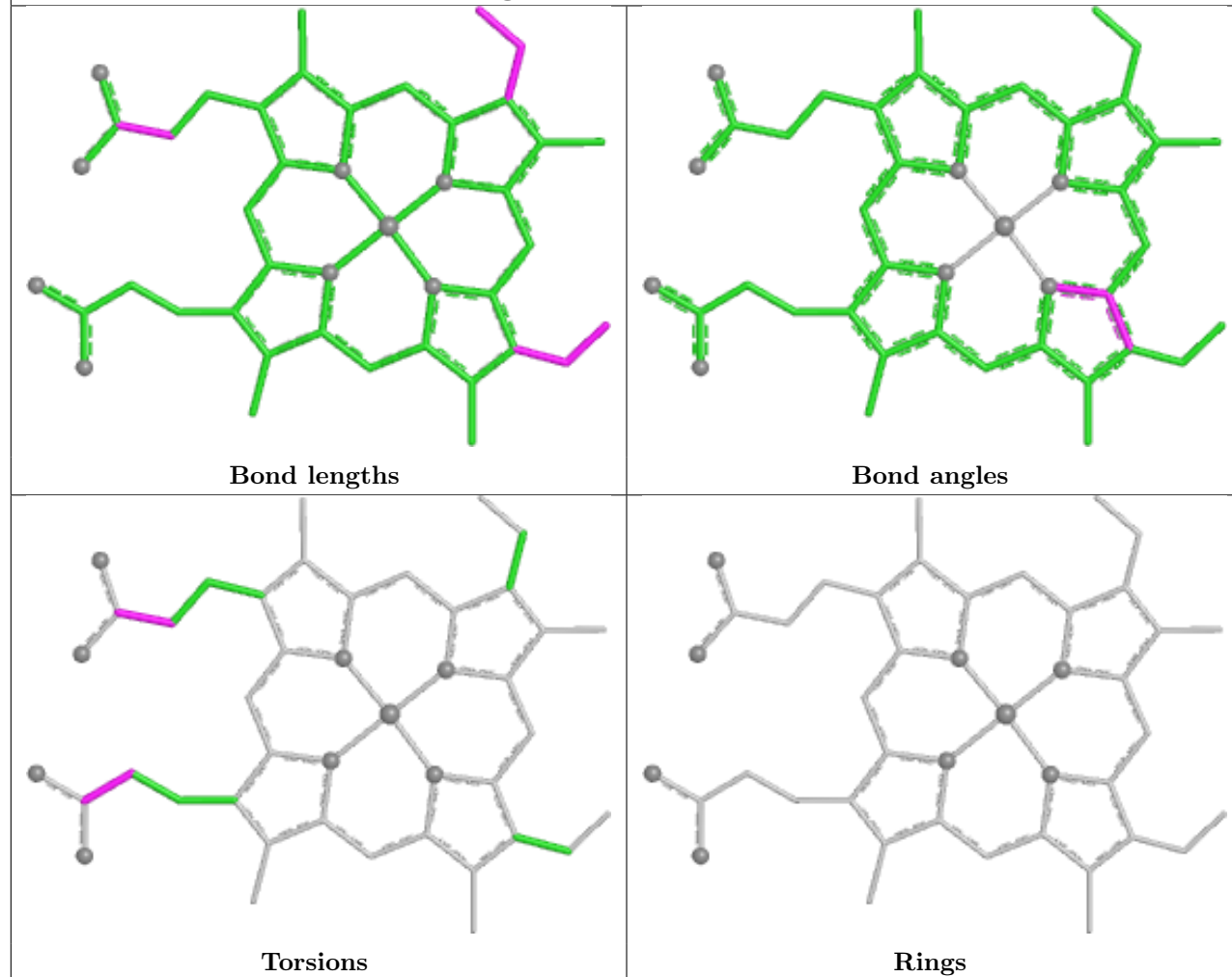
14 monomers are involved in 68 short contacts:

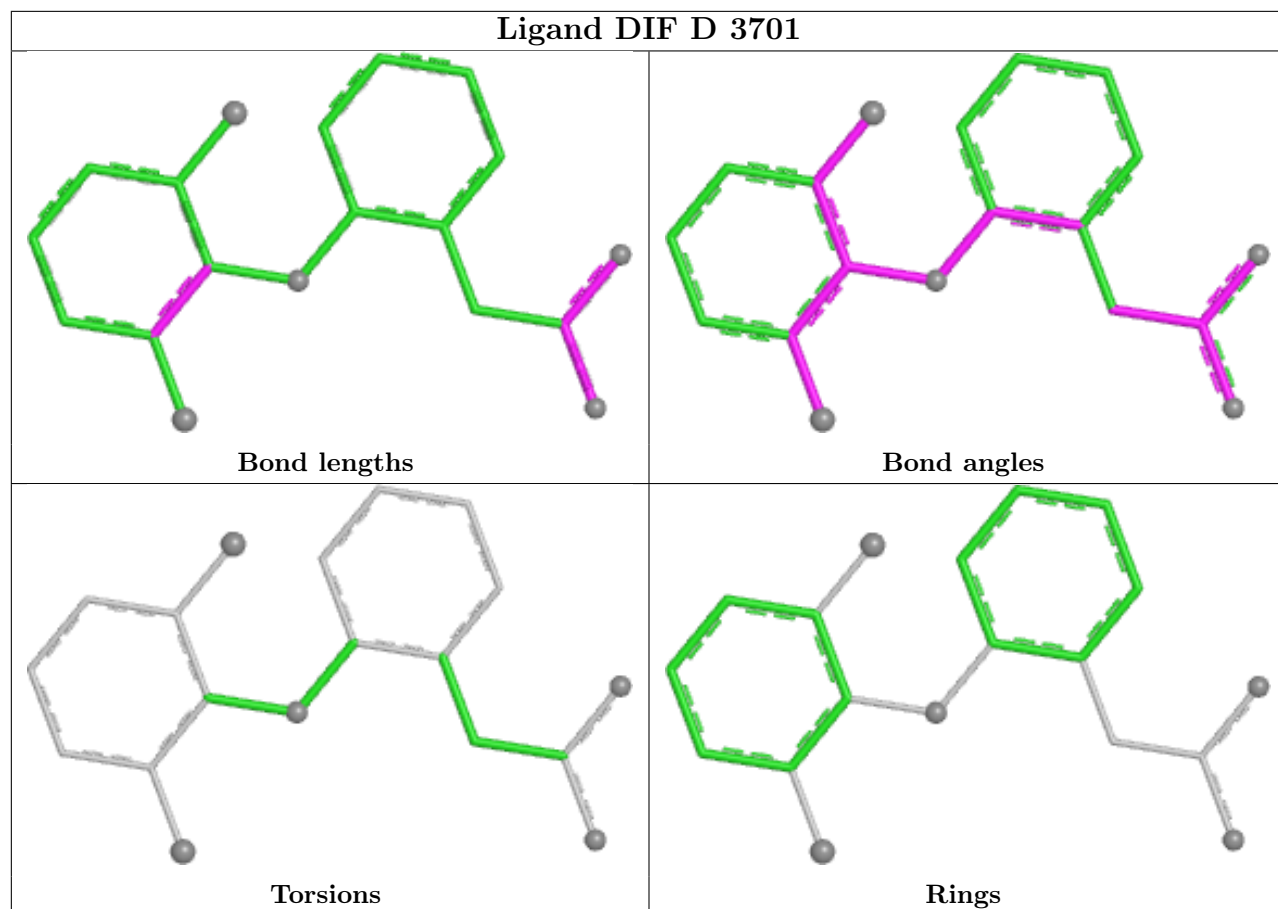
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2701	DIF	4	0
4	D	3703	BOG	9	1
5	D	3601	HEM	4	0
6	D	3701	DIF	1	0
3	D	3661	NAG	4	0
5	B	1601	HEM	7	0
6	B	1701	DIF	3	0
5	C	2601	HEM	4	0
4	A	703	BOG	5	1
6	A	701	DIF	3	0
5	A	704	HEM	4	0
3	B	1661	NAG	6	0
3	A	661	NAG	5	0
3	C	2661	NAG	7	0

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

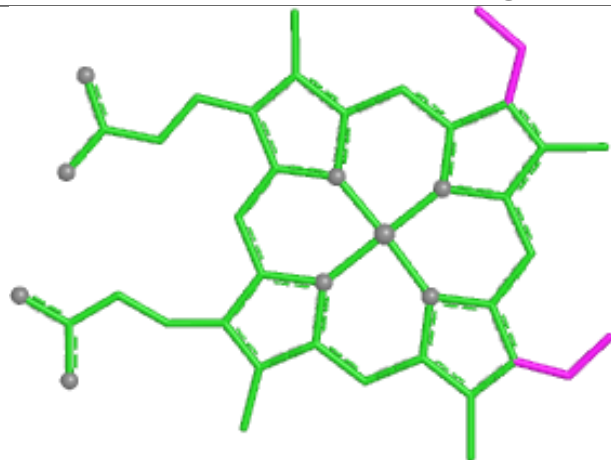


Ligand HEM D 3601

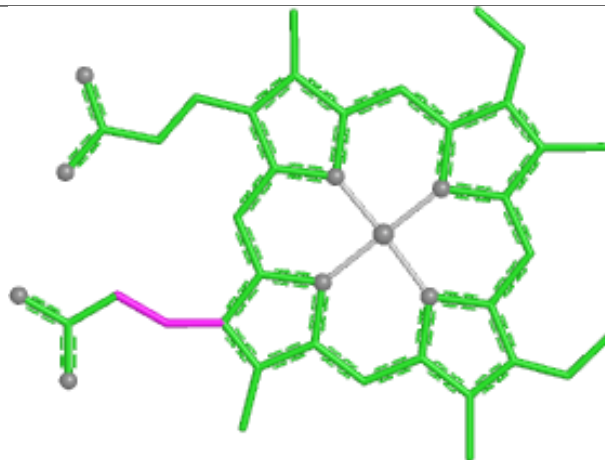




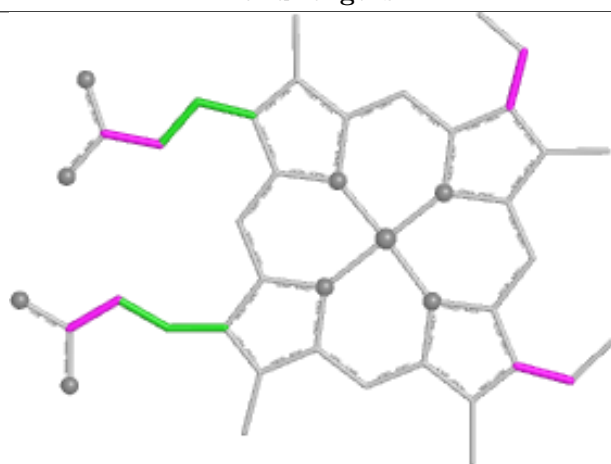
Ligand HEM B 1601



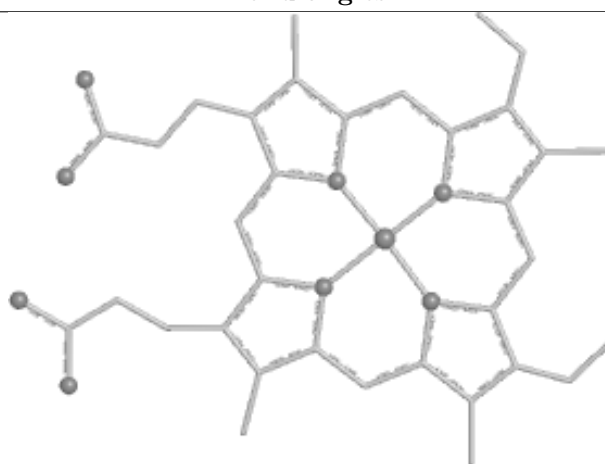
Bond lengths



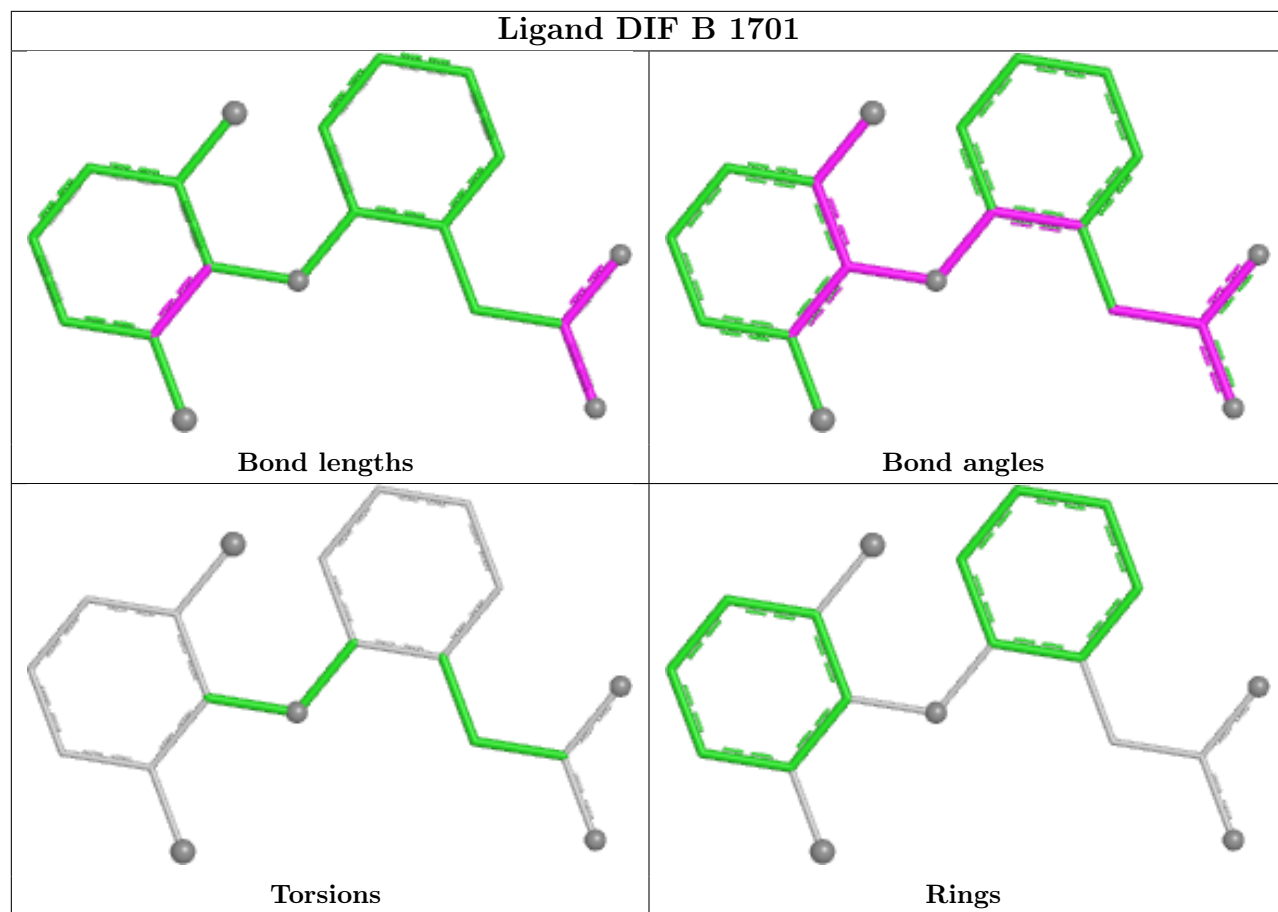
Bond angles



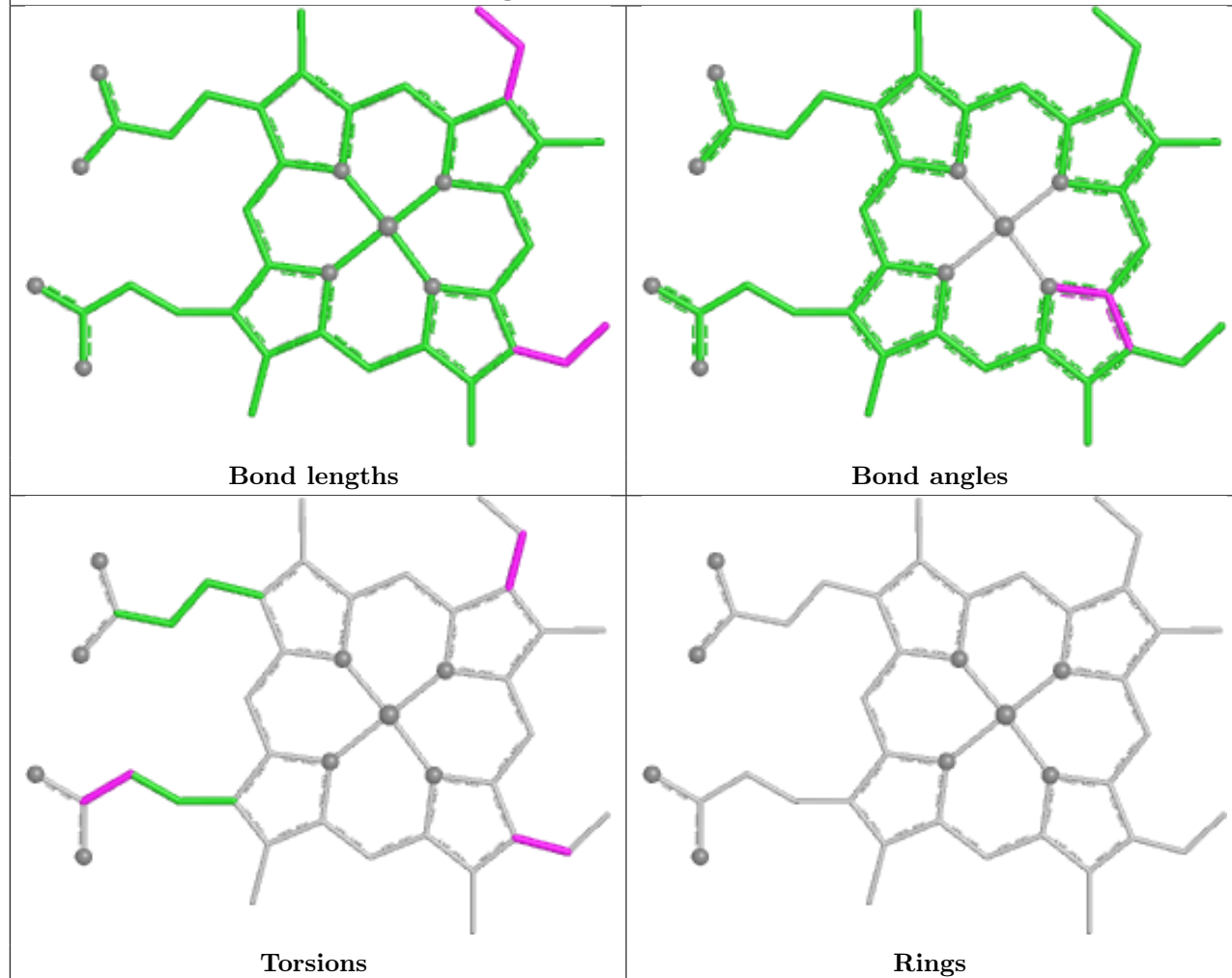
Torsions



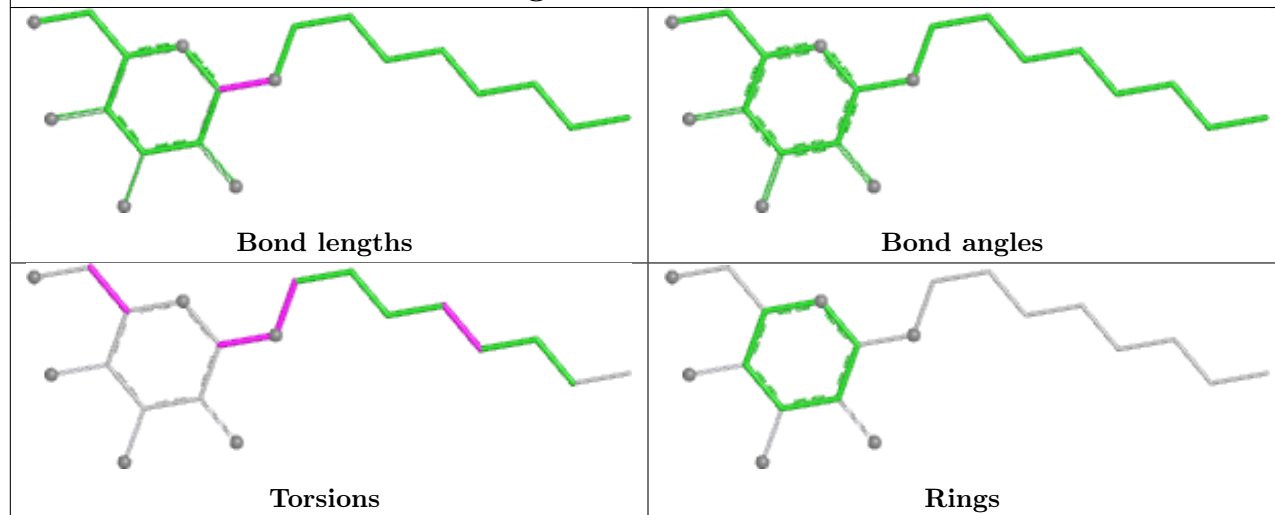
Rings

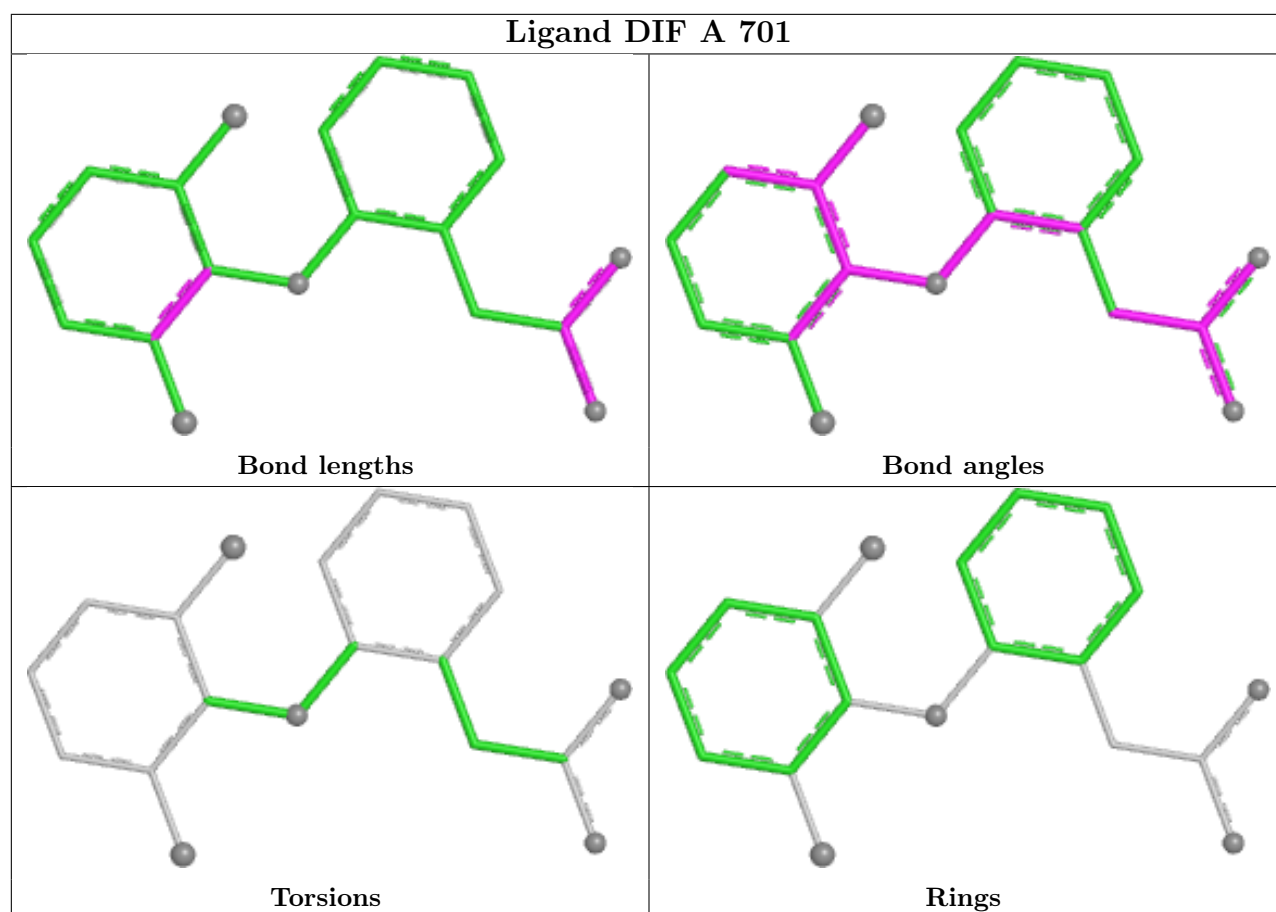


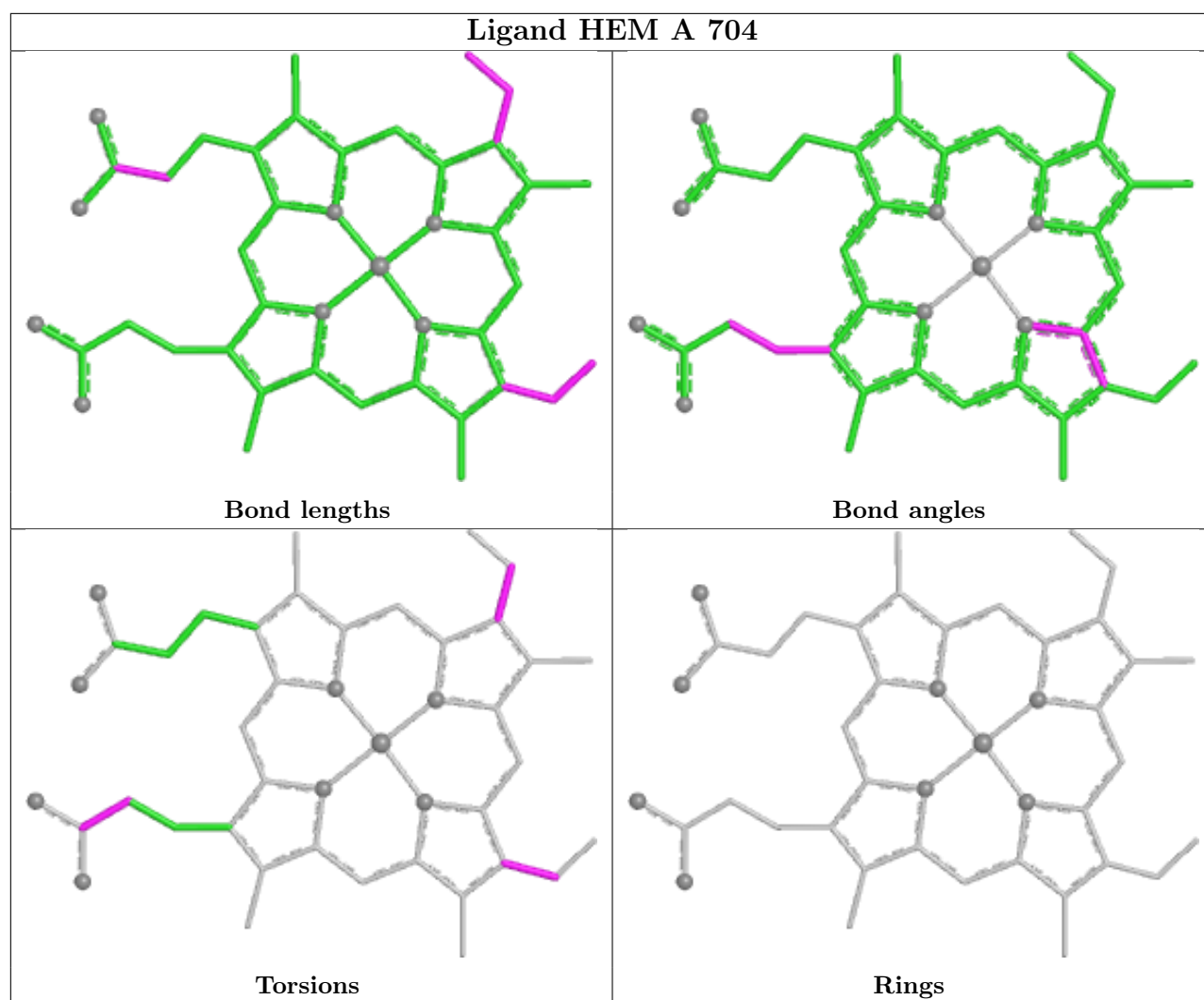
Ligand HEM C 2601



Ligand BOG A 703







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	552/604 (91%)	0.71	32 (5%)	29	22	5, 21, 42, 53	0
1	B	552/604 (91%)	0.88	42 (7%)	20	16	5, 21, 42, 58	0
1	C	552/604 (91%)	0.69	21 (3%)	44	36	3, 21, 41, 62	0
1	D	552/604 (91%)	0.92	57 (10%)	12	10	5, 21, 42, 55	0
All	All	2208/2416 (91%)	0.80	152 (6%)	23	18	3, 21, 42, 62	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1121	SER	5.7
1	B	1583	GLN	5.3
1	A	33	ALA	5.1
1	C	2121	SER	4.8
1	C	2583	GLN	4.7
1	D	3409	TYR	4.4
1	D	3033	ALA	4.3
1	D	3583	GLN	4.3
1	D	3268	ASP	4.2
1	A	121	SER	4.1
1	A	34	ASN	4.0
1	A	107	PHE	4.0
1	D	3049	SER	4.0
1	B	1186	GLU	3.7
1	D	3401	GLU	3.7
1	D	3457	GLU	3.7
1	B	1190	ASP	3.7
1	D	3121	SER	3.7
1	A	583	GLN	3.6
1	A	268	ASP	3.6
1	B	1582	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	3435	ALA	3.4
1	A	409	TYR	3.3
1	D	3575	CYS	3.3
1	B	1484	GLU	3.3
1	D	3101	ASN	3.3
1	B	1416	GLU	3.2
1	D	3034	ASN	3.2
1	B	1399	ASP	3.2
1	B	1039	ASN	3.1
1	B	1575	CYS	3.1
1	B	1441	PRO	3.1
1	B	1053	ASP	3.1
1	C	2248	LYS	3.1
1	D	3441	PRO	3.1
1	A	110	SER	3.0
1	D	3053	ASP	3.0
1	D	3069	CYS	3.0
1	D	3411	ASN	2.9
1	D	3399	ASP	2.9
1	D	3421	GLN	2.8
1	A	122	TYR	2.8
1	A	405	LYS	2.8
1	C	2059	CYS	2.8
1	B	1125	ASP	2.8
1	B	1425	SER	2.8
1	A	214	HIS	2.8
1	D	3403	SER	2.8
1	D	3158	ASP	2.7
1	A	575	CYS	2.7
1	C	2122	TYR	2.7
1	D	3368	ASN	2.7
1	B	1396	ASN	2.6
1	B	1046	GLU	2.6
1	C	2033	ALA	2.6
1	C	2074	PHE	2.6
1	D	3098	GLY	2.6
1	A	248	LYS	2.6
1	C	2370	GLN	2.6
1	D	3059	CYS	2.6
1	D	3410	ASN	2.6
1	D	3107	PHE	2.6
1	D	3190	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1423	VAL	2.6
1	A	36	CYS	2.5
1	D	3397	ILE	2.5
1	C	2325	ASP	2.4
1	D	3393	ASP	2.4
1	C	2219	GLY	2.4
1	B	1409	TYR	2.4
1	B	1411	ASN	2.4
1	C	2034	ASN	2.4
1	B	1576	PRO	2.4
1	C	2575	CYS	2.4
1	A	295	VAL	2.4
1	D	3433	ARG	2.4
1	C	2115	TYR	2.4
1	B	1405	LYS	2.4
1	B	1122	TYR	2.4
1	D	3282	ASN	2.3
1	B	1435	ALA	2.3
1	D	3486	GLU	2.3
1	C	2436	GLY	2.3
1	A	69	CYS	2.3
1	B	1116	VAL	2.3
1	A	444	VAL	2.3
1	D	3280	PRO	2.3
1	D	3359	LEU	2.3
1	C	2569	CYS	2.3
1	D	3582	VAL	2.3
1	D	3293	GLY	2.3
1	D	3398	GLU	2.2
1	B	1436	GLY	2.2
1	B	1422	PHE	2.2
1	D	3186	GLU	2.2
1	D	3281	GLU	2.2
1	A	368	ASN	2.2
1	B	1034	ASN	2.2
1	D	3396	ASN	2.2
1	D	3302	ALA	2.2
1	D	3041	CYS	2.2
1	A	115	TYR	2.2
1	C	2409	TYR	2.2
1	B	1428	ARG	2.2
1	B	1581	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	2.2
1	B	1509	VAL	2.2
1	D	3314	ASP	2.2
1	D	3500	VAL	2.2
1	B	1552	GLY	2.2
1	A	318	GLN	2.1
1	A	53	ASP	2.1
1	A	158	ASP	2.1
1	D	3490	GLU	2.1
1	B	1410	ASN	2.1
1	D	3509	VAL	2.1
1	D	3130	TYR	2.1
1	B	1188	ILE	2.1
1	C	2543	GLN	2.1
1	D	3054	GLN	2.1
1	B	1101	ASN	2.1
1	B	1191	PRO	2.1
1	A	249	ASP	2.1
1	A	294	LEU	2.1
1	D	3414	LEU	2.1
1	D	3357	PHE	2.1
1	C	2036	CYS	2.1
1	B	1368	ASN	2.1
1	B	1290	GLU	2.1
1	C	2272	GLU	2.1
1	D	3416	GLU	2.1
1	D	3480	GLU	2.1
1	D	3484	GLU	2.1
1	C	2504	TYR	2.1
1	A	50	THR	2.0
1	B	1050	THR	2.0
1	A	399	ASP	2.0
1	D	3239	ASP	2.0
1	B	1412	SER	2.0
1	D	3425	SER	2.0
1	A	59	CYS	2.0
1	B	1069	CYS	2.0
1	D	3037	CYS	2.0
1	B	1415	LEU	2.0
1	A	101	ASN	2.0
1	A	533	GLY	2.0
1	D	3285	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLU	2.0
1	A	490	GLU	2.0
1	B	1401	GLU	2.0
1	C	2393	ASP	2.0
1	D	3402	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

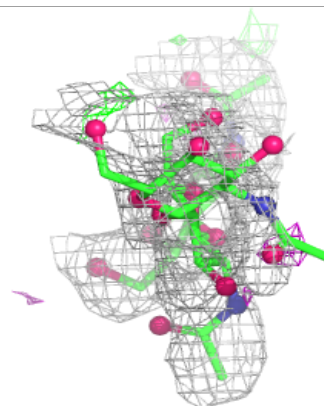
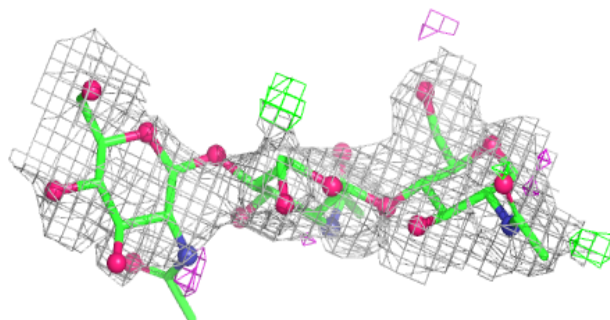
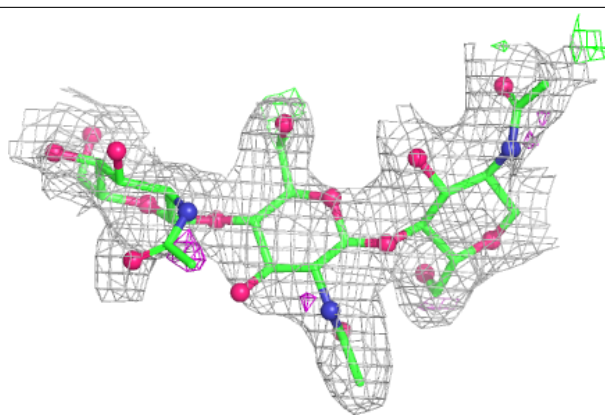
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	3	14/15	0.22	0.26	66,71,73,74	0
2	NAG	H	3	14/15	0.30	0.25	51,66,71,72	0
2	NAG	F	3	14/15	0.37	0.28	41,65,67,69	0
2	NAG	E	3	14/15	0.43	0.22	58,64,72,73	0
2	NAG	E	2	14/15	0.63	0.21	44,51,56,57	0
2	NAG	F	2	14/15	0.67	0.16	51,57,61,61	0
2	NAG	G	2	14/15	0.70	0.15	50,55,62,65	0
2	NAG	H	2	14/15	0.72	0.18	44,50,55,59	0
2	NAG	E	1	14/15	0.84	0.13	18,26,30,38	0
2	NAG	F	1	14/15	0.87	0.13	17,25,39,43	0
2	NAG	H	1	14/15	0.87	0.13	18,23,26,36	0
2	NAG	G	1	14/15	0.90	0.12	22,27,40,46	0

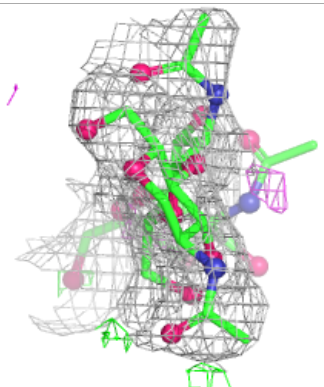
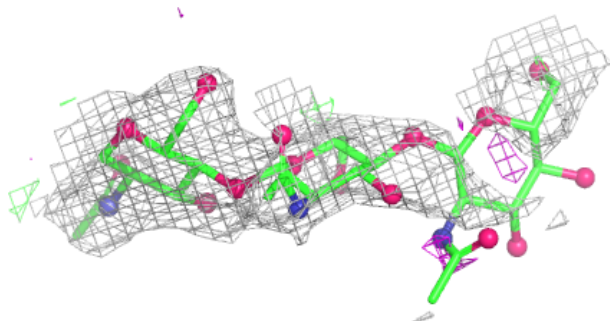
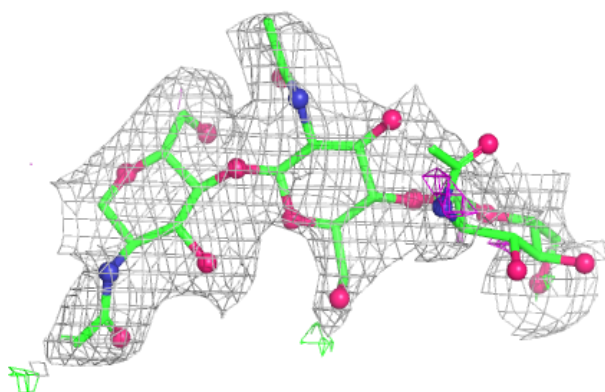
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

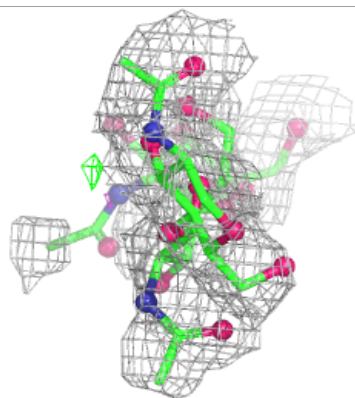
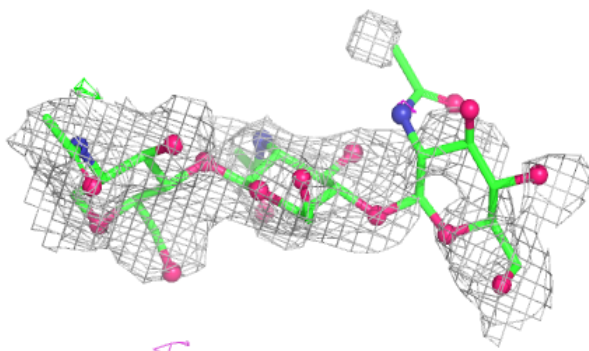
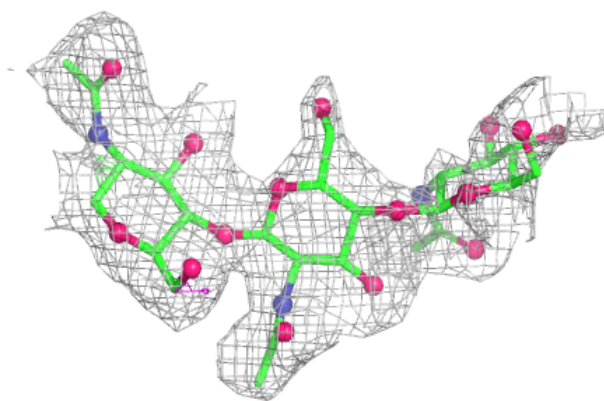
**Electron density around Chain F:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

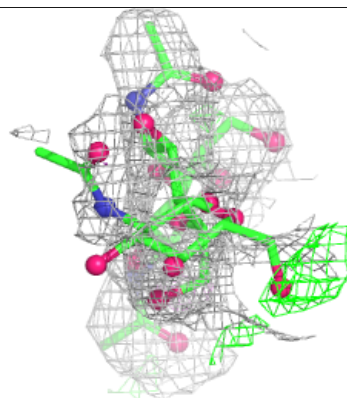
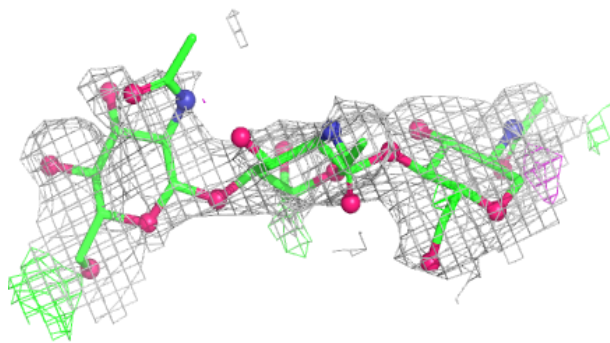
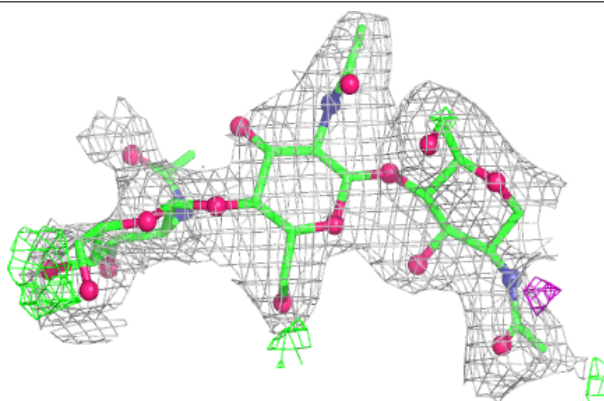


Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain H:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands ⓘ

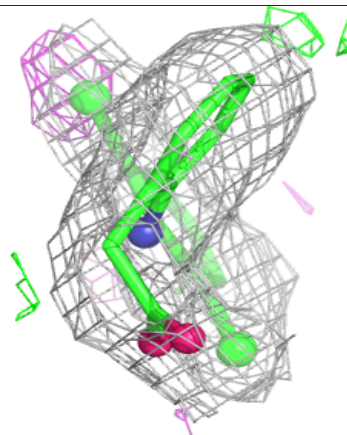
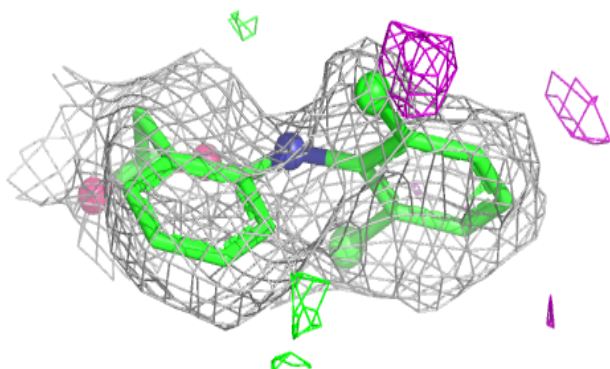
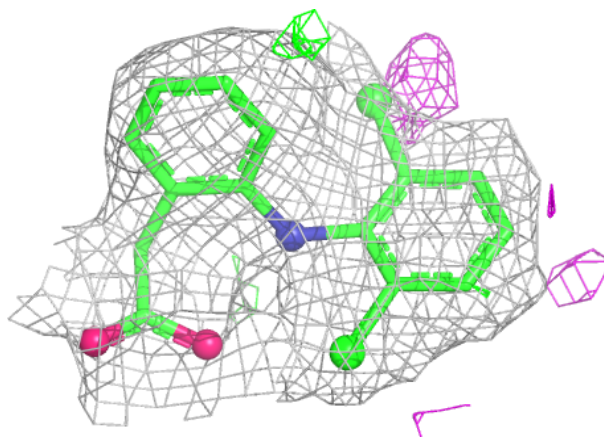
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	3661	14/15	0.62	0.19	51,55,59,61	0
3	NAG	B	1661	14/15	0.67	0.21	55,58,61,62	0
3	NAG	A	681	14/15	0.70	0.18	44,48,51,52	0
3	NAG	C	2661	14/15	0.73	0.15	45,54,61,63	0
3	NAG	B	1681	14/15	0.73	0.21	46,48,56,56	0
3	NAG	A	661	14/15	0.74	0.18	55,57,61,61	0
3	NAG	C	2681	14/15	0.75	0.17	44,46,56,57	0
3	NAG	D	3681	14/15	0.77	0.22	47,51,59,62	0
6	DIF	B	1701	19/19	0.78	0.17	13,31,51,52	0
6	DIF	A	701	19/19	0.82	0.18	28,30,46,48	0
6	DIF	C	2701	19/19	0.84	0.19	9,29,57,58	0
6	DIF	D	3701	19/19	0.84	0.15	17,38,44,55	0
4	BOG	D	3703	19/20	0.85	0.16	19,22,30,30	0
4	BOG	A	703	20/20	0.86	0.17	17,20,24,25	0
5	HEM	B	1601	43/43	0.91	0.15	4,22,48,54	0
5	HEM	D	3601	43/43	0.92	0.14	13,21,41,43	0
5	HEM	A	704	43/43	0.93	0.13	2,15,36,43	0
5	HEM	C	2601	43/43	0.94	0.12	8,20,35,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

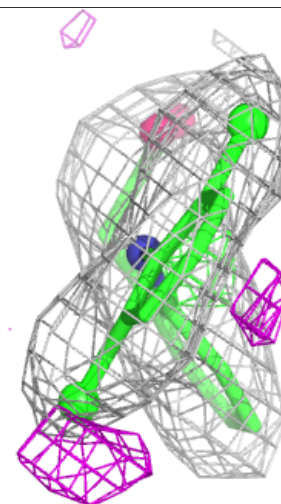
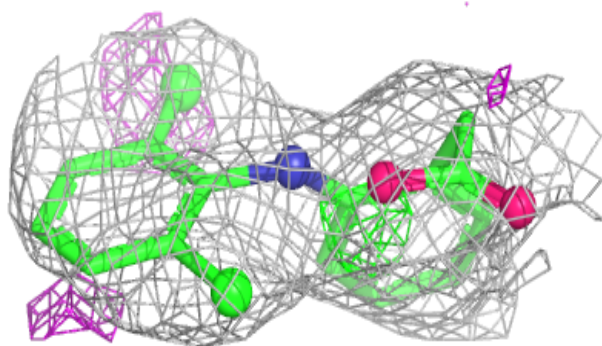
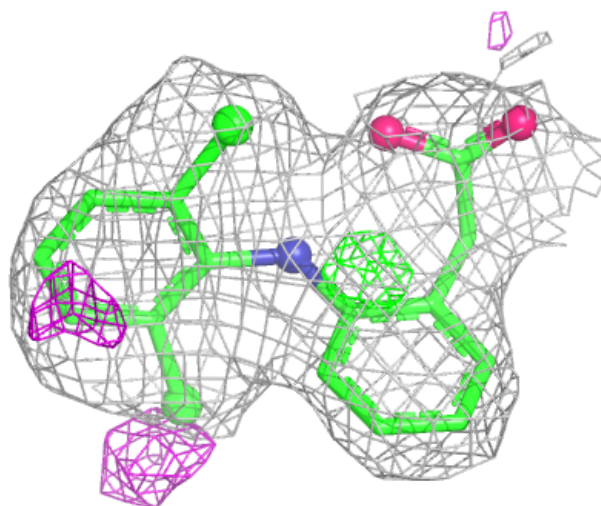
Electron density around DIF B 1701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



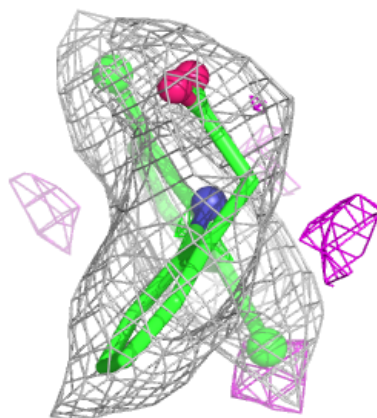
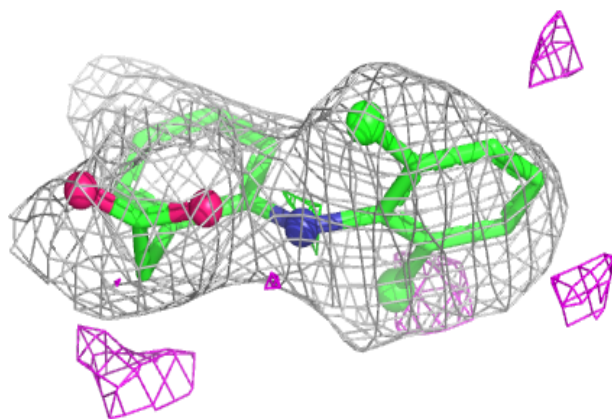
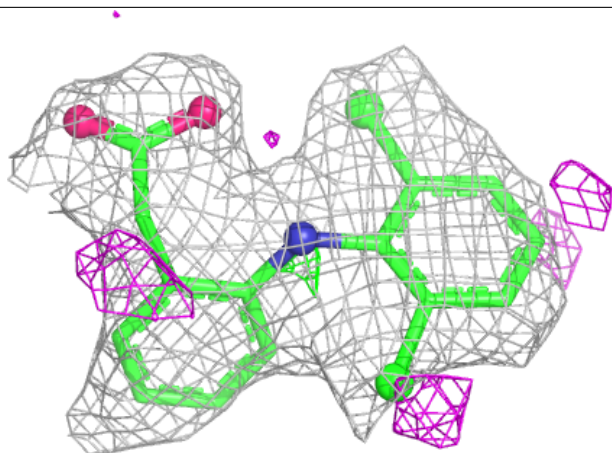
Electron density around DIF A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



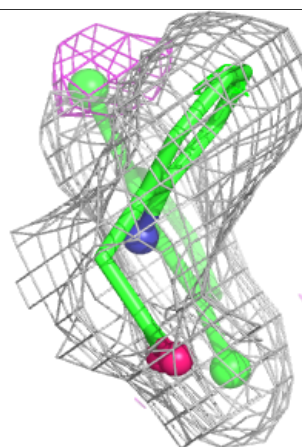
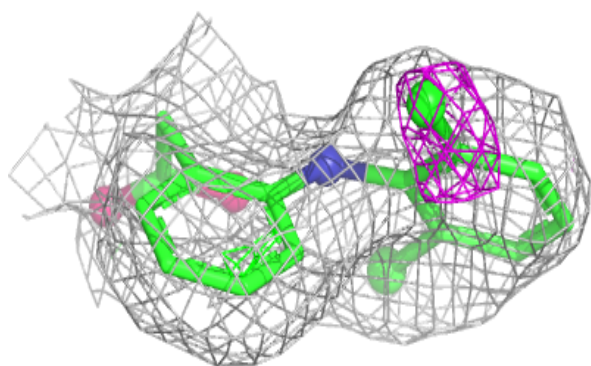
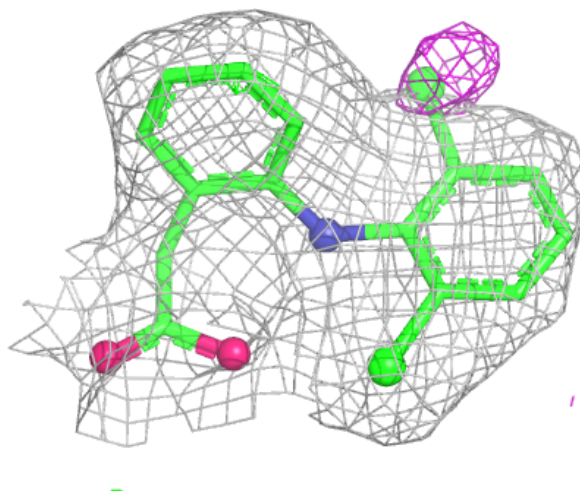
Electron density around DIF C 2701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



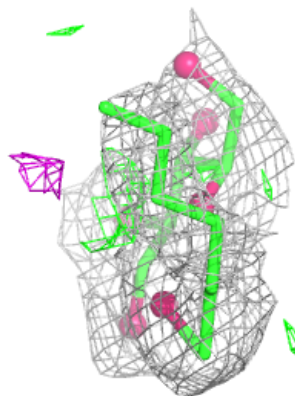
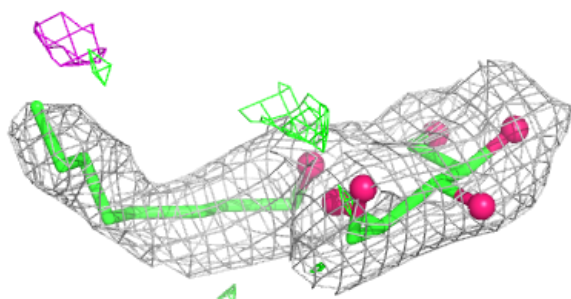
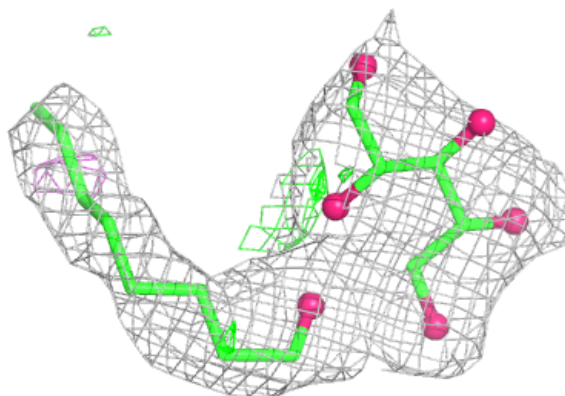
Electron density around DIF D 3701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

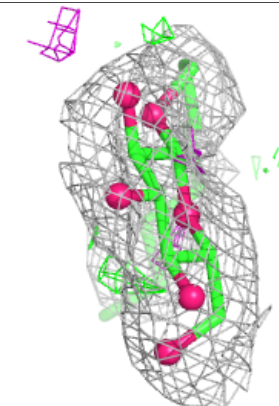
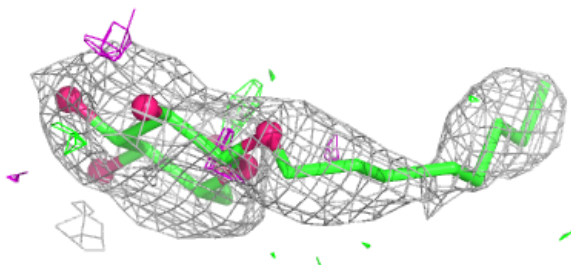
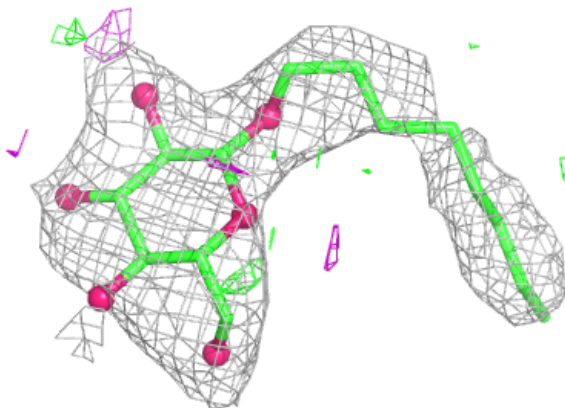


Electron density around BOG D 3703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

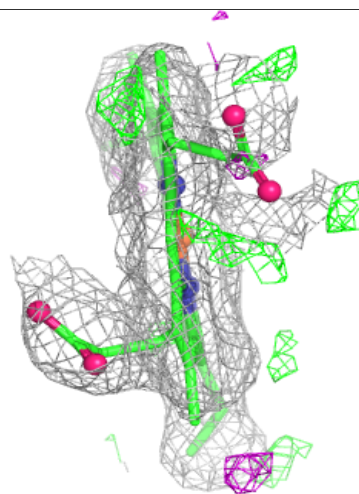
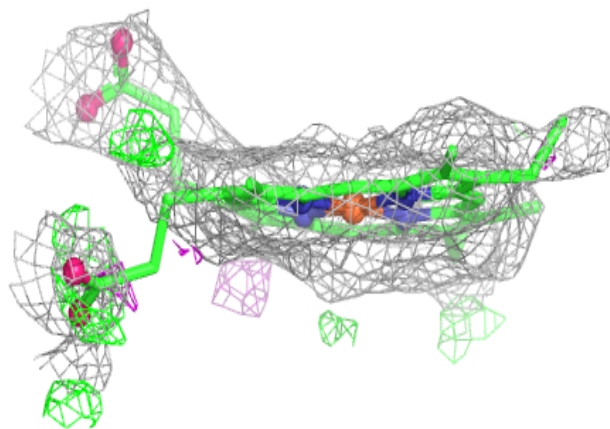
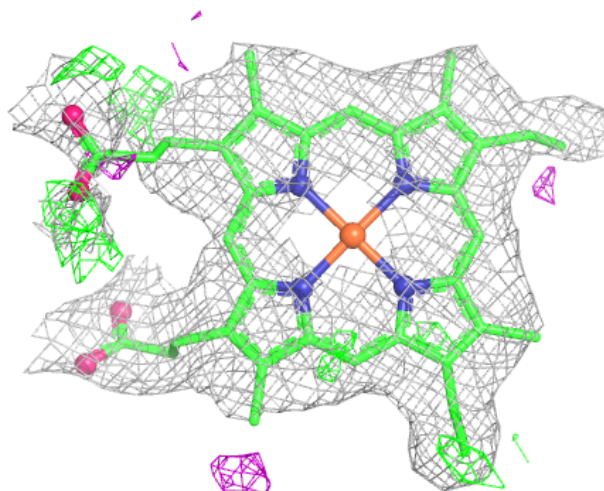
**Electron density around BOG A 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



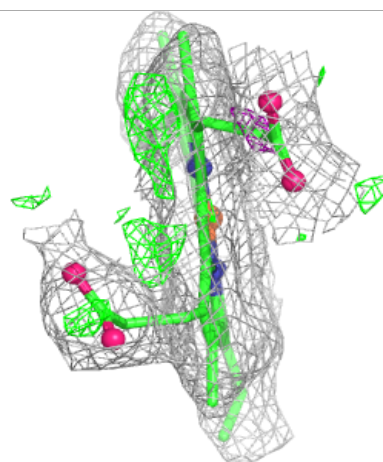
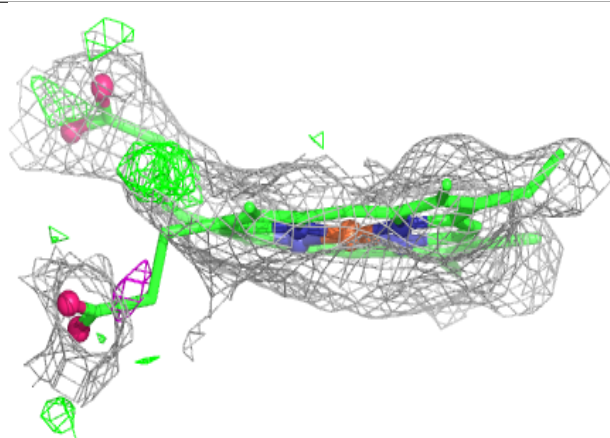
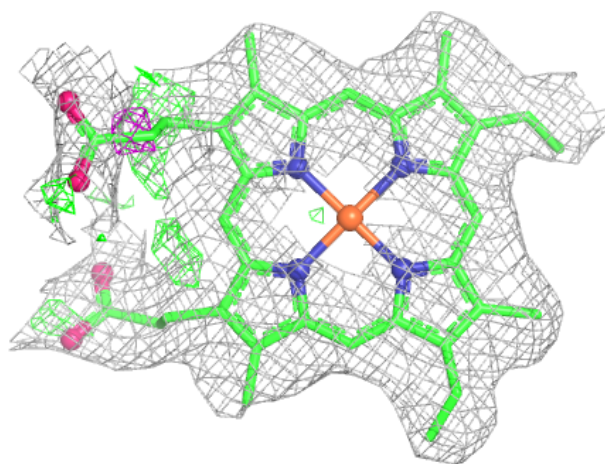
Electron density around HEM B 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



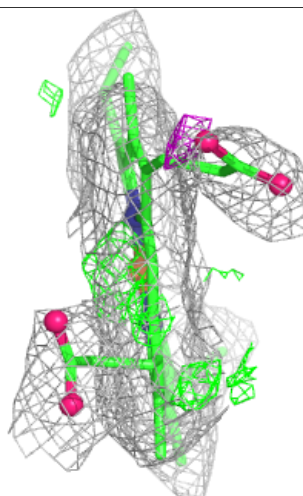
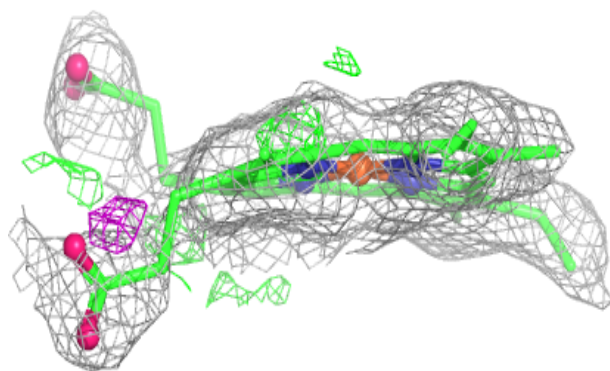
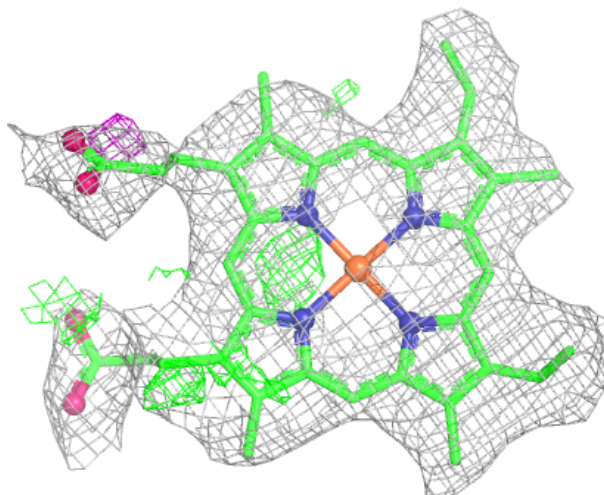
Electron density around HEM D 3601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



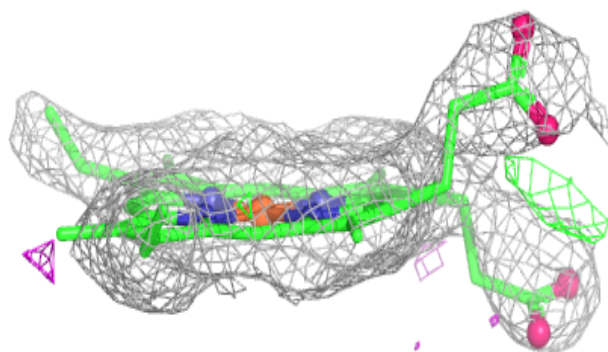
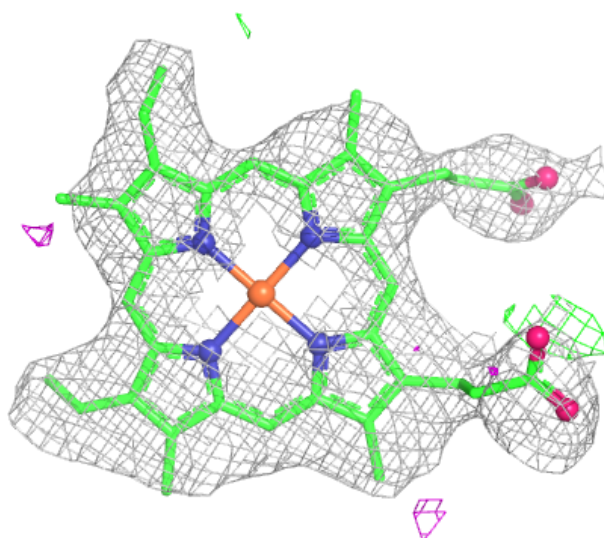
Electron density around HEM A 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 2601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.