



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 05:03 PM EST

PDB ID : 3CCC
Title : Crystal Structure of Human DPP4 in complex with a benzimidazole derivative
Authors : Wallace, M.B.; Skene, R.J.
Deposited on : 2008-02-25
Resolution : 2.71 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:

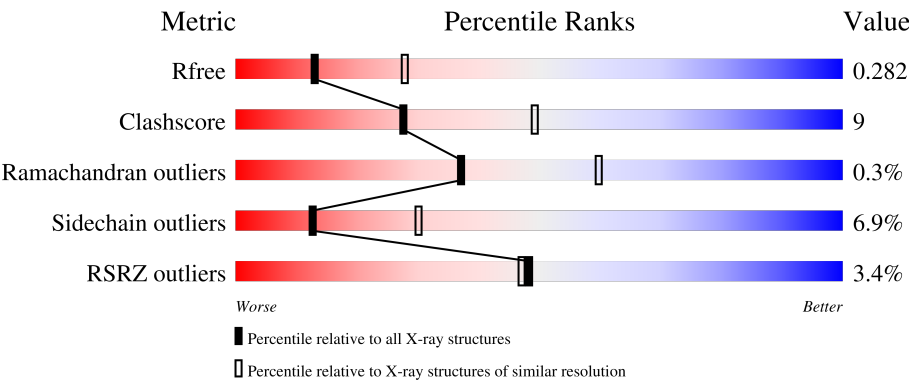
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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.



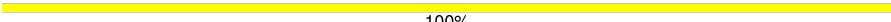


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	740	
1	B	740	
1	C	740	
1	D	740	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50% 50%
2	H	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	804	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24357 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			
1	B	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			
1	C	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



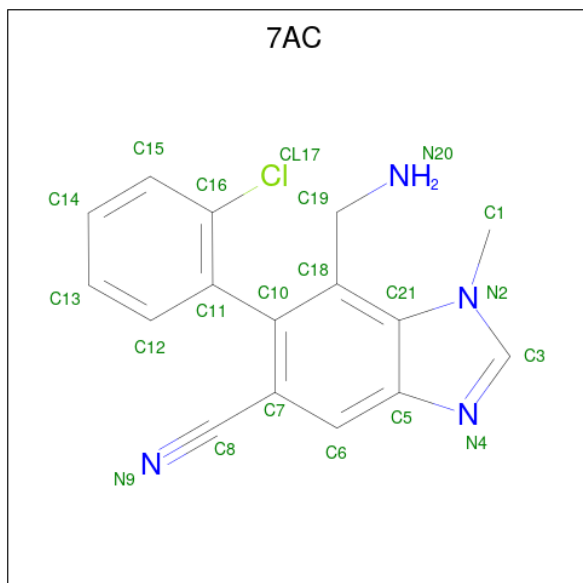
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 7-(aminomethyl)-6-(2-chlorophenyl)-1-methyl-1H-benzimidazole-5-carbonitrile (three-letter code: 7AC) (formula: C₁₆H₁₃ClN₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			21	16	1	4		
4	B	1	Total	C	Cl	N	0	0
			21	16	1	4		
4	C	1	Total	C	Cl	N	0	0
			21	16	1	4		
4	D	1	Total	C	Cl	N	0	0
			21	16	1	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		
5	B	106	Total	O	0	0
			106	106		
5	C	56	Total	O	0	0
			56	56		

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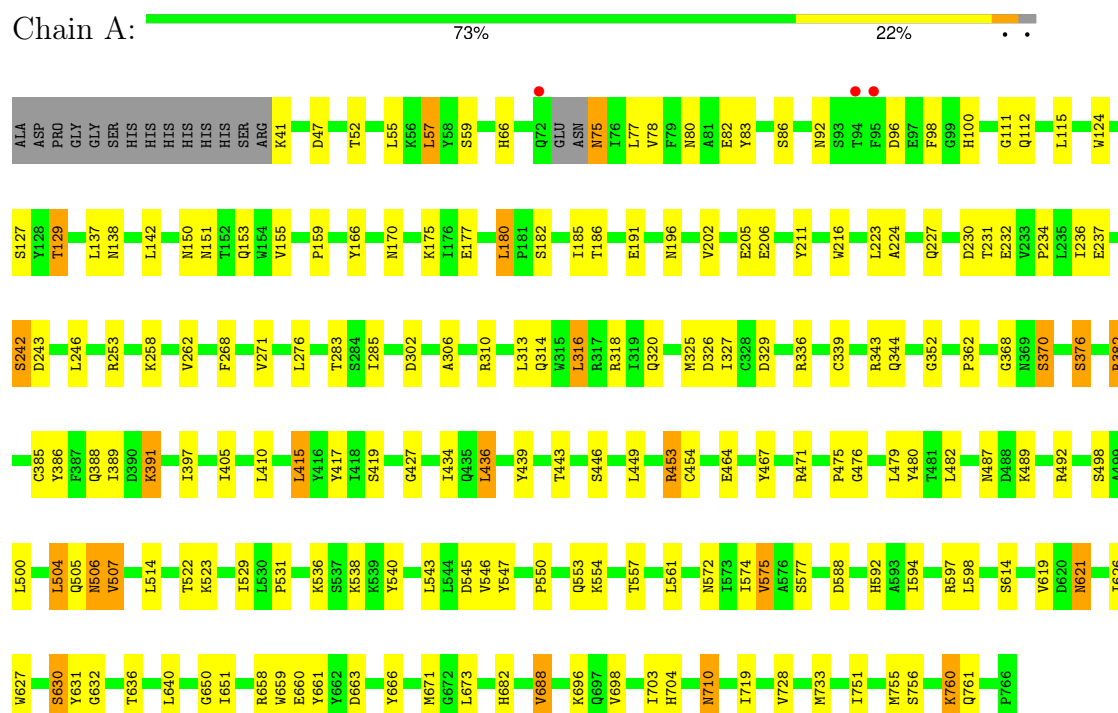
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	30	Total	O	0	0
			30	30		

3 Residue-property plots

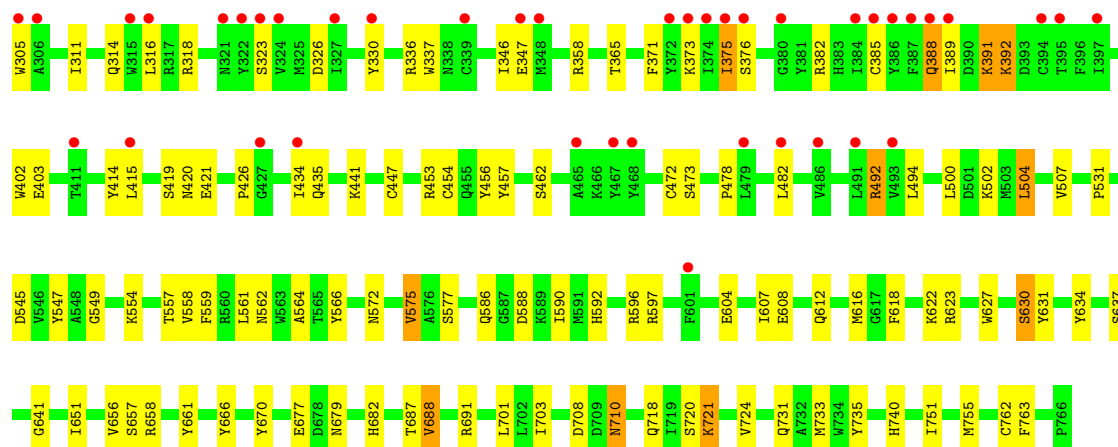
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





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

Chain E:  100%

 MAG1
MAG2

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

Chain F:  100%

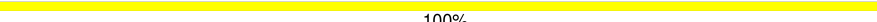
 MAG1
MAG2

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

Chain G:  50% 50%

 MAG1
MAG2

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

Chain H:  100%

 MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.90Å 121.96Å 144.28Å 90.00° 114.94° 90.00°	Depositor
Resolution (Å)	46.13 – 2.71 46.13 – 2.71	Depositor EDS
% Data completeness (in resolution range)	90.9 (46.13-2.71) 91.0 (46.13-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.267 0.223 , 0.282	Depositor DCC
R_{free} test set	4722 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24357	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 7AC, NAG

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	0.47	0/6100	0.62	1/8296 (0.0%)
1	B	0.49	0/6100	0.64	0/8296
1	C	0.46	0/6100	0.61	0/8296
1	D	0.42	0/6100	0.59	0/8296
All	All	0.46	0/24400	0.62	1/33184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5929	0	5649	109	0
1	B	5929	0	5649	109	0
1	C	5929	0	5649	97	0
1	D	5929	0	5651	114	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	56	0	52	0	0
3	B	42	0	39	0	0
3	C	42	0	39	0	0
3	D	28	0	26	0	0
4	A	21	0	13	3	0
4	B	21	0	13	3	0
4	C	21	0	13	1	0
4	D	21	0	13	2	0
5	A	85	0	0	1	0
5	B	106	0	0	0	0
5	C	56	0	0	0	0
5	D	30	0	0	0	0
All	All	24357	0	22906	420	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.40	1.01
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.05	0.99
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.50	0.93
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.54	0.90
1:C:235:LEU:HD23	1:C:253:ARG:HB3	1.54	0.86
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.59	0.82
1:D:720:SER:O	1:D:724:VAL:HG23	1.77	0.82
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.78	0.81
1:A:153:GLN:HE22	1:A:170:ASN:H	1.27	0.80
1:D:414:TYR:HE2	1:D:435:GLN:HG2	1.45	0.79
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.83	0.77
1:A:388:GLN:HB2	1:A:391:LYS:HG2	1.68	0.76
1:A:550:PRO:HG3	1:A:594:ILE:HD11	1.69	0.74
1:D:623:ARG:HH11	1:D:763:PHE:HB3	1.55	0.71
1:D:139:LYS:HG3	1:D:141:GLN:HE22	1.56	0.71
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.71	0.71
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.91	0.71
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.71	0.70
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLN:H	1:D:391:LYS:HE2	1.57	0.69
1:B:336:ARG:HH11	1:B:336:ARG:HB2	1.57	0.69
1:B:630:SER:HB2	4:B:800:7AC:N9	2.08	0.68
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.28	0.68
1:A:77:LEU:HD23	1:A:86:SER:OG	1.94	0.67
1:A:504:LEU:HA	1:A:507:VAL:CG1	2.25	0.66
1:D:80:ASN:O	1:D:84:GLY:HA2	1.96	0.66
1:B:386:TYR:O	1:B:394:CYS:HB2	1.96	0.65
1:A:554:LYS:HB3	1:A:577:SER:HB3	1.78	0.65
1:B:720:SER:O	1:B:724:VAL:HG23	1.97	0.65
1:B:78:VAL:CG2	1:B:89:PHE:HB2	2.27	0.65
1:A:329:ASP:OD2	1:A:343:ARG:NH1	2.30	0.65
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.77	0.64
1:D:588:ASP:HB3	1:D:592:HIS:CD2	2.33	0.64
1:D:102:ILE:HD13	1:D:102:ILE:H	1.63	0.64
1:C:66:HIS:HB3	1:C:467:TYR:HE1	1.63	0.63
1:B:153:GLN:HE22	1:B:170:ASN:H	1.44	0.63
1:B:588:ASP:HB3	1:B:592:HIS:HD2	1.64	0.63
1:D:72:GLN:HG3	1:D:77:LEU:HD22	1.80	0.63
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.79	0.62
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.82	0.62
1:B:148:ILE:HD11	1:B:164:LEU:HD21	1.80	0.62
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.33	0.62
1:D:473:SER:HB3	1:D:558:VAL:HG13	1.82	0.62
1:C:543:LEU:HD23	1:C:567:LEU:HD13	1.82	0.62
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.82	0.62
1:C:153:GLN:HE22	1:C:170:ASN:H	1.48	0.61
1:A:614:SER:HA	1:A:619:VAL:HB	1.82	0.61
1:C:152:THR:HG21	1:C:155:VAL:HG22	1.82	0.61
1:D:290:PRO:HG3	1:D:326:ASP:OD1	2.00	0.61
1:A:185:ILE:HG22	1:A:186:THR:HG23	1.81	0.61
1:D:121:VAL:HB	1:D:129:THR:HG22	1.83	0.61
1:C:51:ASN:HD21	1:C:54:ARG:HD2	1.64	0.61
1:C:170:ASN:N	1:C:170:ASN:HD22	1.97	0.61
1:A:175:LYS:HG2	1:A:182:SER:HB3	1.83	0.61
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.83	0.61
1:A:703:ILE:HG21	1:A:751:ILE:HD12	1.82	0.60
1:A:756:SER:O	1:A:760:LYS:HB2	2.00	0.60
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.36	0.60
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.82	0.60
1:B:82:GLU:HG2	1:B:467:TYR:OH	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.83	0.60
1:C:155:VAL:HG13	1:C:166:TYR:HB3	1.84	0.60
1:D:346:ILE:H	1:D:392:LYS:NZ	2.00	0.60
1:C:630:SER:HB2	4:C:800:7AC:N9	2.17	0.59
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.37	0.59
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.32	0.58
1:D:272:ASN:ND2	1:D:275:SER:HB3	2.17	0.58
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.85	0.58
1:A:388:GLN:HG3	1:A:391:LYS:HE2	1.85	0.58
1:A:155:VAL:HG12	1:A:166:TYR:CB	2.34	0.57
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.05	0.57
1:D:78:VAL:HG23	1:D:89:PHE:HB2	1.87	0.57
1:B:159:PRO:HG3	1:B:217:SER:O	2.05	0.57
1:A:242:SER:OG	1:A:243:ASP:N	2.38	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.87	0.56
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.71	0.56
1:C:124:TRP:HB2	1:C:204:GLU:OE1	2.05	0.56
1:D:630:SER:HB2	4:D:800:7AC:N9	2.21	0.56
1:B:135:TYR:HD1	1:B:142:LEU:HD13	1.70	0.56
1:B:657:SER:HA	1:B:688:VAL:CG1	2.35	0.56
1:D:346:ILE:H	1:D:392:LYS:HZ1	1.50	0.56
1:D:148:ILE:HG22	1:D:149:PRO:HD2	1.88	0.56
1:B:170:ASN:N	1:B:170:ASN:HD22	2.03	0.56
1:D:347:GLU:OE2	1:D:375:ILE:HG23	2.05	0.56
1:A:545:ASP:OD2	1:A:554:LYS:NZ	2.38	0.56
1:C:731:GLN:HE22	1:D:731:GLN:NE2	2.04	0.55
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.55
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.88	0.55
1:A:155:VAL:HG12	1:A:166:TYR:HB3	1.89	0.55
1:C:77:LEU:HD23	1:C:86:SER:HB2	1.88	0.55
1:A:237:GLU:HG2	1:A:253:ARG:HB3	1.89	0.55
1:A:540:TYR:HB2	1:A:574:ILE:HD12	1.88	0.55
1:C:180:LEU:HB3	1:C:181:PRO:HD2	1.89	0.55
1:D:207:VAL:O	1:D:358:ARG:HD3	2.07	0.54
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.88	0.54
1:C:438:ASP:OD2	1:C:440:THR:HB	2.07	0.54
1:C:454:CYS:HB3	1:C:457:TYR:CZ	2.42	0.54
1:B:477:LEU:HD22	1:B:500:LEU:HD23	1.90	0.54
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.43	0.54
1:D:608:GLU:O	1:D:612:GLN:HG2	2.08	0.54
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.43	0.53
1:D:389:ILE:O	1:D:389:ILE:HG22	2.09	0.53
1:D:651:ILE:HD13	1:D:755:MET:HG2	1.90	0.53
1:A:150:ASN:O	1:A:151:ASN:HB2	2.09	0.53
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.90	0.53
1:B:174:VAL:HG23	1:B:185:ILE:HD11	1.90	0.53
1:C:90:LEU:HD21	1:C:95:PHE:HE2	1.73	0.53
1:C:731:GLN:NE2	1:D:731:GLN:HE22	2.06	0.53
1:D:72:GLN:HB2	1:D:77:LEU:HD13	1.90	0.53
1:D:263:ASN:ND2	1:D:299:TYR:HE1	2.07	0.53
1:D:708:ASP:OD2	1:D:740:HIS:HB2	2.08	0.53
1:B:240:PHE:HB3	1:B:250:LYS:HG3	1.90	0.53
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.09	0.53
1:A:310:ARG:NH1	1:A:368:GLY:O	2.41	0.52
1:D:414:TYR:CE2	1:D:435:GLN:HG2	2.36	0.52
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.74	0.52
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.91	0.52
1:D:323:SER:HB3	1:D:347:GLU:HB3	1.91	0.52
1:B:154:TRP:HD1	1:B:214:LEU:HD12	1.74	0.52
1:C:598:LEU:HG	1:C:631:TYR:OH	2.09	0.52
1:A:314:GLN:NE2	1:A:362:PRO:HD3	2.25	0.52
1:C:153:GLN:OE1	1:C:170:ASN:ND2	2.43	0.52
4:B:800:7AC:C1	4:B:800:7AC:H19A	2.40	0.52
1:C:554:LYS:HB3	1:C:577:SER:HB3	1.91	0.52
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.92	0.52
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.45	0.51
1:C:484:SER:O	1:C:488:ASP:HA	2.09	0.51
1:C:731:GLN:HE22	1:D:731:GLN:HE22	1.57	0.51
1:C:64:SER:HA	1:C:463:LYS:HE2	1.91	0.51
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.45	0.51
1:C:453:ARG:NH2	1:C:477:LEU:O	2.43	0.51
1:C:258:LYS:HB3	1:C:660:GLU:O	2.11	0.51
1:D:93:SER:HA	1:D:96:ASP:HB2	1.92	0.51
1:D:679:ASN:OD1	1:D:682:HIS:HB3	2.11	0.51
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.93	0.51
1:D:115:LEU:HD21	1:D:155:VAL:HG21	1.92	0.51
1:A:75:ASN:HB3	1:A:92:ASN:HD22	1.76	0.51
1:C:471:ARG:HG3	1:C:480:TYR:CE1	2.46	0.51
1:A:453:ARG:HB2	1:A:476:GLY:HA3	1.93	0.51
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.91	0.51
1:C:651:ILE:HG21	1:C:755:MET:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HD22	1:A:83:TYR:H	1.59	0.50
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.41	0.50
1:C:543:LEU:HD11	1:C:627:TRP:HD1	1.76	0.50
1:A:318:ARG:HG2	5:A:873:HOH:O	2.11	0.50
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.42	0.50
1:B:195:TYR:HB2	1:B:228:PHE:HB2	1.94	0.50
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.94	0.50
1:D:46:THR:O	1:D:50:LYS:HB2	2.11	0.50
1:D:634:TYR:HD2	1:D:656:VAL:O	1.94	0.50
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.92	0.50
1:C:375:ILE:HD12	1:C:376:SER:O	2.11	0.50
1:C:500:LEU:HG	1:C:504:LEU:HD22	1.93	0.50
1:A:327:ILE:HG21	1:A:389:ILE:HD11	1.93	0.50
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50
1:B:65:ASP:CG	1:B:464:GLU:HB3	2.32	0.50
1:B:123:GLN:HB3	1:B:127:SER:OG	2.11	0.50
1:D:106:SER:HG	1:D:157:TRP:HD1	1.57	0.50
1:B:403:GLU:OE1	1:B:587:GLY:HA2	2.12	0.49
1:D:382:ARG:H	1:D:403:GLU:HG2	1.77	0.49
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.93	0.49
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.26	0.49
1:C:369:ASN:O	1:C:389:ILE:HB	2.11	0.49
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.41	0.49
1:A:626:ILE:O	1:A:650:GLY:HA2	2.11	0.49
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.95	0.49
1:C:714:GLN:NE2	1:D:249:PRO:HD3	2.28	0.49
1:A:206:GLU:CD	1:A:666:TYR:HB2	2.33	0.49
1:D:545:ASP:OD2	1:D:554:LYS:HE3	2.13	0.49
1:C:167:VAL:HG11	1:C:198:ILE:HG12	1.93	0.49
1:C:681:ASP:O	1:C:685:ASN:HB2	2.13	0.49
1:C:543:LEU:HD11	1:C:627:TRP:CD1	2.47	0.49
1:D:718:GLN:OE1	1:D:721:LYS:NZ	2.45	0.49
1:B:517:ILE:HD12	1:B:519:LEU:HD13	1.95	0.49
1:D:371:PHE:HE1	1:D:373:LYS:HG2	1.77	0.49
1:D:492:ARG:HB3	1:D:492:ARG:HH21	1.78	0.49
1:A:41:LYS:HD3	1:A:506:ASN:HB3	1.95	0.49
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.40	0.49
1:B:613:PHE:O	1:B:616:MET:HB2	2.13	0.49
1:C:362:PRO:HA	1:C:373:LYS:HB3	1.95	0.49
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.95	0.48
1:A:206:GLU:HG3	1:A:663:ASP:OD1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:THR:HG23	1:C:151:ASN:HA	1.95	0.48
1:D:588:ASP:HB3	1:D:592:HIS:HD2	1.77	0.48
1:B:156:THR:HG23	1:B:216:TRP:HE1	1.77	0.48
1:C:123:GLN:HB3	1:C:127:SER:OG	2.12	0.48
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.94	0.48
1:D:616:MET:HB3	1:D:618:PHE:CE1	2.49	0.48
1:D:631:TYR:HD1	4:D:800:7AC:H13	1.77	0.48
1:A:232:GLU:HB3	1:A:262:VAL:HG11	1.93	0.48
1:D:415:LEU:O	1:D:434:ILE:HG22	2.13	0.48
1:A:313:LEU:O	1:A:325:MET:HA	2.14	0.48
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.28	0.48
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.96	0.48
1:B:95:PHE:HE1	1:B:135:TYR:CD1	2.30	0.48
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.79	0.48
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.49	0.48
1:D:549:GLY:HA2	1:D:631:TYR:CE2	2.49	0.48
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.44	0.48
1:A:326:ASP:OD2	1:A:344:GLN:HG2	2.14	0.48
1:D:637:SER:HB3	1:D:688:VAL:HG21	1.96	0.48
1:D:375:ILE:HG22	1:D:376:SER:N	2.29	0.47
1:A:75:ASN:HB3	1:A:92:ASN:H	1.79	0.47
1:B:534:PHE:HZ	1:B:618:PHE:CG	2.32	0.47
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.47	0.47
1:B:456:TYR:O	1:B:472:CYS:HA	2.14	0.47
1:A:529:ILE:HB	1:A:575:VAL:HG13	1.96	0.47
1:A:155:VAL:HG12	1:A:166:TYR:HB2	1.97	0.47
1:A:710:ASN:HD22	1:A:710:ASN:C	2.18	0.47
1:B:185:ILE:HD12	1:B:185:ILE:N	2.29	0.47
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.97	0.47
1:C:626:ILE:O	1:C:650:GLY:HA2	2.13	0.47
1:D:482:LEU:HB2	1:D:494:LEU:HD21	1.97	0.47
1:B:116:LEU:O	1:B:132:TYR:HA	2.14	0.47
1:C:543:LEU:O	1:C:575:VAL:HA	2.15	0.47
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.97	0.47
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.96	0.47
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.96	0.47
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.50	0.47
1:D:420:ASN:HB2	1:D:426:PRO:HA	1.97	0.47
1:A:352:GLY:HA3	1:A:592:HIS:ND1	2.30	0.47
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.47
1:C:365:THR:O	1:C:368:GLY:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.97	0.46
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.15	0.46
1:A:112:GLN:HG2	1:A:138:ASN:HD21	1.80	0.46
1:C:157:TRP:CE3	1:C:164:LEU:HD13	2.50	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD2	2.51	0.46
1:B:317:ARG:HD2	1:B:322:TYR:HB3	1.96	0.46
1:D:95:PHE:HE1	1:D:135:TYR:CD1	2.33	0.46
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.49	0.46
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.50	0.46
1:B:334:SER:OG	1:B:336:ARG:HG3	2.15	0.46
1:D:289:ALA:HB3	1:D:294:LEU:HD21	1.96	0.46
1:D:492:ARG:HB3	1:D:492:ARG:NH2	2.30	0.46
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.55	0.46
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.98	0.46
1:D:224:ALA:HB1	1:D:268:PHE:HZ	1.79	0.46
1:A:129:THR:HG22	1:A:151:ASN:HA	1.97	0.46
1:C:499:ALA:O	1:C:502:LYS:HB3	2.16	0.46
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.51	0.46
1:B:438:ASP:OD2	1:B:440:THR:HB	2.15	0.46
1:D:564:ALA:HB1	1:D:575:VAL:HG21	1.97	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.97	0.46
1:A:376:SER:HA	1:A:382:ARG:HA	1.96	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.56	0.46
1:C:201:TRP:CZ2	1:C:710:ASN:HA	2.51	0.46
1:C:455:GLN:HB2	1:C:475:PRO:HD3	1.98	0.46
1:B:289:ALA:HB3	1:B:294:LEU:CD2	2.46	0.45
1:D:657:SER:HA	1:D:688:VAL:CG1	2.46	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD2	1.83	0.45
1:D:119:ASN:HB2	1:D:131:SER:HB2	1.98	0.45
1:D:148:ILE:HD12	1:D:148:ILE:H	1.81	0.45
1:D:376:SER:HA	1:D:382:ARG:HA	1.98	0.45
1:A:446:SER:HA	1:A:449:LEU:HG	1.98	0.45
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.45
1:A:370:SER:OG	1:A:386:TYR:CE2	2.68	0.45
1:A:543:LEU:O	1:A:575:VAL:HA	2.16	0.45
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.99	0.45
1:B:689:MET:HG3	1:B:722:ALA:HB2	1.98	0.45
1:C:527:GLN:HG2	1:C:555:ALA:HA	1.97	0.45
1:C:662:TYR:OH	1:C:710:ASN:ND2	2.49	0.45
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.98	0.45
1:C:232:GLU:HB2	1:C:262:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.46	0.45
1:A:546:VAL:HG23	1:A:632:GLY:HA2	1.99	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.99	0.45
1:C:517:ILE:CD1	1:C:612:GLN:HG3	2.47	0.45
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.98	0.45
1:B:235:LEU:HA	1:B:254:VAL:O	2.17	0.45
1:B:466:LYS:HD2	1:B:467:TYR:CE1	2.51	0.45
1:C:415:LEU:HB3	1:C:434:ILE:HG13	1.97	0.45
1:D:65:ASP:HA	1:D:462:SER:HB2	1.98	0.45
1:B:195:TYR:HB3	1:B:198:ILE:O	2.17	0.45
1:D:169:ASN:O	1:D:170:ASN:HB2	2.17	0.45
1:C:90:LEU:HD21	1:C:95:PHE:CE2	2.52	0.44
1:B:471:ARG:CG	1:B:480:TYR:CE1	3.00	0.44
1:D:191:GLU:O	1:D:192:ASP:HB2	2.17	0.44
1:C:237:GLU:OE2	1:D:251:THR:OG1	2.27	0.44
1:A:153:GLN:HB3	1:A:211:TYR:CE1	2.52	0.44
1:B:81:ALA:O	1:B:492:ARG:NH1	2.51	0.44
1:D:454:CYS:HB3	1:D:457:TYR:CE2	2.52	0.44
1:D:733:MET:HG3	1:D:735:TYR:CE2	2.53	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:336:ARG:HB2	1:B:336:ARG:NH1	2.29	0.44
1:B:598:LEU:HB2	1:B:671:MET:SD	2.57	0.44
1:C:582:GLY:HA2	1:C:594:ILE:HG12	1.99	0.44
1:D:217:SER:HB3	1:D:222:PHE:HB2	2.00	0.44
1:D:559:PHE:CZ	1:D:561:LEU:HD21	2.53	0.44
1:D:666:TYR:CE1	1:D:670:TYR:HE2	2.36	0.44
1:C:109:PRO:HG2	1:C:158:SER:O	2.18	0.44
1:C:191:GLU:O	1:C:193:ILE:HD12	2.17	0.44
1:C:723:LEU:HD22	1:C:728:VAL:HG11	2.00	0.44
1:D:148:ILE:CG2	1:D:149:PRO:HD2	2.47	0.44
1:A:621:ASN:ND2	1:A:621:ASN:H	2.14	0.44
1:A:285:ILE:HG21	1:A:336:ARG:HA	2.00	0.43
1:A:453:ARG:HH21	1:A:479:LEU:HB2	1.83	0.43
1:C:214:LEU:HD23	1:C:225:TYR:HB3	2.00	0.43
1:D:263:ASN:ND2	1:D:299:TYR:CE1	2.86	0.43
1:D:564:ALA:CB	1:D:575:VAL:HG21	2.49	0.43
1:A:554:LYS:HB3	1:A:577:SER:CB	2.47	0.43
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.00	0.43
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.43
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.99	0.43
1:C:261:ALA:O	1:C:318:ARG:NH1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ARG:NH1	1:C:679:ASN:OD1	2.52	0.43
1:A:405:ILE:HG12	1:A:419:SER:HA	2.00	0.43
1:C:415:LEU:HB3	1:C:434:ILE:CG1	2.48	0.43
1:D:246:LEU:HD23	1:D:246:LEU:HA	1.92	0.43
1:C:242:SER:HB3	1:C:246:LEU:HD12	2.01	0.43
1:D:604:GLU:HA	1:D:607:ILE:HD12	1.99	0.43
1:C:134:ILE:HG22	1:C:135:TYR:N	2.34	0.43
1:C:642:SER:OG	1:C:644:SER:HB3	2.18	0.43
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.84	0.43
1:D:657:SER:HA	1:D:688:VAL:HG12	2.00	0.43
1:D:710:ASN:C	1:D:710:ASN:HD22	2.21	0.43
1:A:427:GLY:HA2	1:A:553:GLN:OE1	2.19	0.43
1:A:588:ASP:O	1:A:592:HIS:HB2	2.18	0.43
1:B:77:LEU:HD13	1:B:88:VAL:HA	2.00	0.43
1:B:316:LEU:HD22	1:B:320:GLN:HA	2.01	0.43
1:B:327:ILE:HG12	1:B:389:ILE:HD12	2.00	0.43
1:C:475:PRO:HA	1:C:557:THR:O	2.19	0.43
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.90	0.43
1:B:77:LEU:HD12	1:B:86:SER:HB2	1.99	0.43
1:B:242:SER:OG	1:B:243:ASP:N	2.47	0.43
1:B:356:ARG:NH2	1:B:403:GLU:OE2	2.47	0.43
1:C:42:THR:HG22	1:C:508:GLN:HG3	2.00	0.43
1:D:651:ILE:HG12	1:D:701:LEU:HB3	2.01	0.43
1:B:407:ILE:HG23	1:B:415:LEU:HD21	2.00	0.42
1:D:195:TYR:O	1:D:227:GLN:HA	2.18	0.42
1:A:417:TYR:HE1	1:A:419:SER:HB3	1.84	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.19	0.42
1:B:674:PRO:O	1:B:680:LEU:HD13	2.19	0.42
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.99	0.42
1:D:735:TYR:OH	1:D:751:ILE:HA	2.18	0.42
1:A:598:LEU:O	1:A:682:HIS:NE2	2.50	0.42
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.54	0.42
1:A:696:LYS:HG3	1:A:728:VAL:CG2	2.43	0.42
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.49	0.42
1:D:596:ARG:C	1:D:597:ARG:HD2	2.40	0.42
1:B:290:PRO:HD3	1:B:315:TRP:CD1	2.55	0.42
1:C:376:SER:HA	1:C:382:ARG:HA	2.01	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.42
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.42
1:B:389:ILE:HD13	1:B:389:ILE:HA	1.86	0.42
1:A:417:TYR:CE1	1:A:419:SER:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ALA:HB3	1:B:660:GLU:HA	2.01	0.42
1:B:513:LYS:O	1:B:527:GLN:HA	2.20	0.42
1:D:661:TYR:OH	1:D:718:GLN:HG3	2.20	0.42
1:B:598:LEU:HG	1:B:631:TYR:OH	2.20	0.42
1:A:230:ASP:O	1:A:231:THR:C	2.58	0.42
1:B:117:GLU:HB2	1:B:132:TYR:CE2	2.55	0.42
1:B:340:LEU:HB2	1:B:343:ARG:CG	2.49	0.42
1:D:183:TYR:O	1:D:185:ILE:HD12	2.20	0.42
1:A:487:ASN:OD1	1:A:489:LYS:HG2	2.20	0.42
1:B:167:VAL:HA	1:B:171:ASP:O	2.20	0.42
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.01	0.42
1:C:303:VAL:HG22	1:C:313:LEU:HD12	2.01	0.42
1:A:153:GLN:NE2	1:A:170:ASN:H	2.07	0.41
1:A:631:TYR:HD1	4:A:800:7AC:H13	1.84	0.41
1:B:379:GLU:OE2	1:B:379:GLU:HA	2.20	0.41
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.84	0.41
1:C:654:ALA:N	1:C:655:PRO:HD3	2.35	0.41
1:D:299:TYR:OH	1:D:318:ARG:HG3	2.20	0.41
1:A:47:ASP:HA	1:A:52:THR:OG1	2.20	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HD13	2.02	0.41
1:A:475:PRO:HA	1:A:557:THR:O	2.19	0.41
1:B:336:ARG:NH1	1:B:337:TRP:O	2.54	0.41
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.02	0.41
1:B:654:ALA:N	1:B:655:PRO:CD	2.83	0.41
1:C:51:ASN:ND2	1:C:54:ARG:HD2	2.32	0.41
1:C:627:TRP:HB2	1:C:651:ILE:HB	2.02	0.41
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.56	0.41
1:C:134:ILE:HD11	1:C:148:ILE:HD11	2.03	0.41
1:C:172:ILE:HG22	1:C:185:ILE:HD13	2.01	0.41
1:C:462:SER:O	1:C:463:LYS:C	2.59	0.41
1:B:310:ARG:HH21	1:B:343:ARG:NH1	2.18	0.41
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.56	0.41
1:A:205:GLU:OE1	4:A:800:7AC:N20	2.53	0.41
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.56	0.41
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.56	0.41
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.55	0.41
1:B:214:LEU:HD23	1:B:225:TYR:HB3	2.03	0.41
1:B:293:MET:HG3	1:B:315:TRP:HB3	2.02	0.41
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.56	0.41
1:A:223:LEU:HB3	1:A:271:VAL:HG13	2.02	0.41
1:A:236:ILE:O	1:A:253:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:SER:HB2	4:A:800:7AC:N9	2.36	0.41
1:B:290:PRO:HG3	1:B:326:ASP:OD1	2.21	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:A:598:LEU:HD23	1:A:659:TRP:CE2	2.56	0.41
1:B:630:SER:HB2	1:B:631:TYR:H	1.55	0.41
1:C:703:ILE:HA	1:C:733:MET:O	2.21	0.41
1:B:453:ARG:NH2	1:B:477:LEU:O	2.48	0.40
1:B:545:ASP:HB3	1:B:577:SER:OG	2.21	0.40
1:C:229:ASN:O	1:C:264:PRO:HA	2.20	0.40
1:C:624:ILE:HG22	1:C:647:PHE:CD2	2.57	0.40
1:A:658:ARG:HD3	1:A:661:TYR:CZ	2.56	0.40
1:B:169:ASN:O	1:B:170:ASN:HB2	2.21	0.40
1:B:403:GLU:OE2	1:B:585:TYR:HA	2.21	0.40
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.52	0.40
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.88	0.40
1:C:542:LEU:C	1:C:542:LEU:HD23	2.41	0.40
1:D:257:PRO:HG3	1:D:264:PRO:HD3	2.03	0.40
1:D:641:GLY:O	1:D:691:ARG:HB3	2.21	0.40
1:A:96:ASP:OD1	1:A:96:ASP:N	2.52	0.40
1:A:703:ILE:HA	1:A:733:MET:O	2.22	0.40
1:C:319:ILE:HD12	1:C:319:ILE:H	1.86	0.40
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.50	0.40
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.21	0.40
1:A:111:GLY:O	1:A:137:LEU:HD12	2.22	0.40
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.57	0.40
1:C:612:GLN:HA	1:C:612:GLN:HE21	1.86	0.40
1:C:631:TYR:O	1:C:634:TYR:HB3	2.22	0.40
1:D:90:LEU:HD21	1:D:95:PHE:CE2	2.56	0.40
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.03	0.40
1:B:153:GLN:HB3	1:B:211:TYR:CE1	2.56	0.40
4:B:800:7AC:H19A	4:B:800:7AC:H1B	2.02	0.40
1:C:707:ALA:HB2	1:C:737:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	720/740 (97%)	675 (94%)	44 (6%)	1 (0%)	48	72
1	B	720/740 (97%)	667 (93%)	50 (7%)	3 (0%)	30	53
1	C	720/740 (97%)	668 (93%)	50 (7%)	2 (0%)	37	60
1	D	720/740 (97%)	642 (89%)	76 (11%)	2 (0%)	37	60
All	All	2880/2960 (97%)	2652 (92%)	220 (8%)	8 (0%)	37	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	678	ASP
1	B	366	LEU
1	A	124	TRP
1	D	282	ALA
1	D	447	CYS
1	B	389	ILE
1	C	88	VAL
1	B	88	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	649/662 (98%)	599 (92%)	50 (8%)	10	25
1	B	649/662 (98%)	610 (94%)	39 (6%)	16	36
1	C	649/662 (98%)	602 (93%)	47 (7%)	12	28
1	D	649/662 (98%)	605 (93%)	44 (7%)	13	31
All	All	2596/2648 (98%)	2416 (93%)	180 (7%)	13	30

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	59	SER
1	A	66	HIS
1	A	75	ASN
1	A	78	VAL
1	A	129	THR
1	A	142	LEU
1	A	180	LEU
1	A	191	GLU
1	A	202	VAL
1	A	242	SER
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	339	CYS
1	A	370	SER
1	A	376	SER
1	A	382	ARG
1	A	385	CYS
1	A	391	LYS
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	443	THR
1	A	453	ARG
1	A	464	GLU
1	A	482	LEU
1	A	492	ARG
1	A	498	SER
1	A	504	LEU
1	A	505	GLN
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	522	THR
1	A	523	LYS
1	A	536	LYS
1	A	538	LYS
1	A	547	TYR
1	A	575	VAL
1	A	621	ASN
1	A	630	SER

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Mol	Chain	Res	Type
1	A	660	GLU
1	A	673	LEU
1	A	688	VAL
1	A	704	HIS
1	A	710	ASN
1	A	760	LYS
1	A	761	GLN
1	B	50	LYS
1	B	80	ASN
1	B	83	TYR
1	B	90	LEU
1	B	129	THR
1	B	170	ASN
1	B	190	LYS
1	B	246	LEU
1	B	276	LEU
1	B	316	LEU
1	B	326	ASP
1	B	336	ARG
1	B	339	CYS
1	B	385	CYS
1	B	399	LYS
1	B	413	ASP
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	472	CYS
1	B	482	LEU
1	B	492	ARG
1	B	502	LYS
1	B	505	GLN
1	B	507	VAL
1	B	514	LEU
1	B	536	LYS
1	B	538	LYS
1	B	547	TYR
1	B	566	TYR
1	B	594	ILE
1	B	598	LEU
1	B	630	SER
1	B	639	VAL
1	B	673	LEU

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Mol	Chain	Res	Type
1	B	677	GLU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	C	54	ARG
1	C	66	HIS
1	C	80	ASN
1	C	90	LEU
1	C	91	GLU
1	C	129	THR
1	C	169	ASN
1	C	170	ASN
1	C	202	VAL
1	C	230	ASP
1	C	243	ASP
1	C	246	LEU
1	C	297	ASP
1	C	316	LEU
1	C	326	ASP
1	C	350	THR
1	C	375	ILE
1	C	385	CYS
1	C	392	LYS
1	C	395	THR
1	C	415	LEU
1	C	434	ILE
1	C	441	LYS
1	C	453	ARG
1	C	472	CYS
1	C	482	LEU
1	C	492	ARG
1	C	504	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	533	HIS
1	C	536	LYS
1	C	547	TYR
1	C	566	TYR
1	C	575	VAL
1	C	589	LYS
1	C	598	LEU

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Mol	Chain	Res	Type
1	C	612	GLN
1	C	615	LYS
1	C	627	TRP
1	C	673	LEU
1	C	685	ASN
1	C	688	VAL
1	C	699	GLU
1	C	710	ASN
1	C	761	GLN
1	D	80	ASN
1	D	85	ASN
1	D	92	ASN
1	D	102	ILE
1	D	110	ASP
1	D	129	THR
1	D	134	ILE
1	D	141	GLN
1	D	148	ILE
1	D	151	ASN
1	D	170	ASN
1	D	200	ASP
1	D	227	GLN
1	D	246	LEU
1	D	250	LYS
1	D	254	VAL
1	D	299	TYR
1	D	304	THR
1	D	316	LEU
1	D	336	ARG
1	D	365	THR
1	D	375	ILE
1	D	385	CYS
1	D	388	GLN
1	D	391	LYS
1	D	392	LYS
1	D	419	SER
1	D	441	LYS
1	D	453	ARG
1	D	492	ARG
1	D	502	LYS
1	D	504	LEU
1	D	507	VAL

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Mol	Chain	Res	Type
1	D	547	TYR
1	D	566	TYR
1	D	575	VAL
1	D	622	LYS
1	D	627	TRP
1	D	630	SER
1	D	677	GLU
1	D	688	VAL
1	D	710	ASN
1	D	721	LYS
1	D	762	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	80	ASN
1	A	92	ASN
1	A	123	GLN
1	A	138	ASN
1	A	141	GLN
1	A	153	GLN
1	A	170	ASN
1	A	344	GLN
1	A	455	GLN
1	A	505	GLN
1	A	506	ASN
1	A	572	ASN
1	A	621	ASN
1	A	710	ASN
1	A	761	GLN
1	B	80	ASN
1	B	100	HIS
1	B	112	GLN
1	B	123	GLN
1	B	141	GLN
1	B	151	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	338	ASN
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	572	ASN
1	B	592	HIS
1	B	595	ASN
1	B	697	GLN
1	B	710	ASN
1	B	731	GLN
1	C	51	ASN
1	C	80	ASN
1	C	123	GLN
1	C	138	ASN
1	C	151	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	227	GLN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	572	ASN
1	C	592	HIS
1	C	710	ASN
1	D	80	ASN
1	D	85	ASN
1	D	92	ASN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	388	GLN
1	D	430	ASN
1	D	505	GLN
1	D	572	ASN
1	D	710	ASN
1	D	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	E	1	1,2	14,14,15	0.58	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.77	0
2	NAG	F	1	1,2	14,14,15	0.52	0	17,19,21	1.07	1 (5%)
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	0.99	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.65	0	17,19,21	0.87	0
2	NAG	G	2	2	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
2	NAG	H	2	2	14,14,15	0.64	0	17,19,21	1.22	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	3.61	117.03	112.19
2	F	2	NAG	C4-C3-C2	2.67	114.93	111.02
2	F	1	NAG	C2-N2-C7	-2.61	119.40	122.90
2	H	1	NAG	C1-O5-C5	2.28	115.25	112.19
2	H	2	NAG	O4-C4-C5	2.02	114.30	109.32

There are no chirality outliers.

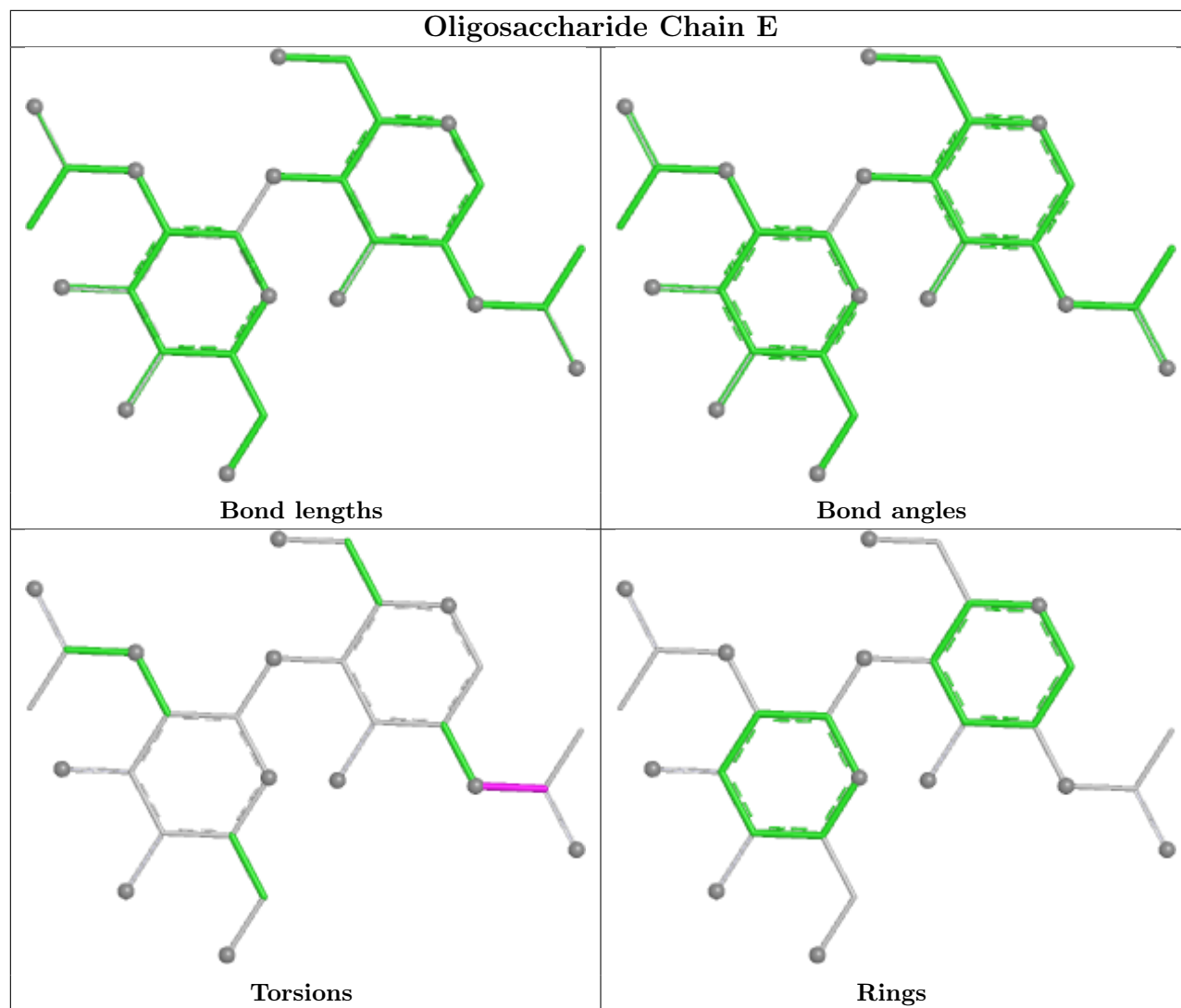
All (14) torsion outliers are listed below:

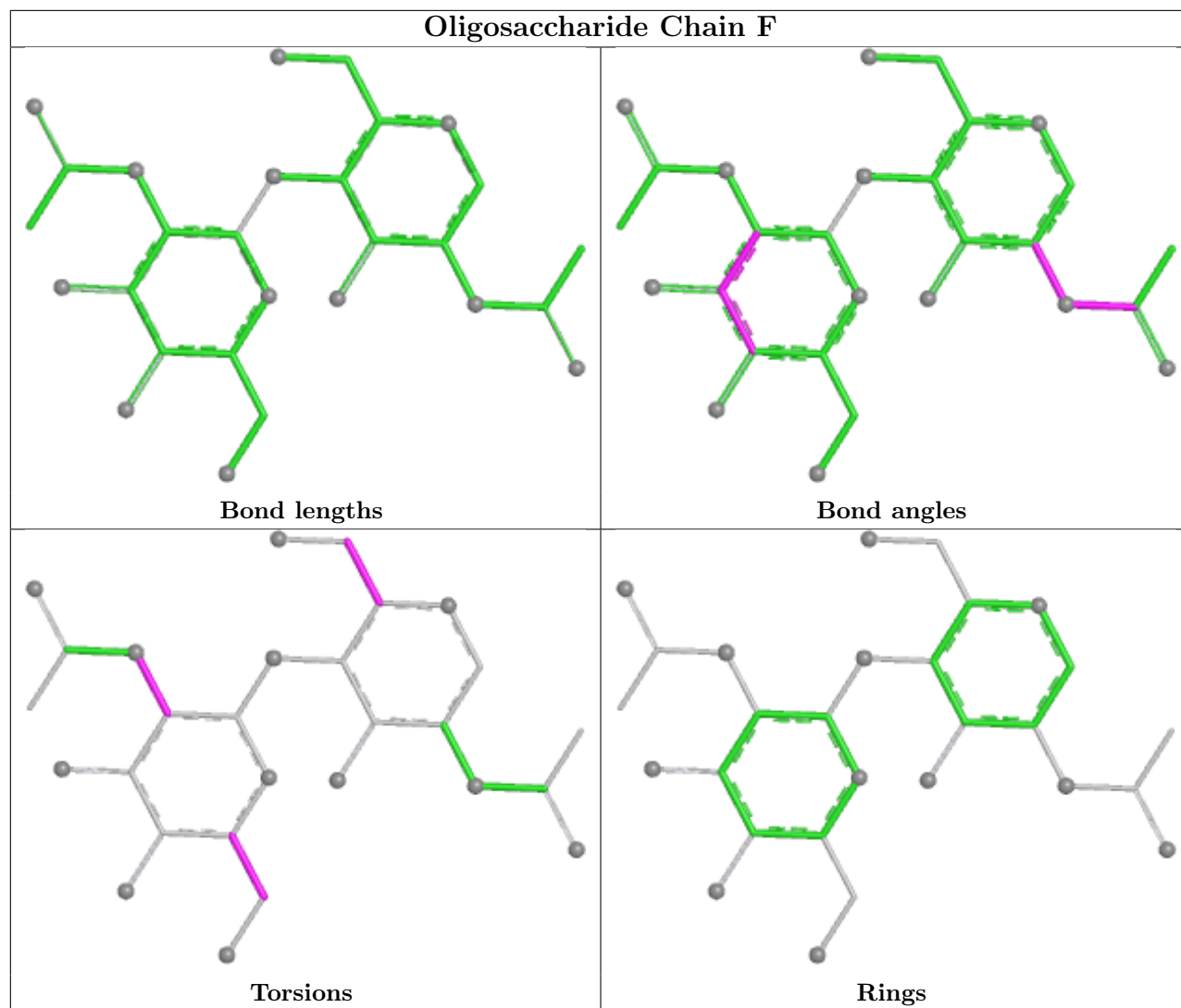
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	F	1	NAG	O5-C5-C6-O6

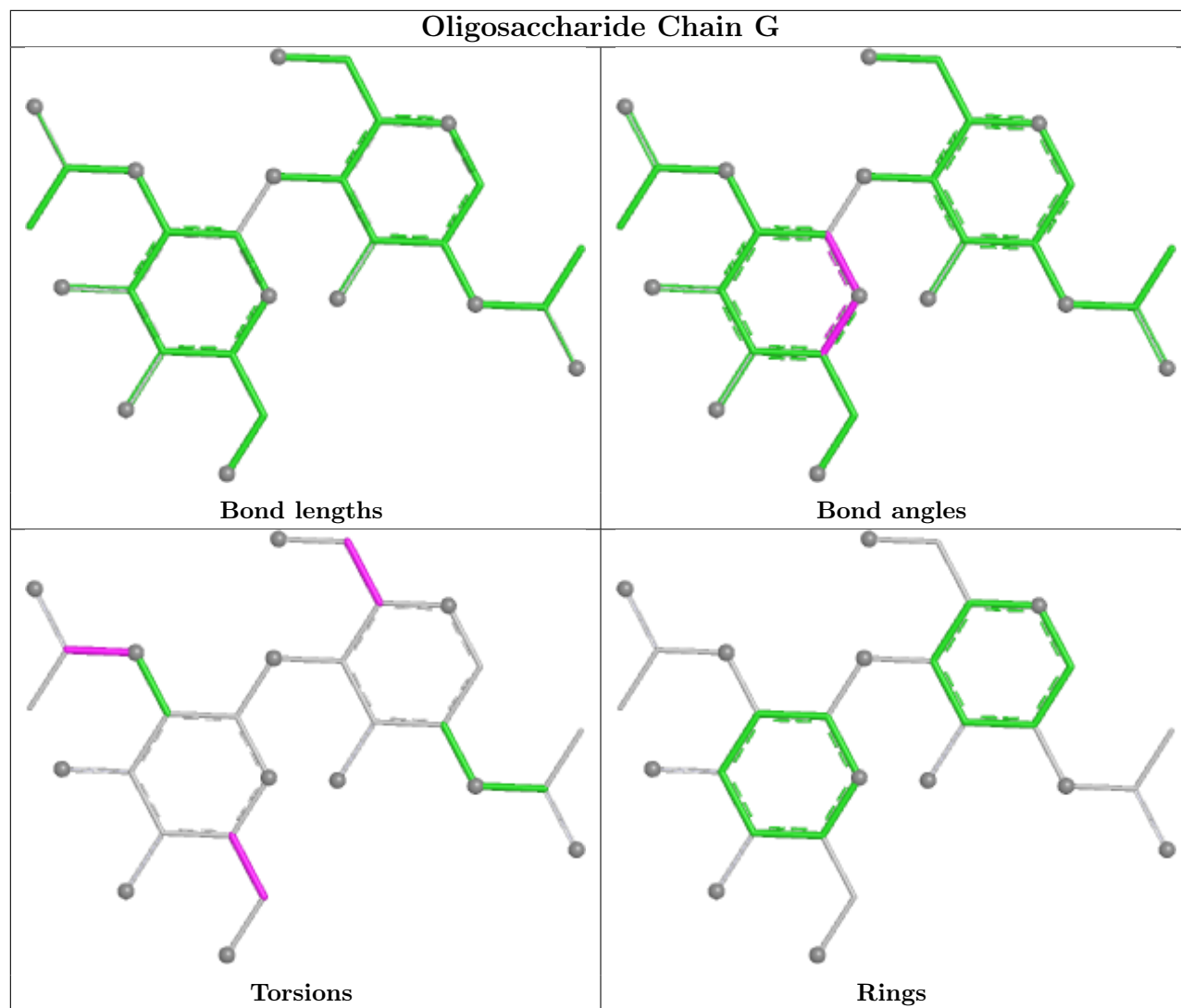
There are no ring outliers.

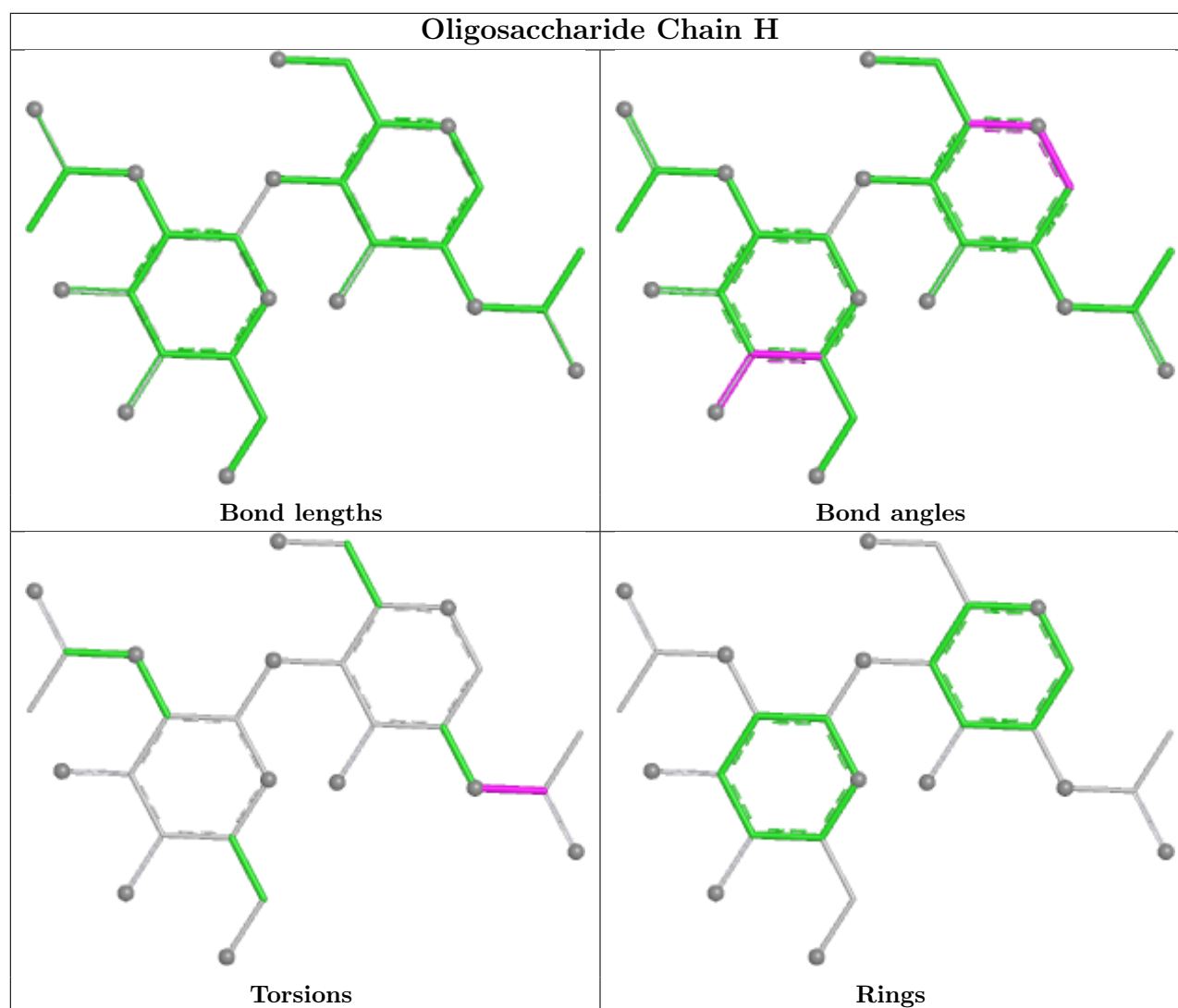
No monomer is involved in short contacts.

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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.70	2 (11%)
3	NAG	D	804	1	14,14,15	0.74	1 (7%)	17,19,21	1.29	1 (5%)
3	NAG	B	802	1	14,14,15	0.84	1 (7%)	17,19,21	1.64	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	801	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
3	NAG	C	804	1	14,14,15	0.82	1 (7%)	17,19,21	1.24	2 (11%)
3	NAG	D	801	1	14,14,15	0.65	0	17,19,21	1.41	1 (5%)
3	NAG	B	801	1	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
4	7AC	C	800	-	19,23,23	1.13	2 (10%)	19,33,33	1.13	2 (10%)
3	NAG	B	805	1	14,14,15	0.63	0	17,19,21	1.42	1 (5%)
3	NAG	A	802	1	14,14,15	0.53	0	17,19,21	1.55	2 (11%)
4	7AC	D	800	-	19,23,23	1.20	2 (10%)	19,33,33	1.40	2 (10%)
4	7AC	A	800	-	19,23,23	1.40	3 (15%)	19,33,33	1.48	3 (15%)
3	NAG	A	803	1	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	NAG	C	801	1	14,14,15	0.73	0	17,19,21	1.24	1 (5%)
4	7AC	B	800	-	19,23,23	1.29	3 (15%)	19,33,33	1.75	2 (10%)
3	NAG	C	805	1	14,14,15	0.64	0	17,19,21	1.48	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
3	NAG	A	806	1	-	2/6/23/26	0/1/1/1
3	NAG	D	804	1	-	4/6/23/26	0/1/1/1
3	NAG	B	802	1	-	5/6/23/26	0/1/1/1
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1
3	NAG	C	804	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	D	801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	801	1	-	4/6/23/26	0/1/1/1
4	7AC	C	800	-	-	0/3/8/8	0/3/3/3
3	NAG	B	805	1	-	4/6/23/26	0/1/1/1
3	NAG	A	802	1	-	2/6/23/26	0/1/1/1
4	7AC	D	800	-	-	0/3/8/8	0/3/3/3
4	7AC	A	800	-	-	0/3/8/8	0/3/3/3
3	NAG	A	803	1	-	2/6/23/26	0/1/1/1
3	NAG	C	801	1	-	4/6/23/26	0/1/1/1
4	7AC	B	800	-	-	0/3/8/8	0/3/3/3
3	NAG	C	805	1	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	7AC	C18-C10	-4.22	1.39	1.42
4	B	800	7AC	C18-C10	-3.20	1.39	1.42
4	D	800	7AC	C18-C10	-2.84	1.40	1.42
4	C	800	7AC	C3-N4	-2.62	1.29	1.34
4	C	800	7AC	C18-C10	-2.54	1.40	1.42
3	C	804	NAG	C1-C2	2.49	1.55	1.52
4	D	800	7AC	C3-N4	-2.43	1.30	1.34
4	B	800	7AC	C3-N4	-2.37	1.30	1.34
3	D	804	NAG	C1-C2	2.31	1.55	1.52
4	A	800	7AC	C3-N4	-2.23	1.30	1.34
3	B	802	NAG	C1-C2	2.22	1.55	1.52
4	A	800	7AC	C7-C10	-2.06	1.41	1.44
4	B	800	7AC	C18-C21	-2.04	1.39	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	806	NAG	C1-O5-C5	5.16	119.10	112.19
3	D	801	NAG	C1-O5-C5	5.06	118.97	112.19
4	B	800	7AC	C10-C7-C8	-5.05	117.68	123.49
3	B	805	NAG	C1-O5-C5	4.99	118.88	112.19
3	B	802	NAG	C4-C3-C2	4.73	117.94	111.02
3	D	804	NAG	C1-O5-C5	4.61	118.36	112.19
3	A	802	NAG	C1-O5-C5	4.51	118.23	112.19
3	C	805	NAG	C1-O5-C5	4.23	117.86	112.19
4	B	800	7AC	C16-C11-C12	4.19	120.17	115.38
3	A	801	NAG	C1-O5-C5	3.98	117.52	112.19
4	D	800	7AC	C10-C7-C8	-3.97	118.92	123.49
3	C	801	NAG	C4-C3-C2	3.80	116.58	111.02
4	A	800	7AC	C16-C11-C12	3.70	119.62	115.38
4	A	800	7AC	C10-C7-C8	-3.66	119.28	123.49
4	D	800	7AC	C16-C11-C12	3.26	119.11	115.38
4	C	800	7AC	C16-C11-C12	3.21	119.05	115.38
3	B	801	NAG	C1-O5-C5	3.05	116.27	112.19
3	C	804	NAG	C4-C3-C2	2.77	115.08	111.02
3	A	801	NAG	O5-C5-C6	2.51	112.55	107.66
3	B	802	NAG	C2-N2-C7	2.48	126.23	122.90
3	A	803	NAG	C1-O5-C5	2.47	115.50	112.19
3	A	806	NAG	O5-C5-C6	2.33	112.20	107.66
3	C	804	NAG	O5-C5-C6	2.32	112.19	107.66
3	A	802	NAG	O5-C5-C6	2.25	112.04	107.66
4	C	800	7AC	C10-C7-C8	-2.15	121.01	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	7AC	C13-C12-C11	-2.04	118.16	120.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	804	NAG	C1

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	B	801	NAG	C8-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	B	802	NAG	C8-C7-N2-C2
3	B	802	NAG	O7-C7-N2-C2
3	C	801	NAG	C8-C7-N2-C2
3	C	801	NAG	O7-C7-N2-C2
3	C	804	NAG	C8-C7-N2-C2
3	C	804	NAG	O7-C7-N2-C2
3	D	804	NAG	C8-C7-N2-C2
3	D	804	NAG	O7-C7-N2-C2
3	B	802	NAG	C4-C5-C6-O6
3	D	804	NAG	C4-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	D	804	NAG	O5-C5-C6-O6
3	A	802	NAG	O5-C5-C6-O6
3	A	802	NAG	C4-C5-C6-O6
3	B	802	NAG	O5-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	A	806	NAG	O5-C5-C6-O6
3	D	801	NAG	O5-C5-C6-O6
3	B	805	NAG	C8-C7-N2-C2
3	C	801	NAG	C4-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	B	805	NAG	O7-C7-N2-C2
3	C	805	NAG	C8-C7-N2-C2
3	D	801	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	805	NAG	O7-C7-N2-C2
3	A	806	NAG	C4-C5-C6-O6
3	B	805	NAG	C4-C5-C6-O6
3	B	802	NAG	C3-C2-N2-C7
3	B	805	NAG	O5-C5-C6-O6

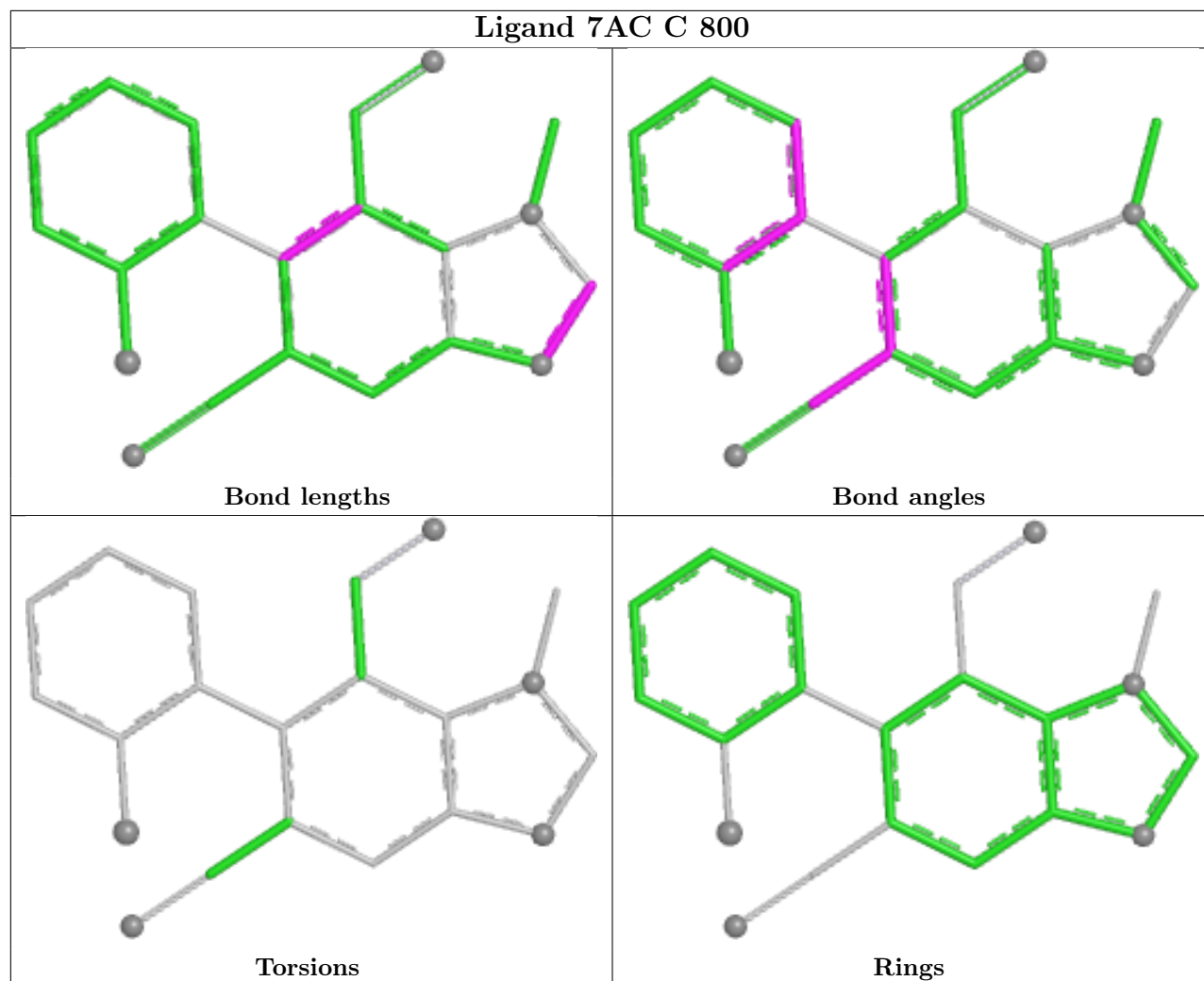
There are no ring outliers.

4 monomers are involved in 9 short contacts:

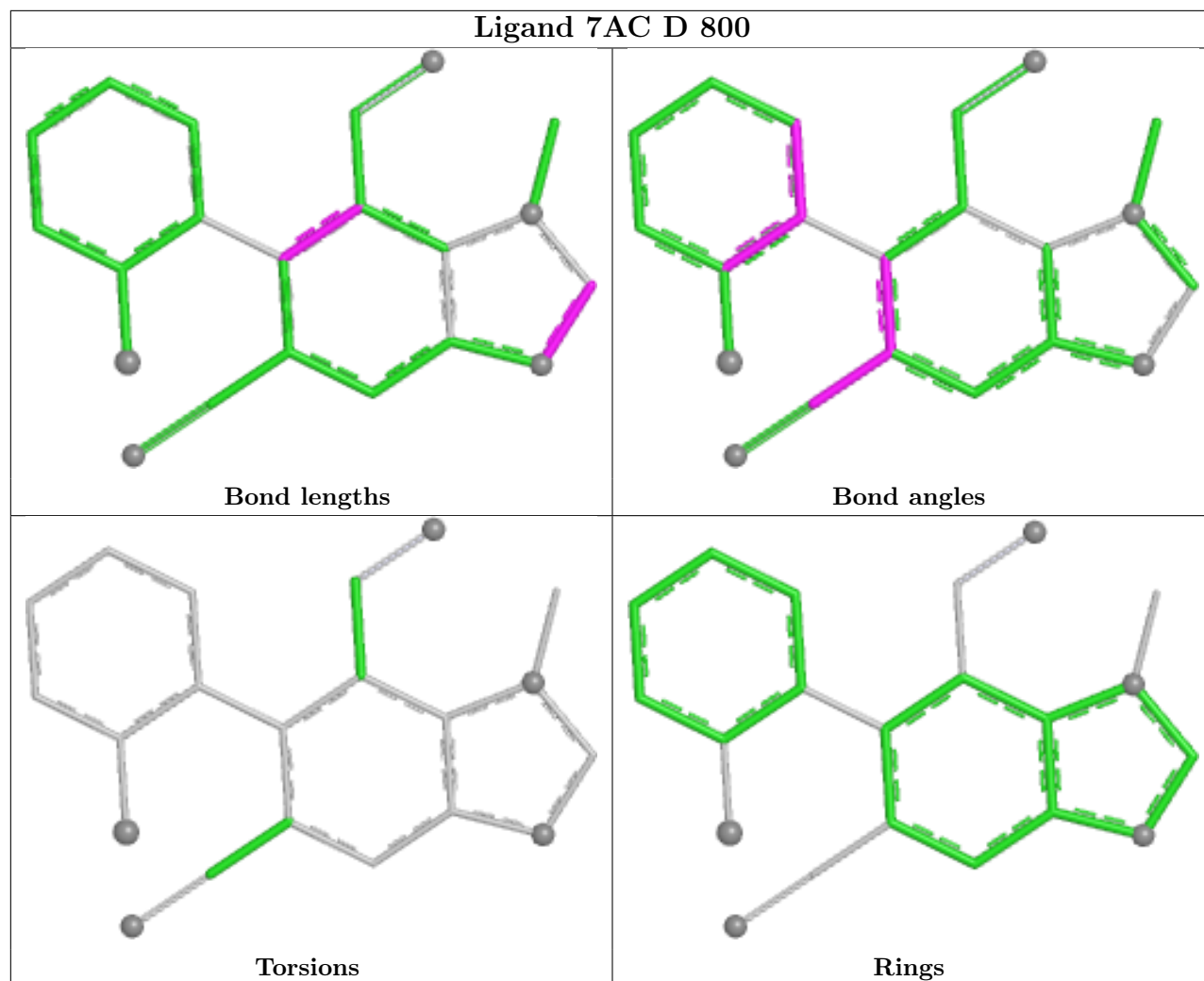
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	800	7AC	1	0
4	D	800	7AC	2	0
4	A	800	7AC	3	0
4	B	800	7AC	3	0

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.

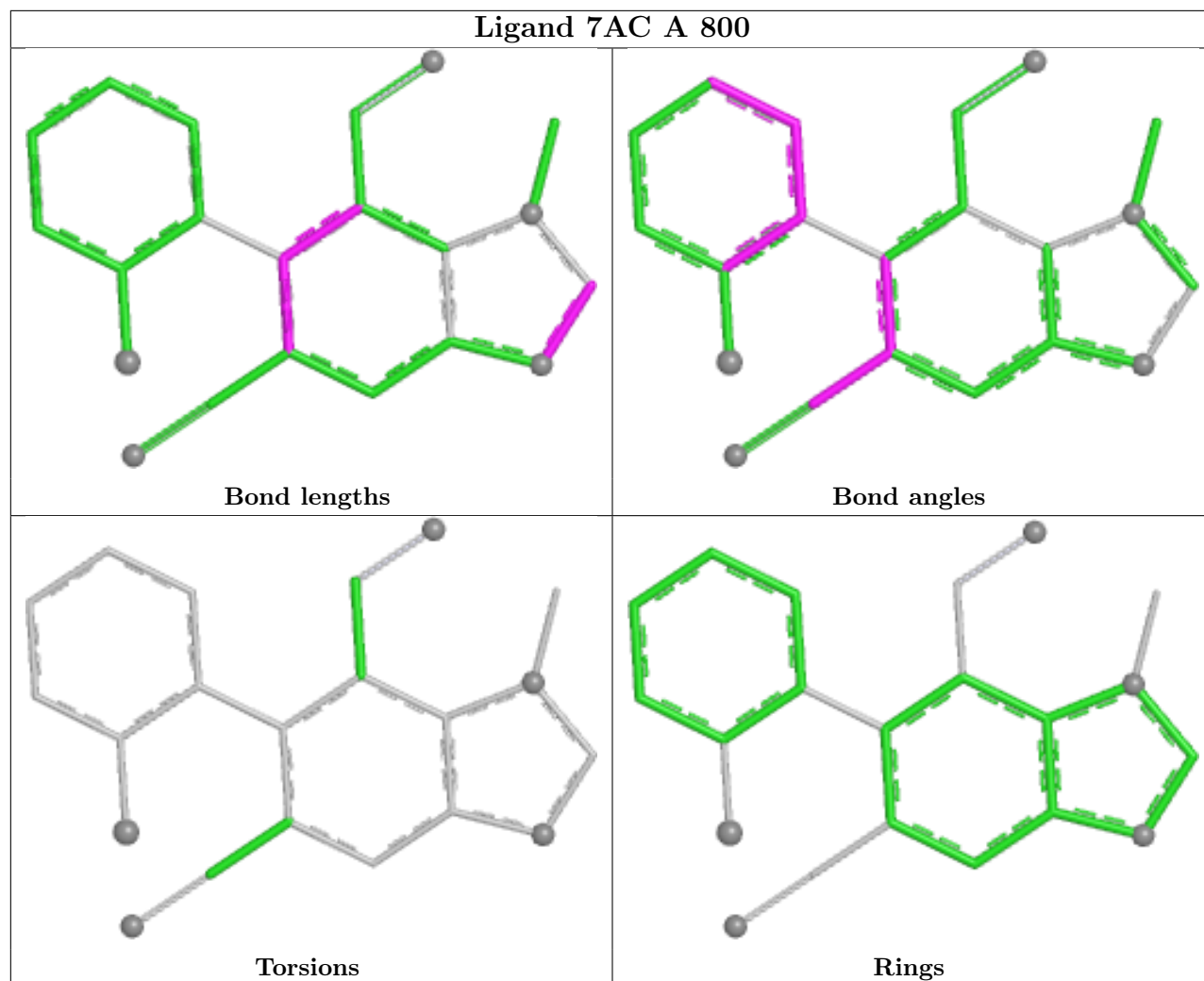
Ligand 7AC C 800

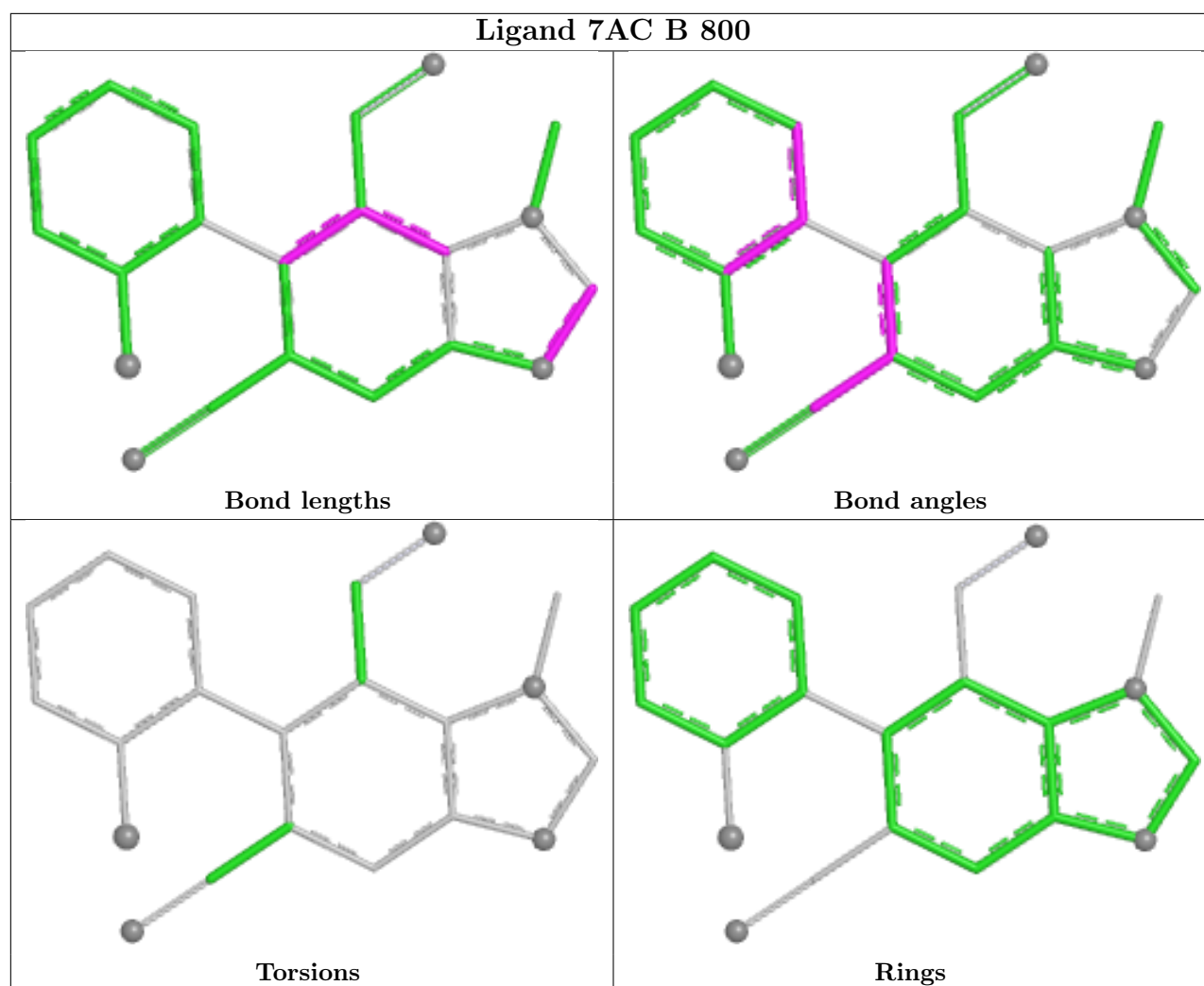


Ligand 7AC D 800



Ligand 7AC A 800





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	724/740 (97%)	-0.02	3 (0%) 89 88	32, 52, 73, 108	0
1	B	724/740 (97%)	-0.13	4 (0%) 85 85	28, 49, 75, 102	0
1	C	724/740 (97%)	0.19	17 (2%) 61 60	30, 57, 84, 99	0
1	D	724/740 (97%)	0.73	75 (10%) 13 13	40, 69, 95, 124	0
All	All	2896/2960 (97%)	0.19	99 (3%) 48 47	28, 55, 86, 124	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	GLY	4.0
1	C	143	ILE	3.9
1	D	63	ILE	3.8
1	D	384	ILE	3.8
1	D	322	TYR	3.6
1	D	102	ILE	3.6
1	D	385	CYS	3.4
1	D	90	LEU	3.3
1	C	88	VAL	3.3
1	C	490	GLY	3.3
1	D	375	ILE	3.2
1	D	69	LEU	3.2
1	D	372	TYR	3.2
1	D	306	ALA	3.2
1	D	415	LEU	3.2
1	D	388	GLN	3.1
1	D	176	ILE	3.1
1	B	148	ILE	3.1
1	D	395	THR	3.1
1	D	467	TYR	3.0
1	D	479	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	411	THR	3.0
1	D	373	LYS	2.9
1	A	95	PHE	2.8
1	D	323	SER	2.8
1	D	601	PHE	2.8
1	D	397	ILE	2.7
1	D	292	SER	2.7
1	D	394	CYS	2.7
1	D	164	LEU	2.7
1	C	90	LEU	2.7
1	D	141	GLN	2.7
1	C	142	LEU	2.7
1	D	339	CYS	2.7
1	C	491	LEU	2.6
1	C	152	THR	2.6
1	C	226	ALA	2.6
1	D	380	GLY	2.6
1	D	348	MET	2.6
1	B	137	LEU	2.6
1	C	137	LEU	2.6
1	D	387	PHE	2.5
1	D	389	ILE	2.5
1	C	145	GLU	2.5
1	D	142	LEU	2.5
1	C	330	TYR	2.5
1	A	72	GLN	2.5
1	D	162	HIS	2.5
1	D	276	LEU	2.5
1	D	167	VAL	2.5
1	D	327	ILE	2.5
1	C	89	PHE	2.4
1	D	324	VAL	2.4
1	D	291	ALA	2.4
1	D	222	PHE	2.4
1	D	330	TYR	2.4
1	D	78	VAL	2.3
1	C	176	ILE	2.3
1	D	376	SER	2.3
1	D	468	TYR	2.3
1	D	113	PHE	2.3
1	D	214	LEU	2.3
1	D	315	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	305	TRP	2.3
1	D	223	LEU	2.3
1	B	274	ASP	2.2
1	C	102	ILE	2.2
1	D	491	LEU	2.2
1	D	273	THR	2.2
1	D	95	PHE	2.2
1	D	134	ILE	2.2
1	D	374	ILE	2.2
1	D	434	ILE	2.2
1	D	62	TRP	2.2
1	D	93	SER	2.2
1	D	149	PRO	2.2
1	D	321	ASN	2.2
1	D	88	VAL	2.2
1	D	486	VAL	2.2
1	D	137	LEU	2.2
1	D	386	TYR	2.1
1	D	159	PRO	2.1
1	A	94	THR	2.1
1	C	282	ALA	2.1
1	D	76	ILE	2.1
1	D	148	ILE	2.1
1	D	174	VAL	2.1
1	D	316	LEU	2.1
1	D	427	GLY	2.1
1	D	301	CYS	2.1
1	B	399	LYS	2.1
1	D	221	THR	2.1
1	C	270	VAL	2.1
1	C	149	PRO	2.0
1	D	347	GLU	2.0
1	D	114	ILE	2.0
1	D	482	LEU	2.0
1	D	493	VAL	2.0
1	D	465	ALA	2.0

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

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

6.3 Carbohydrates

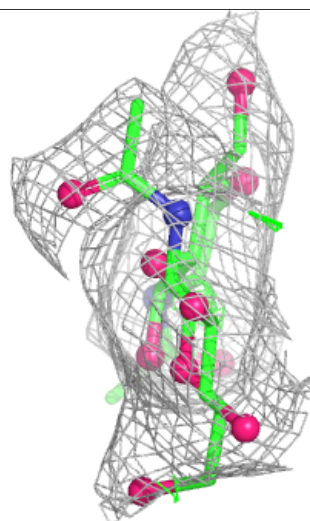
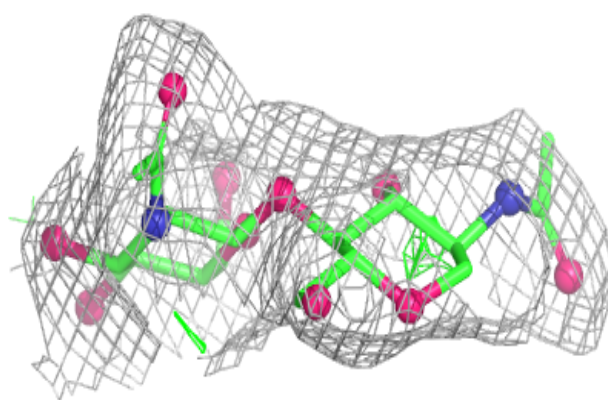
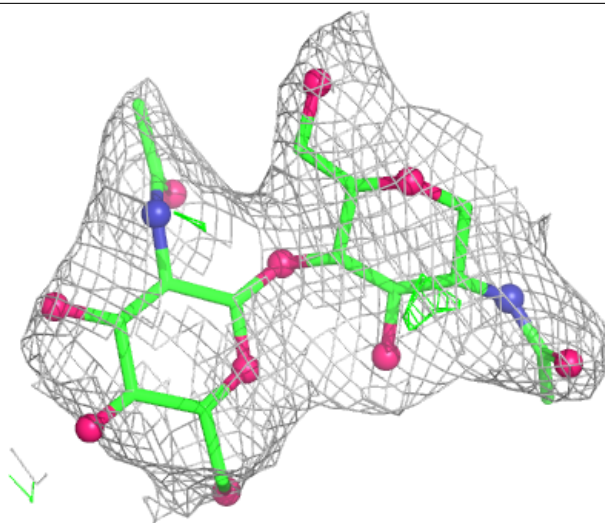
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2	14/15	0.74	0.12	86,89,90,90	0
2	NAG	H	2	14/15	0.76	0.11	82,83,84,84	0
2	NAG	E	2	14/15	0.77	0.11	82,83,85,86	0
2	NAG	H	1	14/15	0.85	0.10	76,77,78,80	0
2	NAG	F	2	14/15	0.86	0.09	74,75,77,77	0
2	NAG	E	1	14/15	0.88	0.11	67,71,75,79	0
2	NAG	G	1	14/15	0.89	0.10	71,74,78,82	0
2	NAG	F	1	14/15	0.92	0.10	63,66,69,71	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.

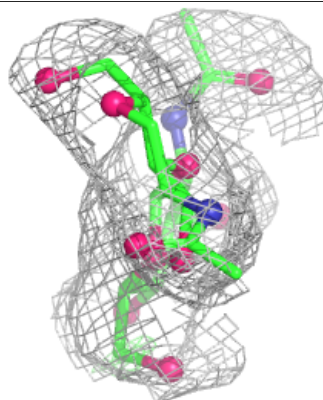
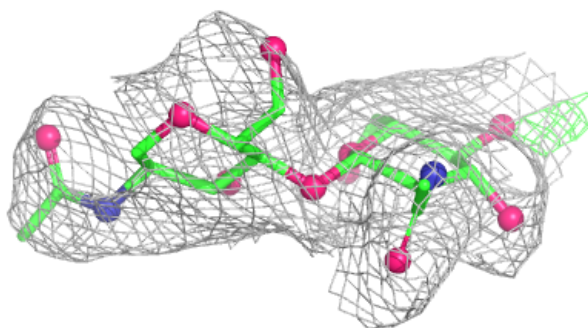
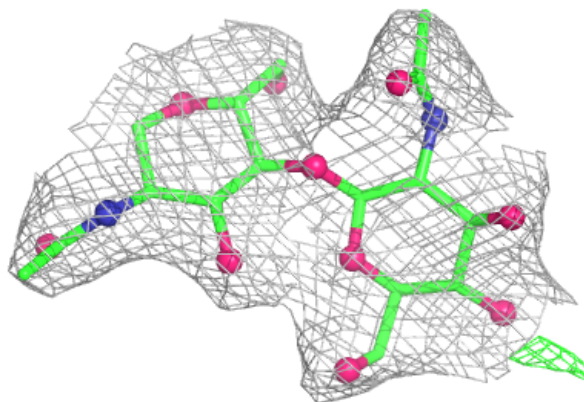
Electron density around Chain E:

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

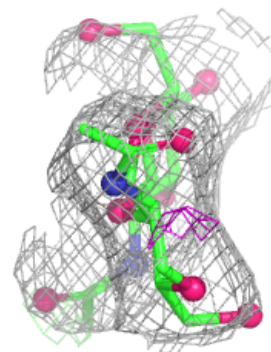
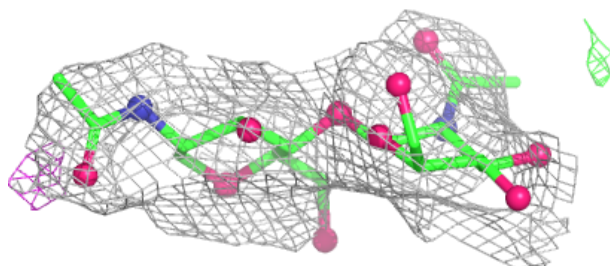
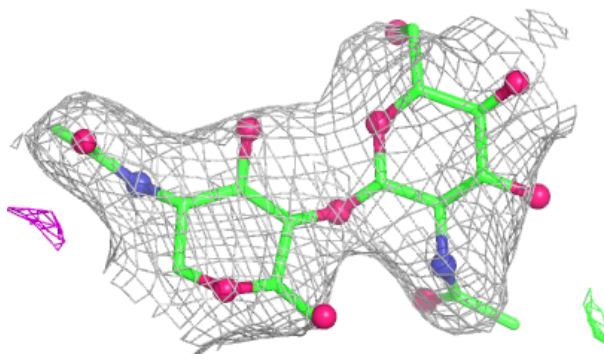


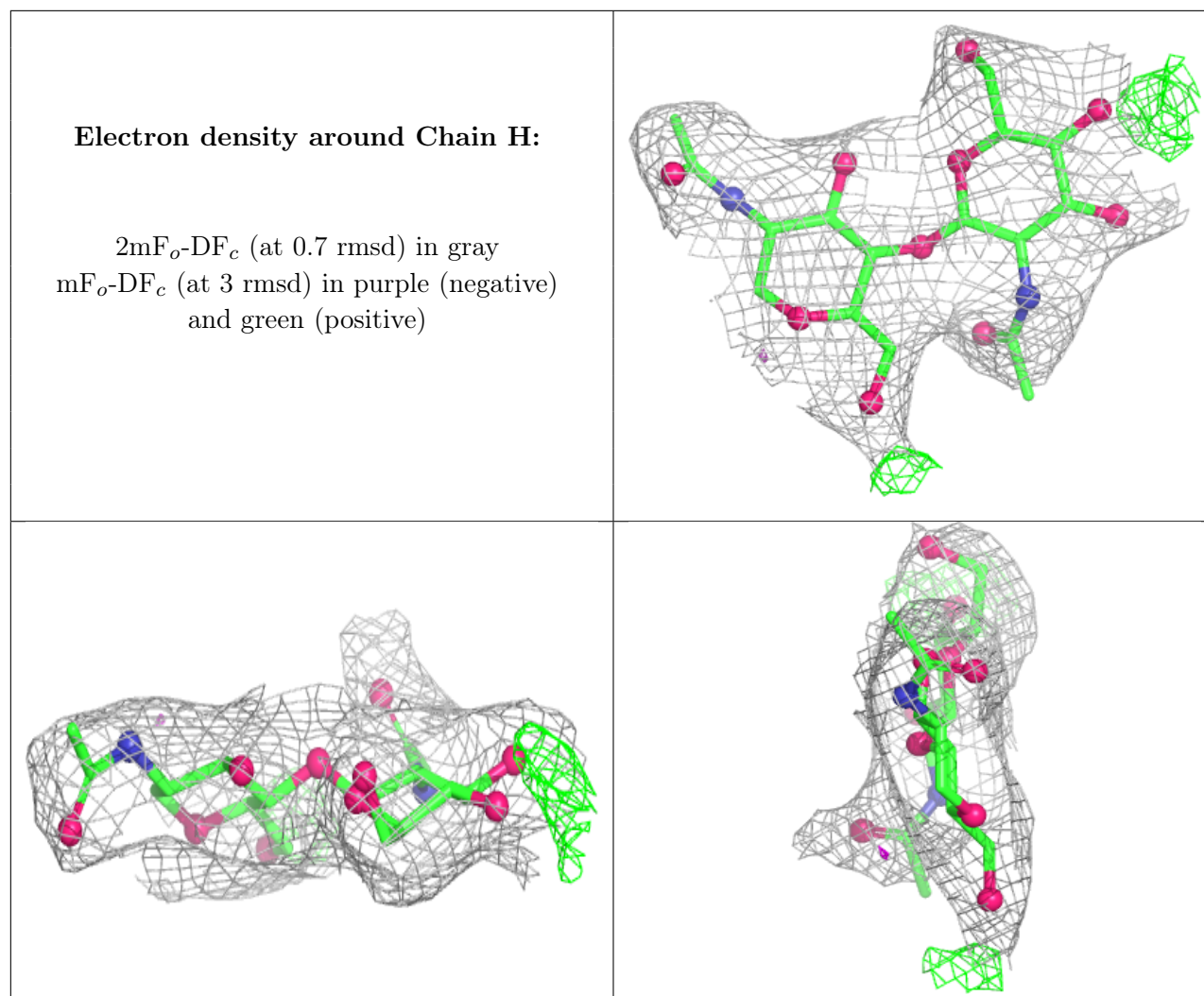
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands [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(\AA^2)	Q<0.9
3	NAG	A	801	14/15	0.56	0.17	78,80,81,82	0
3	NAG	B	802	14/15	0.62	0.14	80,83,85,85	0
3	NAG	B	801	14/15	0.65	0.14	76,77,78,78	0
3	NAG	C	804	14/15	0.68	0.14	93,95,96,96	0
3	NAG	D	801	14/15	0.70	0.14	71,72,72,72	0
3	NAG	D	804	14/15	0.70	0.13	91,92,93,93	0
3	NAG	C	805	14/15	0.71	0.15	73,76,77,77	0
3	NAG	A	802	14/15	0.75	0.14	62,67,69,69	0
3	NAG	A	803	14/15	0.75	0.12	73,76,78,79	0

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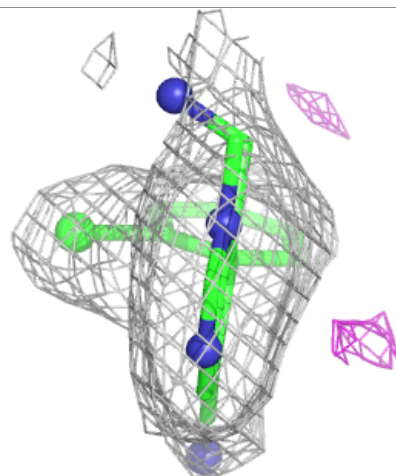
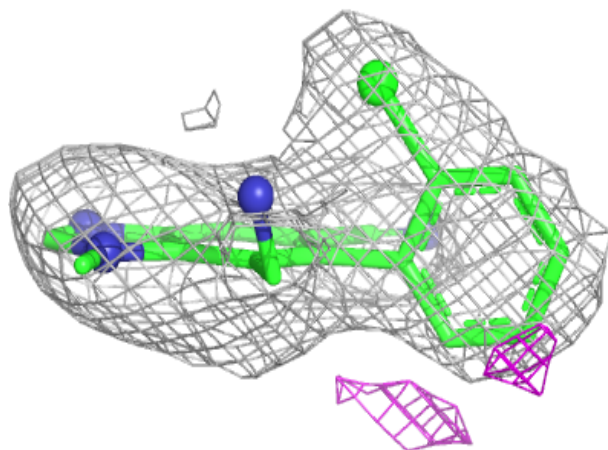
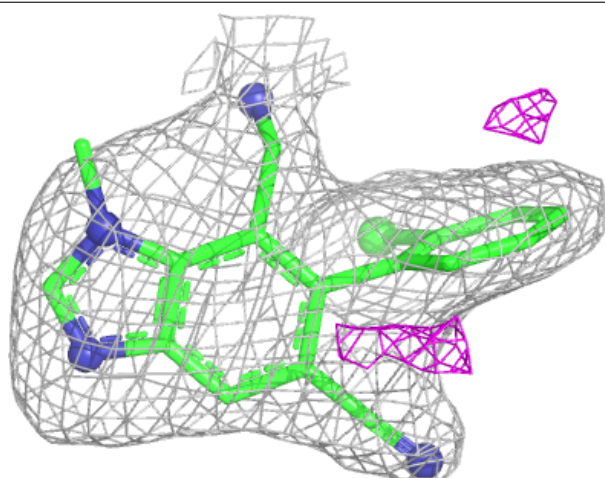
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	806	14/15	0.77	0.11	65,68,70,70	0
3	NAG	B	805	14/15	0.81	0.12	75,78,79,79	0
3	NAG	C	801	14/15	0.83	0.09	73,75,75,76	0
4	7AC	D	800	21/21	0.91	0.13	67,68,68,68	0
4	7AC	A	800	21/21	0.93	0.12	57,58,59,60	0
4	7AC	C	800	21/21	0.94	0.11	55,59,59,59	0
4	7AC	B	800	21/21	0.94	0.11	55,58,59,59	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.

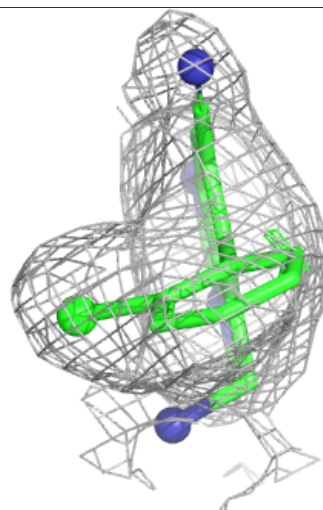
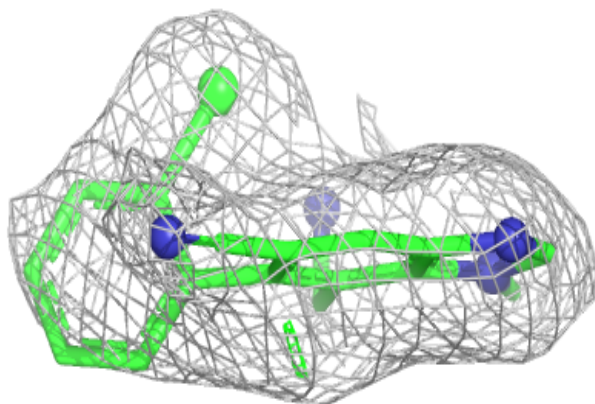
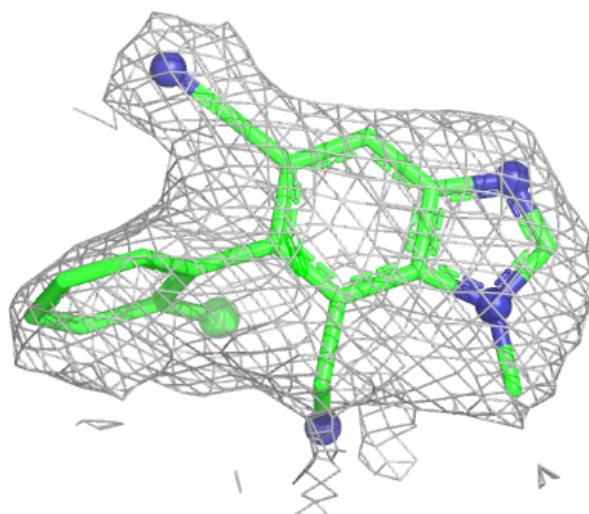
Electron density around 7AC D 800:

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



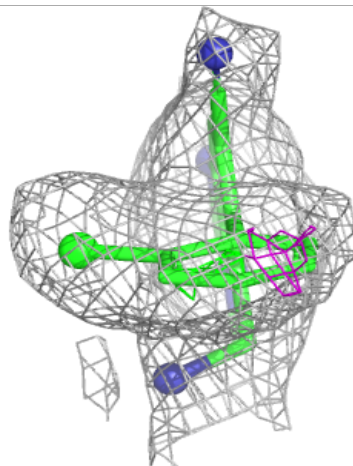
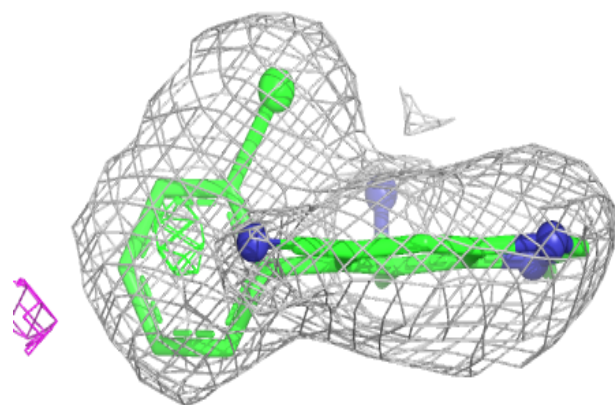
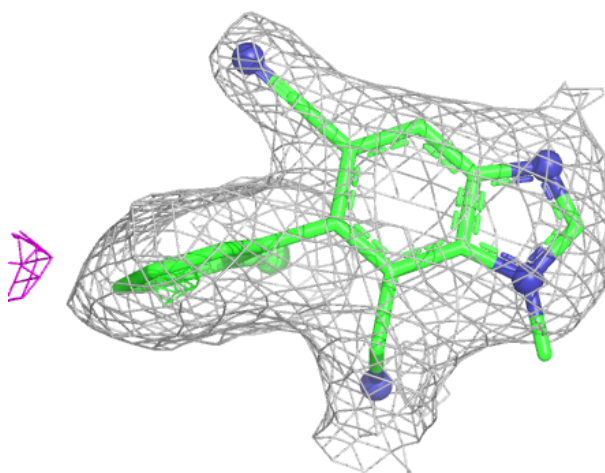
Electron density around 7AC A 800:

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



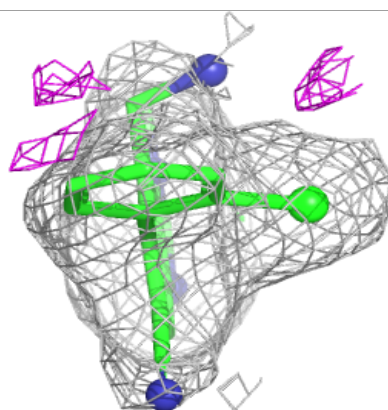
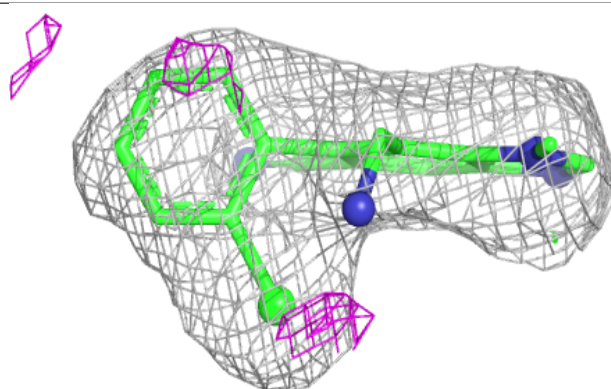
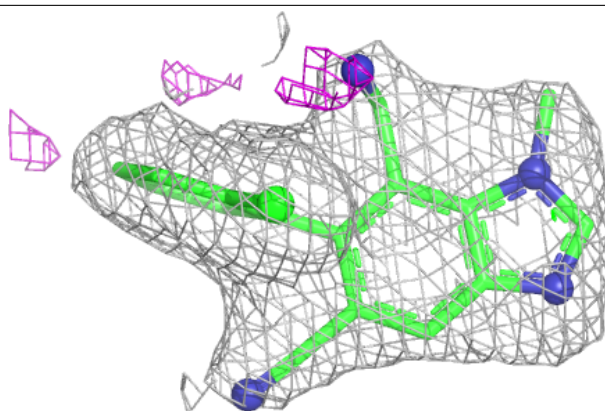
Electron density around 7AC C 800:

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



Electron density around 7AC B 800:

$2mF_o-DF_c$ (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.