



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 4Y49 / pdb_00004y49
Title : Crystal structure of yeast N-terminal acetyltransferase (ppGpp) NatE in complex with a bisubstrate
Authors : Dong, J.; Wang, S.; York, J.D.
Deposited on : 2015-02-10
Resolution : 3.95 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

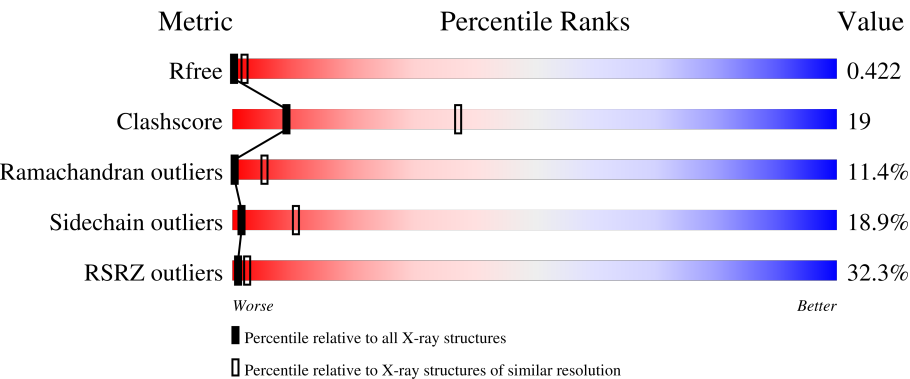
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	854	27% 56% 26% 6% 10%
1	G	854	31% 58% 24% 7% 10%
1	M	854	29% 58% 24% 7% 10%
2	B	238	23% 37% 24% 8% 31%
2	H	238	26% 43% 20% 5% 31%

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Mol	Chain	Length	Quality of chain
2	N	238	22%41%22%6%31%
3	C	176	24%61%19%7%11%
3	I	176	31%55%26%6%12%
3	O	176	24%65%16%6%13%
4	E	8	25%75%25%
4	K	8	25%75%25%
4	Q	8	25%75%25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20122 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 N-terminal acetyltransferase A complex subunit NAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	0	0	0
			4636	2891	860	877	8			
1	G	770	Total	C	N	O	S	0	0	0
			4656	2910	855	881	10			
1	M	769	Total	C	N	O	S	0	0	0
			4624	2889	848	877	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	TYR	GLU	conflict	UNP P12945
G	31	TYR	GLU	conflict	UNP P12945
M	31	TYR	GLU	conflict	UNP P12945

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1024	640	188	188	8			
2	H	164	Total	C	N	O	S	0	0	0
			1025	635	190	192	8			
2	N	164	Total	C	N	O	S	0	0	0
			1025	636	189	192	8			

- Molecule 3 is a protein called N-terminal acetyltransferase A complex subunit NAT5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	4	0	0
			888	555	168	163	2			
3	I	155	Total	C	N	O	S	3	0	0
			879	545	167	165	2			

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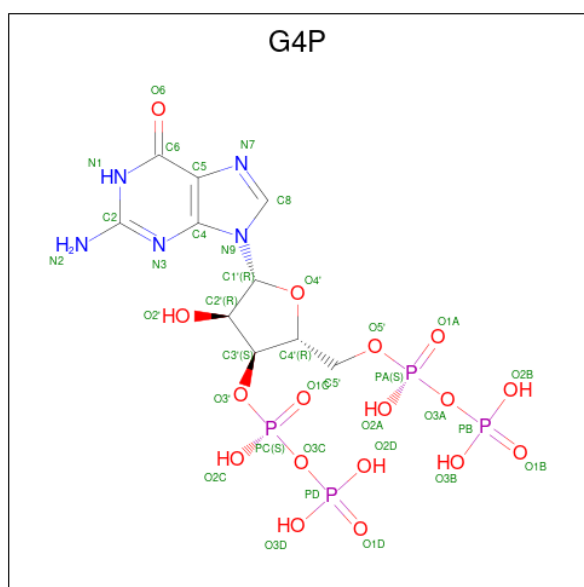
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	154	Total	C	N	O	S	1	1	0
			861	532	165	162	2			

- Molecule 4 is a protein called ALA-ALA-ALA-ALA-ALA-ALA.

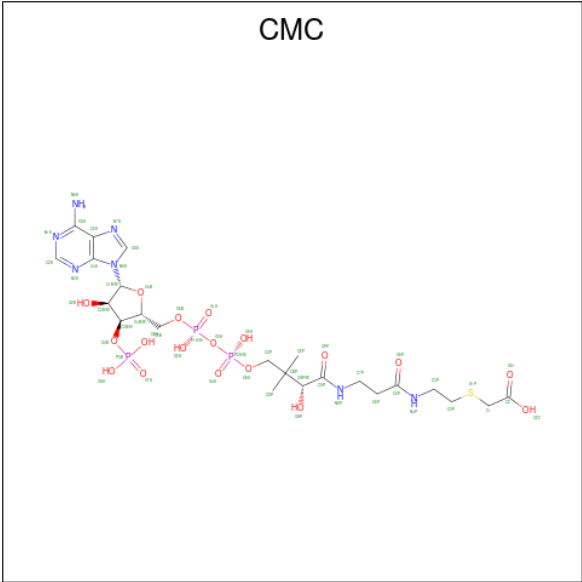
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O		0	0	0
			30	18	6	6				
4	K	6	Total	C	N	O		0	0	0
			30	18	6	6				
4	Q	6	Total	C	N	O		0	0	0
			30	18	6	6				

- Molecule 5 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



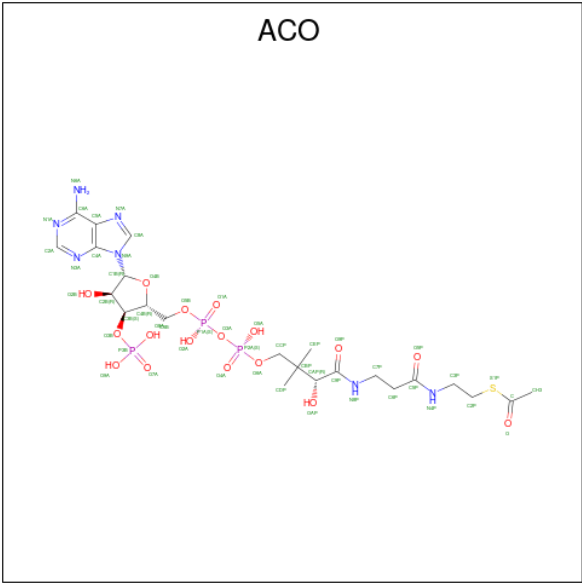
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	G	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	M	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 6 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		
6	H	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		
6	N	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		

- Molecule 7 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

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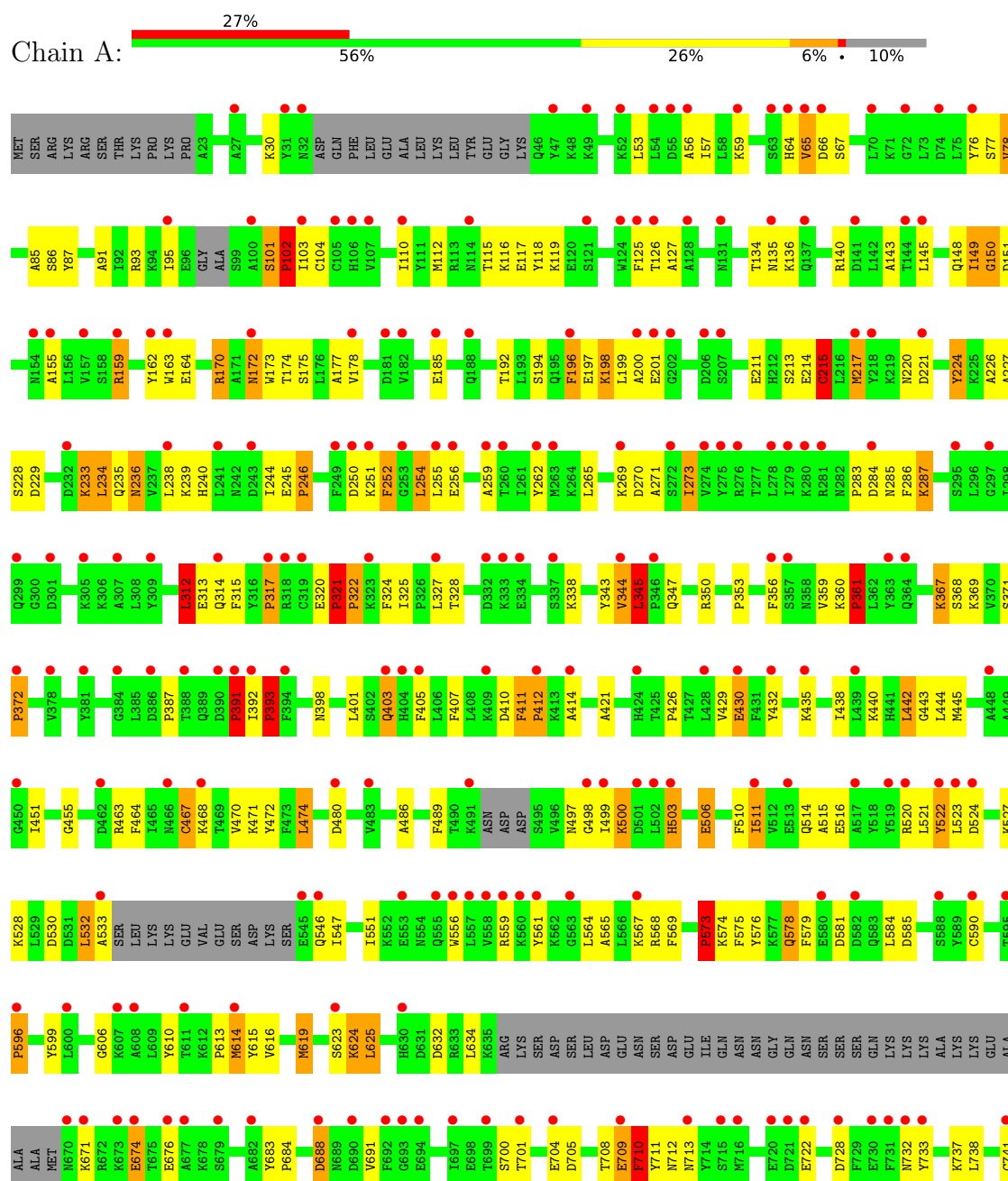
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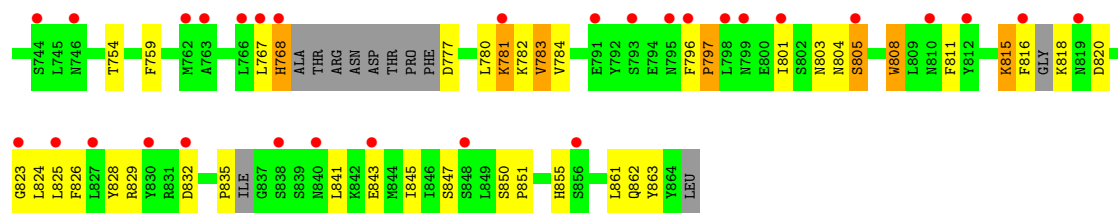
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
7	O	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

3 Residue-property plots

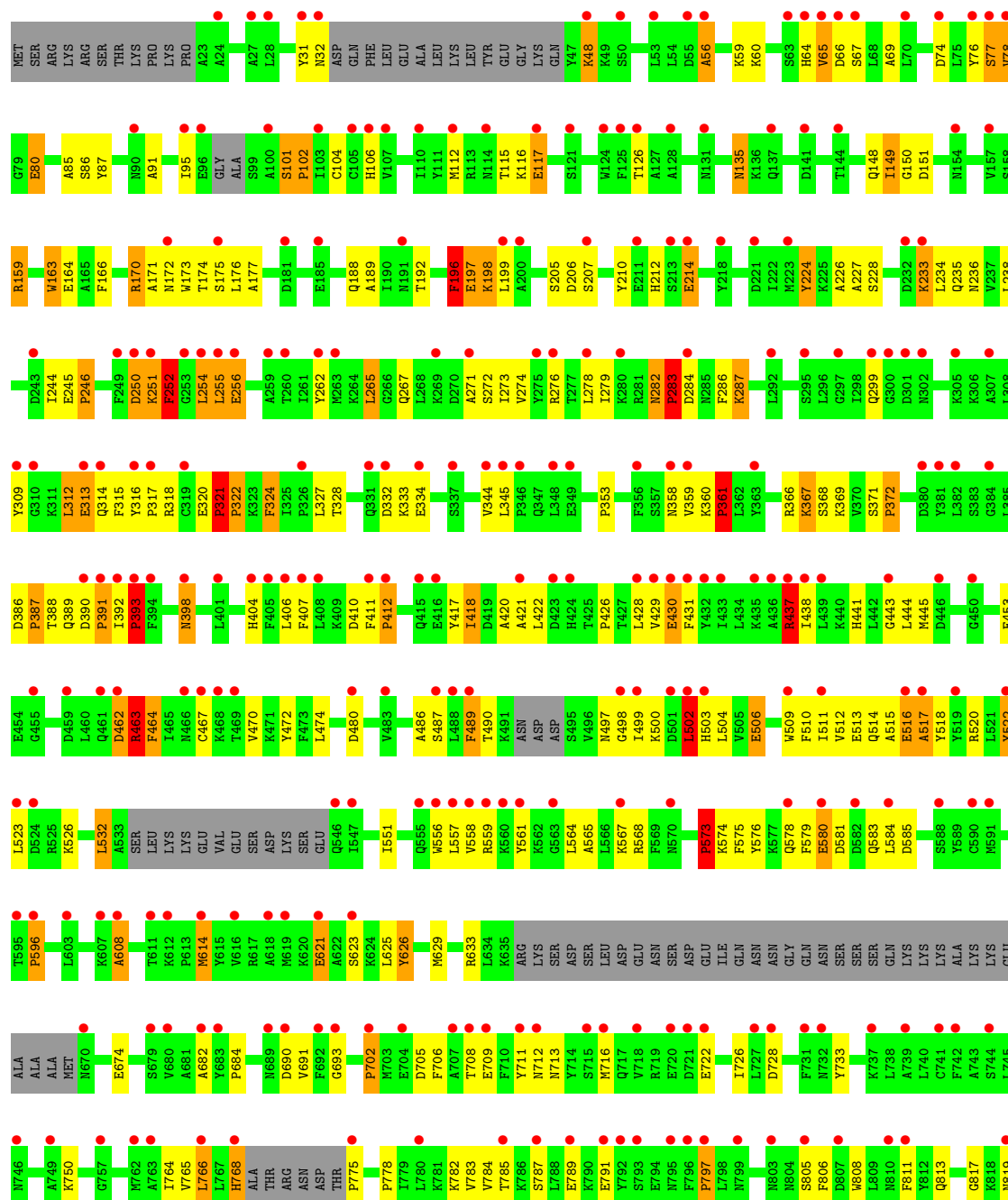
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

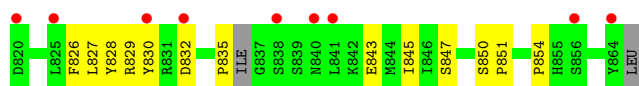
- Molecule 1: N-terminal acetyltransferase A complex subunit NAT1



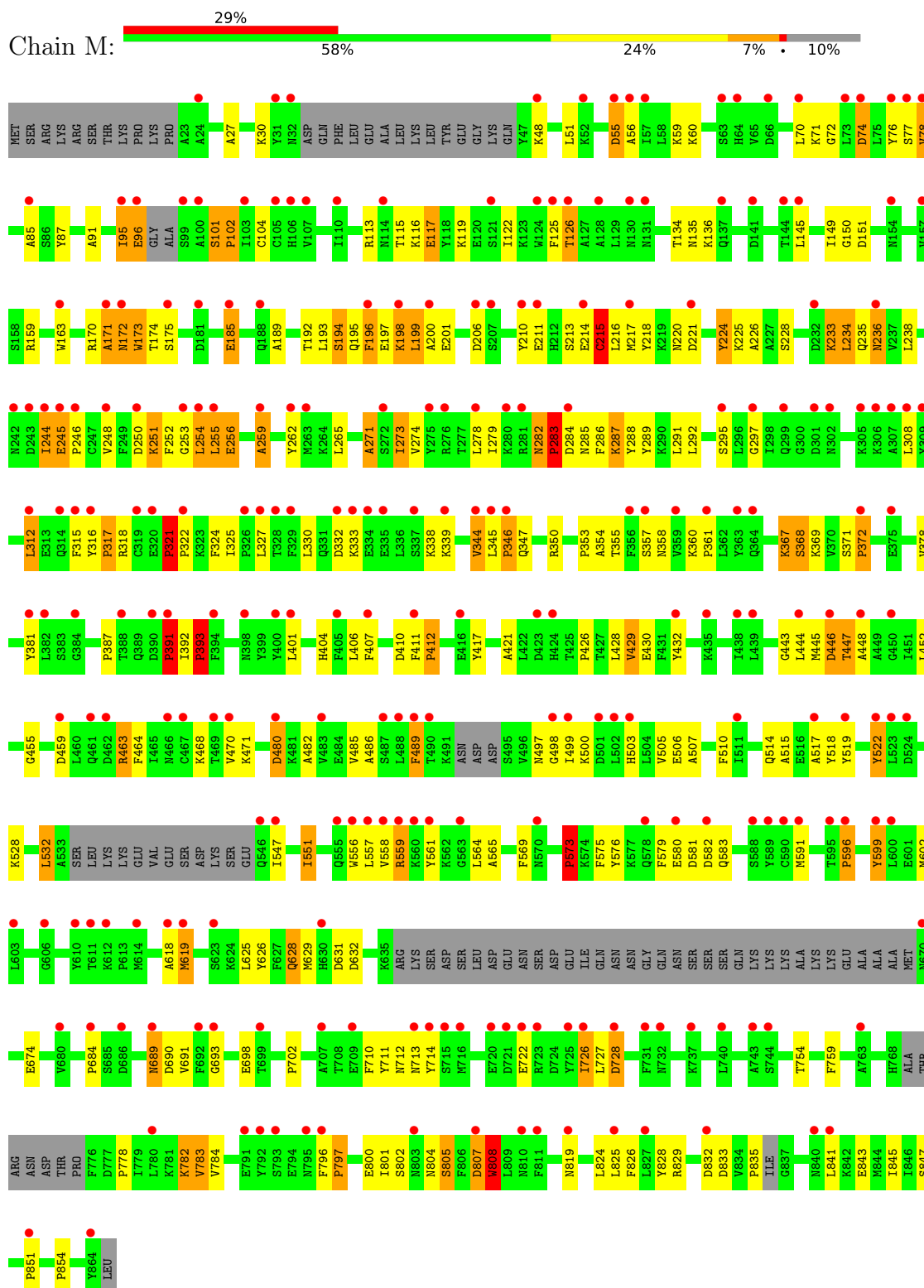


● Molecule 1: N-terminal acetyltransferase A complex subunit NAT1

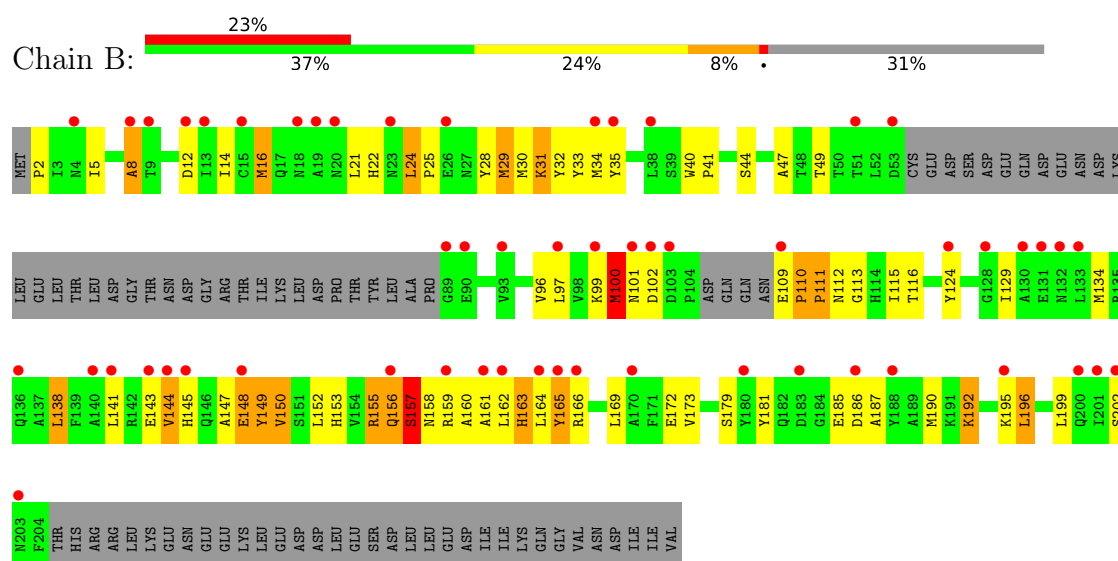




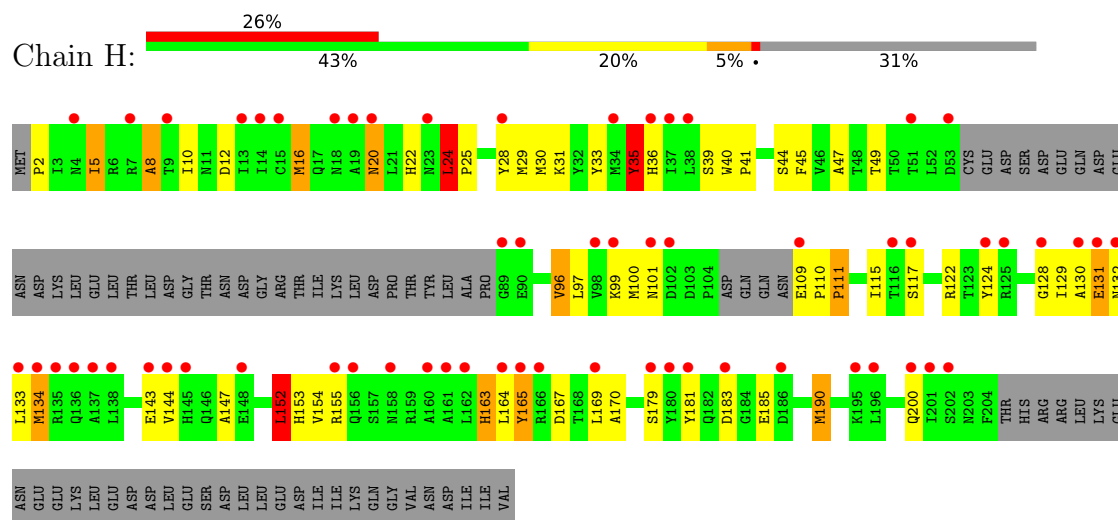
• Molecule 1: N-terminal acetyltransferase A complex subunit NAT1



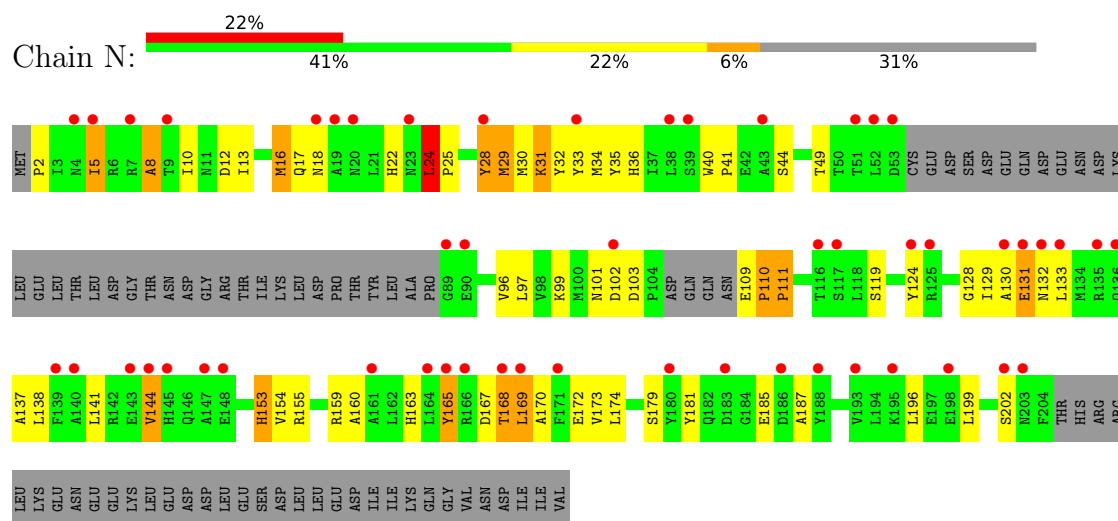
• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1



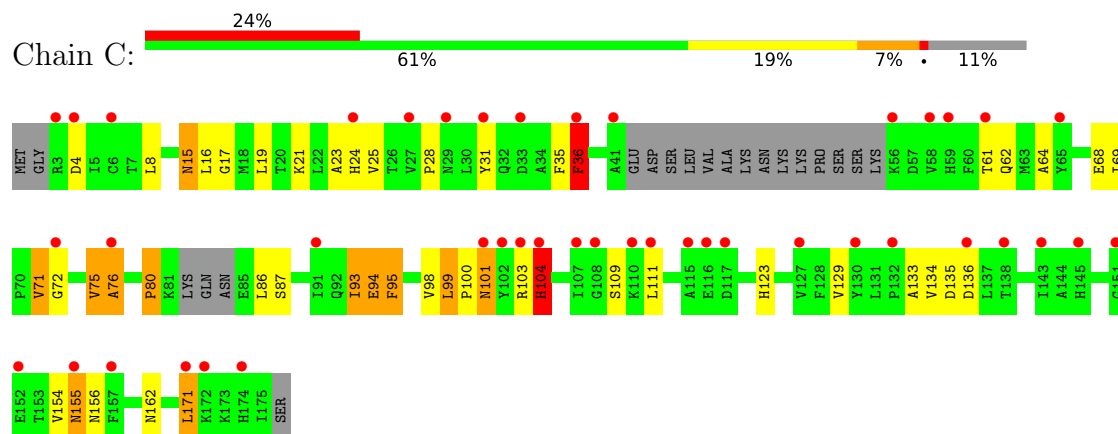
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1



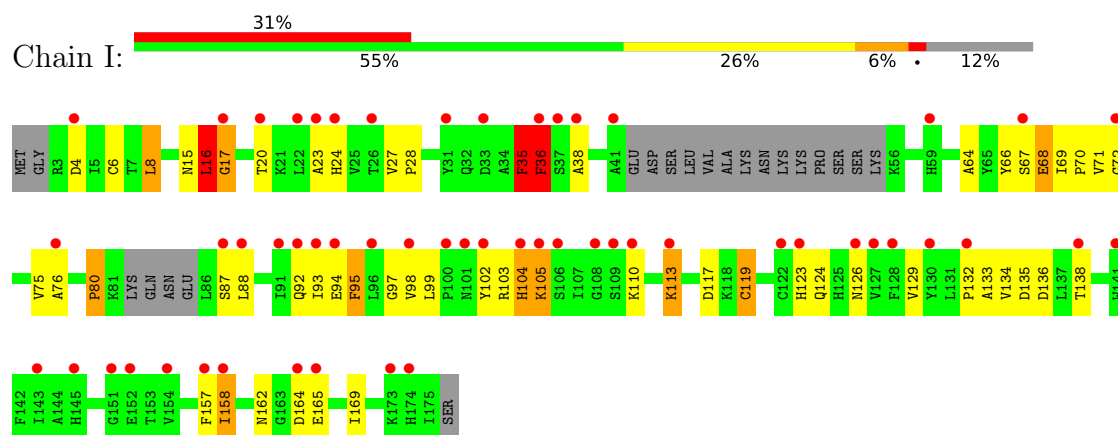
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1



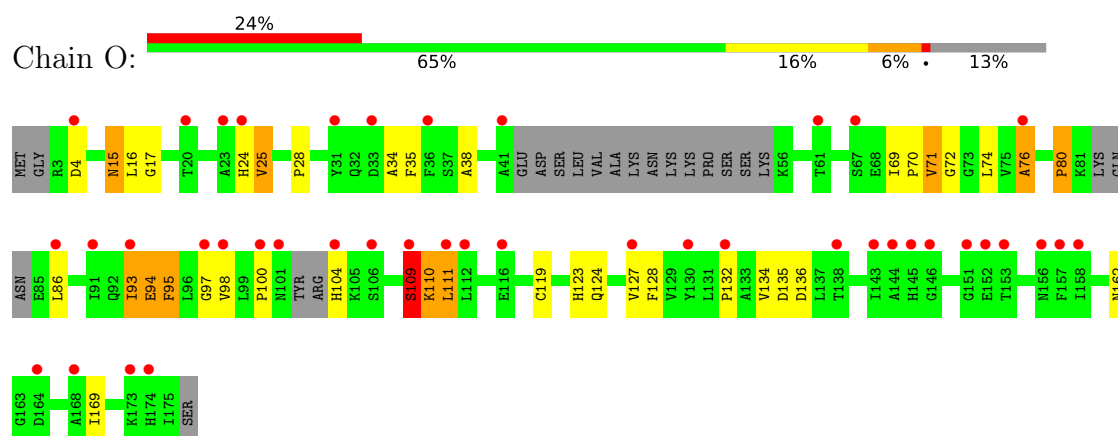
- Molecule 3: N-terminal acetyltransferase A complex subunit NAT5



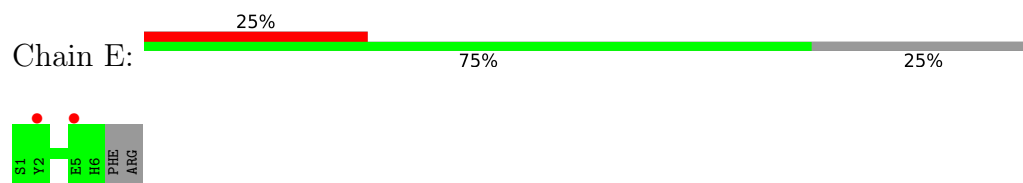
- Molecule 3: N-terminal acetyltransferase A complex subunit NAT5



- Molecule 3: N-terminal acetyltransferase A complex subunit NAT5

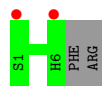


- Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA



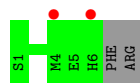
- Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA

Chain K: 



- Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA

Chain Q: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.72Å 146.49Å 254.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.95 49.63 – 3.95	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.63-3.95) 96.5 (49.63-3.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.355 , 0.421 0.366 , 0.422	Depositor DCC
R_{free} test set	1815 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20122	wwPDB-VP
Average B, all atoms (Å ²)	85.0	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 92.28 % 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 9.9860e-09. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, CMC, ACO

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	1.37	26/4701 (0.6%)	1.24	34/6458 (0.5%)
1	G	1.31	18/4725 (0.4%)	1.29	38/6500 (0.6%)
1	M	1.19	15/4689 (0.3%)	1.25	32/6453 (0.5%)
2	B	1.44	16/1040 (1.5%)	1.33	10/1424 (0.7%)
2	H	1.26	5/1041 (0.5%)	1.26	7/1424 (0.5%)
2	N	1.14	5/1040 (0.5%)	1.23	10/1423 (0.7%)
3	C	2.02	4/900 (0.4%)	1.46	12/1243 (1.0%)
3	I	1.85	9/889 (1.0%)	1.45	13/1224 (1.1%)
3	O	1.05	0/870	1.24	10/1197 (0.8%)
4	E	1.48	0/29	1.65	0/39
4	K	1.59	0/29	1.51	0/39
4	Q	1.49	0/29	1.20	0/39
All	All	1.35	98/19982 (0.5%)	1.28	166/27463 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	M	0	2
3	C	0	1
3	I	0	1
All	All	0	6

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	35	PHE	C-N	-33.66	0.90	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	36	PHE	C-O	33.03	1.63	1.24
1	G	768	HIS	C-O	32.03	1.87	1.23
3	I	36	PHE	N-CA	31.89	1.87	1.46
1	A	768	HIS	C-O	25.36	1.74	1.23
3	I	16	LEU	CA-C	21.52	1.81	1.52
3	C	36	PHE	CA-CB	-20.86	1.20	1.53
1	A	619	MET	SD-CE	19.38	2.27	1.79
1	G	614	MET	SD-CE	18.63	2.26	1.79
1	A	614	MET	SD-CE	17.37	2.23	1.79
1	A	215	CYS	CB-SG	16.86	2.36	1.81
1	A	709	GLU	CD-OE1	16.84	1.57	1.25
2	B	29	MET	CG-SD	13.92	2.15	1.80
1	A	709	GLU	CD-OE2	13.16	1.50	1.25
1	M	185	GLU	CG-CD	12.85	1.84	1.52
1	A	676	GLU	CD-OE1	12.33	1.48	1.25
1	M	126	THR	C-O	11.69	1.37	1.24
1	M	185	GLU	CD-OE2	11.00	1.46	1.25
1	M	689	ASN	C-O	10.49	1.38	1.24
1	A	533	ALA	C-O	10.35	1.44	1.23
2	N	109	GLU	C-N	9.49	1.44	1.33
3	I	164	ASP	CG-OD2	9.01	1.42	1.25
3	I	97	GLY	C-O	8.87	1.35	1.23
3	I	36	PHE	CA-C	8.87	1.64	1.52
1	M	199	LEU	C-O	8.79	1.33	1.24
3	I	36	PHE	CA-CB	8.71	1.68	1.53
1	G	126	THR	C-O	8.60	1.34	1.24
1	A	467	CYS	CB-SG	8.46	2.09	1.81
1	G	775	PRO	C-N	8.38	1.46	1.33
1	G	614	MET	CB-CG	8.31	1.77	1.52
1	M	215	CYS	CB-SG	8.21	2.08	1.81
2	H	134	MET	CG-SD	7.86	2.00	1.80
1	M	591	MET	CG-SD	7.75	2.00	1.80
2	B	100	MET	SD-CE	7.72	1.98	1.79
2	B	109	GLU	C-N	7.55	1.42	1.33
1	M	503	HIS	N-CA	7.49	1.55	1.46
1	G	614	MET	CG-SD	7.48	1.99	1.80
3	C	19	LEU	C-O	7.42	1.33	1.24
1	A	126	THR	C-O	7.37	1.33	1.24
2	B	149	TYR	C-O	-7.32	1.15	1.24
2	B	14	ILE	C-O	7.27	1.32	1.24
2	B	147	ALA	CA-C	-7.19	1.44	1.52
3	I	138	THR	CA-C	7.15	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	TYR	C-O	7.02	1.33	1.24
1	A	805	SER	CA-C	6.97	1.60	1.52
1	G	437	ARG	CZ-NH1	6.79	1.42	1.32
1	G	56	ALA	CA-C	6.57	1.59	1.52
1	G	453	GLU	CD-OE1	6.57	1.37	1.25
2	B	16	MET	SD-CE	6.56	1.96	1.79
1	G	516	GLU	C-O	6.55	1.32	1.24
1	A	624	LYS	C-O	6.43	1.32	1.24
2	H	109	GLU	C-N	6.39	1.41	1.33
1	M	619	MET	CG-SD	6.26	1.96	1.80
1	A	110	ILE	N-CA	6.26	1.54	1.46
2	B	29	MET	SD-CE	6.15	1.95	1.79
1	A	221	ASP	CA-C	6.15	1.61	1.52
1	G	276	ARG	CA-C	6.11	1.60	1.52
1	A	140	ARG	C-O	6.10	1.31	1.23
1	A	215	CYS	CA-CB	5.95	1.63	1.53
1	M	698	GLU	C-O	5.90	1.31	1.24
2	H	134	MET	SD-CE	5.82	1.94	1.79
2	B	150	VAL	C-O	-5.82	1.17	1.24
2	B	186	ASP	C-N	5.79	1.42	1.33
2	B	100	MET	CG-SD	5.79	1.95	1.80
1	G	709	GLU	CD-OE2	5.72	1.36	1.25
1	M	559	ARG	CA-C	5.71	1.60	1.52
1	M	206	ASP	CB-CG	5.64	1.66	1.52
1	A	674	GLU	N-CA	5.61	1.53	1.46
2	N	144	VAL	C-O	5.59	1.30	1.24
1	A	619	MET	CG-SD	5.58	1.94	1.80
1	A	503	HIS	N-CA	5.53	1.53	1.46
2	H	20	ASN	CG-OD1	5.52	1.34	1.23
1	G	608	ALA	C-O	5.52	1.30	1.24
1	M	221	ASP	CA-C	5.51	1.60	1.52
1	A	732	ASN	CA-C	5.50	1.60	1.52
2	B	143	GLU	N-CA	5.50	1.53	1.46
2	B	186	ASP	C-O	5.45	1.30	1.24
1	G	511	ILE	CA-C	5.42	1.59	1.52
1	G	845	ILE	C-O	5.42	1.29	1.23
1	G	621	GLU	CA-C	5.40	1.60	1.52
1	M	618	ALA	CA-C	-5.37	1.45	1.52
1	A	704	GLU	CG-CD	5.36	1.65	1.52
1	G	827	LEU	N-CA	5.34	1.53	1.46
2	H	190	MET	CA-CB	5.34	1.57	1.53
2	N	202	SER	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	92	GLN	N-CA	5.26	1.52	1.46
2	N	111	PRO	C-O	5.26	1.30	1.24
2	B	202	SER	CA-C	5.24	1.58	1.53
1	G	64	HIS	CA-C	5.24	1.58	1.52
2	N	169	LEU	CA-C	5.22	1.59	1.52
2	B	16	MET	CG-SD	5.21	1.93	1.80
3	I	126	ASN	N-CA	5.21	1.52	1.45
1	A	145	LEU	N-CA	5.13	1.51	1.46
1	M	689	ASN	C-N	5.12	1.41	1.33
1	A	516	GLU	C-O	5.11	1.30	1.24
1	A	112	MET	CG-SD	5.05	1.93	1.80
2	B	150	VAL	CA-CB	-5.04	1.47	1.54
1	A	777	ASP	C-N	5.03	1.39	1.33

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	35	PHE	O-C-N	-21.17	96.58	122.20
3	I	36	PHE	N-CA-CB	14.02	134.18	110.49
3	C	36	PHE	O-C-N	-13.73	107.57	122.12
1	G	851	PRO	N-CA-CB	12.68	111.35	102.35
1	A	851	PRO	N-CA-CB	12.36	110.90	102.25
3	C	36	PHE	CA-CB-CG	9.80	123.60	113.80
3	I	35	PHE	CA-C-N	-9.32	103.73	121.54
3	I	35	PHE	C-N-CA	-9.32	103.73	121.54
1	G	768	HIS	CA-C-O	-9.29	105.00	120.80
3	C	35	PHE	CA-C-N	8.98	132.69	120.38
3	C	35	PHE	C-N-CA	8.98	132.69	120.38
3	O	28	PRO	N-CA-CB	8.97	111.30	103.31
3	I	132	PRO	N-CA-CB	8.90	111.20	103.19
3	C	28	PRO	N-CA-CB	8.65	111.01	103.31
1	A	573	PRO	N-CA-CB	8.41	112.08	103.25
1	M	573	PRO	N-CA-CB	8.32	111.99	103.25
2	B	149	TYR	N-CA-C	7.92	121.88	108.02
2	B	41	PRO	N-CA-CB	7.67	110.49	103.20
2	N	28	TYR	N-CA-C	7.67	120.82	109.24
1	A	684	PRO	N-CA-CB	7.57	110.51	103.39
2	B	111	PRO	N-CA-CB	7.57	111.20	103.25
3	I	70	PRO	N-CA-CB	7.56	109.99	103.19
3	O	132	PRO	N-CA-CB	7.55	109.89	103.25
2	H	111	PRO	N-CA-CB	7.54	111.17	103.25
2	N	25	PRO	N-CA-CB	7.45	110.64	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	111	PRO	N-CA-CB	7.35	110.97	103.25
1	M	596	PRO	N-CA-CB	7.33	110.95	103.25
2	H	25	PRO	N-CA-CB	7.32	110.94	103.25
1	G	464	PHE	N-CA-C	-7.32	103.98	113.12
3	I	16	LEU	CA-C-O	-7.29	110.08	120.51
1	M	851	PRO	N-CA-CB	7.23	111.20	103.39
2	N	110	PRO	N-CA-CB	7.16	110.03	103.08
1	M	689	ASN	O-C-N	7.16	132.26	122.46
1	G	517	ALA	N-CA-C	-7.15	102.34	112.13
1	A	317	PRO	N-CA-CB	7.12	110.72	103.25
1	G	393	PRO	N-CA-CB	7.12	110.72	103.25
3	I	28	PRO	N-CA-CB	7.11	109.95	103.34
2	H	134	MET	CG-SD-CE	-7.09	85.31	100.90
2	H	153	HIS	N-CA-C	7.07	119.04	107.23
1	A	387	PRO	N-CA-CB	7.06	110.66	103.25
1	G	596	PRO	N-CA-CB	7.04	110.65	103.25
1	G	573	PRO	N-CA-CB	7.02	110.62	103.25
1	G	324	PHE	N-CA-C	7.01	119.57	111.02
1	M	102	PRO	N-CA-CB	7.00	110.60	103.25
2	N	41	PRO	N-CA-CB	6.98	110.21	103.51
2	B	31	LYS	N-CA-C	-6.97	102.24	111.24
1	M	797	PRO	N-CA-CB	6.96	110.56	103.25
1	M	854	PRO	N-CA-CB	6.95	110.66	103.23
1	A	835	PRO	N-CA-CB	6.90	110.59	103.00
1	M	835	PRO	N-CA-CB	6.87	110.56	103.00
1	G	102	PRO	N-CA-CB	6.85	110.45	103.25
1	A	797	PRO	N-CA-CB	6.85	110.44	103.25
1	A	619	MET	CG-SD-CE	-6.84	85.85	100.90
3	O	70	PRO	N-CA-CB	6.84	109.27	103.25
1	G	246	PRO	N-CA-CB	6.78	109.97	103.19
1	A	391	PRO	N-CA-CB	6.78	110.37	103.25
1	G	684	PRO	N-CA-CB	6.76	109.00	103.32
1	M	391	PRO	N-CA-CB	6.76	110.35	103.25
2	B	110	PRO	N-CA-CB	6.75	109.63	103.08
1	G	372	PRO	N-CA-CB	6.74	110.33	103.25
1	M	387	PRO	N-CA-CB	6.72	110.30	103.25
1	G	797	PRO	N-CA-CB	6.69	110.27	103.25
1	A	393	PRO	N-CA-CB	6.68	110.26	103.25
1	A	426	PRO	N-CA-CB	6.67	109.18	102.17
1	M	807	ASP	N-CA-C	6.63	120.40	111.24
1	G	808	TRP	N-CA-C	6.58	120.17	111.75
1	M	372	PRO	N-CA-CB	6.55	110.13	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	ILE	N-CA-C	6.55	116.86	106.32
1	G	426	PRO	N-CA-CB	6.55	110.13	103.25
1	A	372	PRO	N-CA-CB	6.55	110.12	103.25
2	H	41	PRO	N-CA-CB	6.54	110.09	102.76
1	G	387	PRO	N-CA-CB	6.54	110.12	103.25
1	A	474	LEU	N-CA-C	-6.53	106.27	114.56
1	M	321	PRO	N-CA-C	6.52	118.65	110.70
1	M	353	PRO	N-CA-CB	6.52	110.00	103.48
1	M	819	ASN	N-CA-C	6.52	120.23	112.93
2	B	148	GLU	N-CA-C	6.51	119.70	111.69
1	A	361	PRO	N-CA-CB	6.48	110.05	103.25
1	M	346	PRO	N-CA-CB	6.45	110.02	103.25
1	G	778	PRO	N-CA-CB	6.43	110.00	103.25
1	G	835	PRO	N-CA-CB	6.43	110.07	103.00
1	M	689	ASN	CA-C-O	-6.42	111.76	119.27
1	M	684	PRO	N-CA-CB	6.42	110.12	103.38
3	I	80	PRO	N-CA-CB	6.41	109.98	103.25
3	C	100	PRO	N-CA-CB	6.40	109.97	103.25
3	O	80	PRO	N-CA-CB	6.40	109.97	103.25
3	C	76	ALA	N-CA-C	6.38	119.86	109.59
3	C	80	PRO	N-CA-CB	6.38	109.95	103.25
3	O	100	PRO	N-CA-CB	6.38	109.94	103.25
1	G	850	SER	O-C-N	6.34	124.65	120.27
1	A	217	MET	N-CA-C	-6.29	103.08	111.96
1	A	246	PRO	N-CA-CB	6.29	110.18	103.39
3	I	36	PHE	N-CA-C	-6.26	97.45	110.80
1	G	391	PRO	N-CA-CB	6.20	110.39	103.44
3	I	126	ASN	N-CA-C	6.16	118.85	110.35
3	I	69	ILE	N-CA-C	6.13	115.29	108.05
1	M	412	PRO	N-CA-CB	6.12	109.82	103.15
1	M	426	PRO	N-CA-CB	6.10	109.53	102.33
2	H	5	ILE	N-CA-C	6.09	115.38	106.55
1	G	361	PRO	N-CA-CB	6.06	109.62	103.25
2	N	31	LYS	N-CA-C	-6.05	104.64	112.68
1	A	613	PRO	N-CA-CB	6.04	109.59	103.25
1	A	321	PRO	N-CA-C	6.03	118.05	110.70
3	O	109	SER	CA-C-N	6.00	132.51	121.70
3	O	109	SER	C-N-CA	6.00	132.51	121.70
1	G	353	PRO	N-CA-CB	6.00	109.27	103.51
1	M	393	PRO	N-CA-CB	5.98	109.53	103.25
1	A	215	CYS	CA-CB-SG	-5.96	100.69	114.40
1	M	728	ASP	N-CA-C	-5.96	103.75	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	76	ALA	N-CA-C	5.96	119.18	109.59
1	A	850	SER	O-C-N	5.95	124.38	120.27
2	N	5	ILE	N-CA-C	5.94	115.91	106.88
1	A	353	PRO	N-CA-CB	5.92	109.80	103.52
1	A	464	PHE	N-CA-C	-5.92	106.60	113.88
1	G	321	PRO	N-CA-C	5.90	117.90	110.70
1	G	196	PHE	N-CA-C	-5.89	104.23	112.12
1	A	102	PRO	N-CA-CB	5.88	109.43	103.25
1	A	777	ASP	CA-C-N	5.85	126.66	120.11
1	A	777	ASP	C-N-CA	5.85	126.66	120.11
1	G	69	ALA	N-CA-C	5.85	117.33	111.07
3	I	36	PHE	CA-C-O	5.83	128.85	120.51
1	A	705	ASP	N-CA-C	-5.82	105.27	112.72
1	M	459	ASP	N-CA-C	5.76	117.52	107.49
1	G	462	ASP	N-CA-C	-5.76	98.54	110.80
1	G	77	SER	N-CA-C	-5.71	104.55	112.03
2	B	138	LEU	N-CA-C	-5.70	104.45	111.40
1	A	674	GLU	N-CA-C	5.69	120.08	113.20
3	C	69	ILE	CA-C-N	5.68	125.69	119.90
3	C	69	ILE	C-N-CA	5.68	125.69	119.90
1	M	172	ASN	N-CA-C	-5.68	106.27	113.43
1	G	854	PRO	N-CA-CB	5.66	109.19	103.25
1	M	471	LYS	N-CA-C	-5.63	104.42	112.13
2	N	168	THR	N-CA-C	-5.63	103.98	111.24
1	A	606	GLY	N-CA-C	5.60	119.41	112.64
2	N	170	ALA	N-CA-CB	5.59	119.93	110.49
1	G	523	LEU	N-CA-C	5.54	120.45	111.37
3	C	69	ILE	N-CA-C	5.50	113.93	107.77
1	G	299	GLN	N-CA-C	-5.44	104.22	111.24
2	H	8	ALA	N-CA-C	5.43	122.37	110.80
1	G	702	PRO	N-CA-CB	5.42	108.94	103.25
1	G	412	PRO	N-CA-CB	5.41	109.43	103.26
2	B	157	SER	N-CA-C	5.40	126.13	111.00
3	O	69	ILE	N-CA-C	5.39	114.42	108.05
1	A	412	PRO	N-CA-CB	5.37	109.00	103.15
2	N	169	LEU	N-CA-C	5.35	119.53	112.89
1	M	807	ASP	CA-C-N	5.35	131.32	121.70
1	M	807	ASP	C-N-CA	5.35	131.32	121.70
3	I	133	ALA	N-CA-C	5.34	117.53	111.02
1	G	252	PHE	N-CA-C	5.32	117.16	111.36
3	O	71	VAL	N-CA-C	5.27	120.30	109.34
1	G	48	LYS	N-CA-C	5.24	116.25	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	PHE	N-CA-C	-5.24	103.55	111.56
1	A	471	LYS	N-CA-C	-5.23	105.72	112.68
1	G	283	PRO	N-CA-CB	5.22	108.73	103.25
1	A	590	CYS	N-CA-C	-5.19	107.00	113.38
1	M	185	GLU	CG-CD-OE2	5.19	130.33	118.40
1	M	244	ILE	N-CA-C	5.15	115.37	110.42
1	A	710	PHE	CA-C-O	5.13	123.33	119.68
1	M	808	TRP	N-CA-CB	5.11	119.19	110.50
1	A	464	PHE	CB-CA-C	5.11	117.30	109.03
2	B	47	ALA	N-CA-C	5.08	116.32	107.93
1	M	283	PRO	N-CA-CB	5.08	108.59	103.25
1	G	787	SER	N-CA-C	-5.05	105.68	111.14
1	G	716	MET	N-CA-C	-5.04	107.52	113.97
1	M	778	PRO	N-CA-CB	5.03	109.00	103.26
1	G	567	LYS	N-CA-C	5.01	116.75	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	781	LYS	Peptide
3	C	36	PHE	Mainchain
1	G	806	PHE	Peptide
3	I	16	LEU	Mainchain
1	M	171	ALA	Peptide
1	M	689	ASN	Mainchain

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	4636	0	2969	146	0
1	G	4656	0	2966	140	0
1	M	4624	0	2960	154	0
2	B	1024	0	710	42	0
2	H	1025	0	695	28	0
2	N	1025	0	699	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	888	0	539	29	0
3	I	879	0	527	32	0
3	O	861	0	511	17	0
4	E	30	0	14	0	0
4	K	30	0	14	0	0
4	Q	30	0	14	0	0
5	A	36	0	11	1	0
5	G	36	0	11	3	0
5	M	36	0	11	0	0
6	B	51	0	31	0	0
6	H	51	0	31	0	0
6	N	51	0	31	0	0
7	C	51	0	34	10	0
7	I	51	0	34	9	0
7	O	51	0	34	5	0
All	All	20122	0	12846	606	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 19.

All (606) 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:G:614:MET:CB	1:G:614:MET:CG	1.77	1.62
1:M:185:GLU:CD	1:M:185:GLU:CG	1.84	1.49
1:M:215:CYS:CB	1:M:215:CYS:SG	2.08	1.42
1:A:467:CYS:SG	1:A:467:CYS:CB	2.09	1.41
2:B:29:MET:CG	2:B:29:MET:SD	2.15	1.33
1:A:768:HIS:O	1:A:768:HIS:C	1.74	1.29
1:A:614:MET:SD	1:A:614:MET:CE	2.23	1.27
1:G:614:MET:SD	1:G:614:MET:CE	2.26	1.24
1:A:619:MET:SD	1:A:619:MET:CE	2.28	1.22
1:G:768:HIS:O	1:G:768:HIS:C	1.87	1.18
1:A:215:CYS:CB	1:A:215:CYS:SG	2.36	1.13
1:G:437:ARG:HD3	5:G:901:G4P:O1C	1.56	1.04
3:I:104:HIS:N	7:I:201:ACO:O1A	1.96	0.98
1:M:807:ASP:HA	1:M:808:TRP:HB2	1.51	0.92
3:I:98:VAL:HG12	7:I:201:ACO:H142	1.49	0.91
1:A:816:PHE:C	1:A:818:LYS:N	2.31	0.88
1:A:312:LEU:O	1:A:315:PHE:N	2.08	0.87
1:M:344:VAL:O	1:M:346:PRO:N	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:O	1:G:315:PHE:N	2.12	0.83
3:I:16:LEU:CA	3:I:17:GLY:N	2.42	0.82
7:I:201:ACO:H131	7:I:201:ACO:H72	1.60	0.81
1:M:807:ASP:CA	1:M:808:TRP:HB2	2.11	0.80
1:G:532:LEU:HD21	1:G:551:ILE:CG1	2.11	0.80
2:B:156:GLN:HA	2:B:158:ASN:N	1.97	0.79
1:M:74:ASP:O	1:M:78:VAL:N	2.15	0.79
1:M:470:VAL:CB	1:M:486:ALA:HB2	2.12	0.79
1:G:467:CYS:HG	1:G:509:TRP:HH2	1.30	0.79
1:A:199:LEU:O	1:A:201:GLU:N	2.17	0.77
1:M:170:ARG:NH2	1:M:215:CYS:SG	2.57	0.77
2:N:12:ASP:O	2:N:16:MET:HB2	1.84	0.77
1:G:463:ARG:HB3	1:G:489:PHE:CZ	2.20	0.77
3:I:103:ARG:CB	7:I:201:ACO:O4A	2.34	0.76
1:G:843:GLU:O	1:G:847:SER:N	2.19	0.76
3:I:23:ALA:O	3:I:24:HIS:ND1	2.18	0.75
1:G:367:LYS:O	1:G:369:LYS:N	2.20	0.75
1:A:244:ILE:O	1:A:246:PRO:N	2.21	0.74
1:G:244:ILE:O	1:G:246:PRO:N	2.21	0.74
3:I:72:GLY:HA2	3:I:98:VAL:HG23	1.70	0.73
1:G:443:GLY:O	1:G:445:MET:N	2.20	0.73
3:O:104:HIS:N	7:O:201:ACO:O4A	2.21	0.73
1:G:312:LEU:O	1:G:314:GLN:N	2.21	0.73
3:I:103:ARG:O	3:I:105:LYS:N	2.22	0.72
1:M:252:PHE:CE1	1:M:278:LEU:HD11	2.24	0.72
3:C:103:ARG:C	7:C:201:ACO:O4A	2.33	0.72
1:G:706:PHE:HE2	1:G:711:TYR:HB2	1.55	0.72
1:M:255:LEU:HD11	1:M:278:LEU:HD13	1.72	0.72
1:G:437:ARG:CD	5:G:901:G4P:O1C	2.38	0.71
2:H:163:HIS:O	2:H:165:TYR:N	2.22	0.71
1:A:711:TYR:O	1:A:713:ASN:N	2.21	0.71
1:M:367:LYS:O	1:M:369:LYS:N	2.24	0.71
1:M:401:LEU:HA	1:M:404:HIS:HB3	1.72	0.71
2:B:169:LEU:HD23	2:B:192:LYS:HE2	1.73	0.71
1:M:446:ASP:O	1:M:448:ALA:N	2.24	0.71
1:A:262:TYR:HD2	1:A:270:ASP:O	1.74	0.71
1:A:367:LYS:O	1:A:369:LYS:N	2.23	0.71
1:A:470:VAL:CB	1:A:486:ALA:HB2	2.20	0.70
3:C:103:ARG:CB	7:C:201:ACO:P2A	2.79	0.70
1:M:259:ALA:HB2	1:M:274:VAL:HG11	1.71	0.70
1:G:467:CYS:SG	1:G:509:TRP:HH2	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:NZ	5:A:901:G4P:O6	2.27	0.68
1:A:101:SER:O	1:A:104:CYS:N	2.21	0.68
1:G:282:ASN:O	1:G:284:ASP:N	2.26	0.68
2:H:100:MET:HE1	2:H:147:ALA:HB2	1.76	0.67
1:A:781:LYS:HA	1:A:781:LYS:HE2	1.77	0.67
2:B:12:ASP:O	2:B:16:MET:HB2	1.95	0.67
1:G:532:LEU:HD21	1:G:551:ILE:HG13	1.77	0.67
1:A:177:ALA:HB2	1:A:192:THR:CG2	2.25	0.66
1:G:515:ALA:C	1:G:517:ALA:H	2.04	0.66
3:C:104:HIS:N	7:C:201:ACO:O4A	2.28	0.66
1:G:177:ALA:HB2	1:G:192:THR:CG2	2.25	0.66
3:O:109:SER:HB3	3:O:110:LYS:HB2	1.78	0.65
1:M:282:ASN:O	1:M:284:ASP:N	2.29	0.65
2:N:8:ALA:HB3	2:N:44:SER:O	1.97	0.65
1:M:443:GLY:O	1:M:445:MET:N	2.30	0.65
2:N:101:ASN:O	2:N:103:ASP:N	2.30	0.64
1:M:807:ASP:HA	1:M:808:TRP:CB	2.26	0.64
2:H:155:ARG:HG2	2:H:181:TYR:CE2	2.33	0.64
1:A:56:ALA:O	1:A:59:LYS:N	2.31	0.64
1:A:443:GLY:O	1:A:445:MET:N	2.31	0.63
1:G:614:MET:CB	1:G:614:MET:SD	2.86	0.63
1:M:217:MET:O	1:M:220:ASN:N	2.31	0.63
1:M:807:ASP:N	1:M:808:TRP:HB2	2.14	0.63
1:M:101:SER:O	1:M:104:CYS:N	2.26	0.63
2:B:161:ALA:O	2:B:163:HIS:N	2.29	0.63
1:A:596:PRO:HA	1:A:599:TYR:HB3	1.81	0.63
3:I:95:PHE:HA	7:I:201:ACO:S1P	2.38	0.63
1:G:614:MET:CG	1:G:614:MET:CA	2.73	0.62
2:H:16:MET:HE1	2:H:97:LEU:HB3	1.80	0.62
1:G:205:SER:O	1:G:207:SER:N	2.31	0.62
3:C:134:VAL:O	3:C:136:ASP:N	2.32	0.62
3:I:15:ASN:O	3:I:17:GLY:N	2.31	0.62
1:G:234:LEU:HD23	1:G:265:LEU:HD23	1.80	0.62
1:A:65:VAL:O	1:A:67:SER:N	2.33	0.62
1:A:578:GLN:HA	1:A:581:ASP:HB2	1.81	0.62
2:B:153:HIS:O	2:B:181:TYR:OH	2.12	0.61
1:M:628:GLN:HA	1:M:631:ASP:HB3	1.82	0.61
1:G:785:THR:O	1:G:789:GLU:N	2.33	0.61
2:N:155:ARG:HG2	2:N:181:TYR:HE2	1.64	0.61
1:G:556:TRP:O	1:G:559:ARG:N	2.29	0.61
1:G:706:PHE:CE2	1:G:711:TYR:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:ARG:HG2	2:H:181:TYR:HE2	1.64	0.60
3:C:103:ARG:O	7:C:201:ACO:O1A	2.19	0.60
1:G:828:TYR:O	1:G:830:TYR:N	2.34	0.60
3:C:101:ASN:HD22	3:C:101:ASN:C	2.09	0.60
1:M:532:LEU:HG	1:M:551:ILE:HD11	1.83	0.60
1:G:250:ASP:O	1:G:251:LYS:C	2.44	0.60
1:A:843:GLU:O	1:A:847:SER:N	2.34	0.60
3:I:66:TYR:O	3:I:68:GLU:N	2.35	0.60
3:C:15:ASN:O	3:C:17:GLY:N	2.34	0.60
2:H:154:VAL:HA	2:H:181:TYR:OH	2.02	0.60
1:G:227:ALA:HB2	1:G:233:LYS:HB2	1.83	0.60
3:C:98:VAL:HG22	7:C:201:ACO:H142	1.83	0.59
1:M:196:PHE:O	1:M:199:LEU:N	2.35	0.59
1:M:87:TYR:O	1:M:91:ALA:N	2.35	0.59
1:A:159:ARG:NH1	1:A:175:SER:OG	2.35	0.59
2:N:153:HIS:O	2:N:181:TYR:OH	2.18	0.59
3:I:103:ARG:C	7:I:201:ACO:O1A	2.44	0.59
1:G:782:LYS:O	1:G:784:VAL:O	2.21	0.59
1:M:843:GLU:O	1:M:847:SER:N	2.34	0.59
3:O:134:VAL:O	3:O:136:ASP:N	2.36	0.59
1:M:312:LEU:O	1:M:316:TYR:N	2.35	0.59
1:A:514:GLN:OE1	1:A:568:ARG:NH1	2.36	0.59
2:H:131:GLU:O	2:H:133:LEU:N	2.35	0.59
1:M:358:ASN:O	2:N:2:PRO:HG3	2.03	0.59
3:I:104:HIS:O	7:I:201:ACO:C5A	2.50	0.58
1:M:170:ARG:O	1:M:173:TRP:N	2.36	0.58
1:G:74:ASP:O	1:G:77:SER:N	2.33	0.58
1:M:200:ALA:HB3	1:M:201:GLU:HA	1.84	0.58
1:A:861:LEU:O	1:A:863:TYR:N	2.36	0.58
2:B:8:ALA:HB3	2:B:44:SER:O	2.03	0.58
1:M:782:LYS:O	1:M:783:VAL:C	2.47	0.58
3:O:15:ASN:O	3:O:17:GLY:N	2.37	0.58
3:I:16:LEU:CA	3:I:16:LEU:O	2.52	0.58
1:A:498:GLY:O	1:A:500:LYS:N	2.37	0.58
2:B:163:HIS:O	2:B:165:TYR:N	2.36	0.58
1:M:250:ASP:O	1:M:253:GLY:N	2.37	0.58
1:M:170:ARG:O	1:M:172:ASN:N	2.37	0.57
3:I:8:LEU:HA	3:I:64:ALA:HA	1.85	0.57
1:G:65:VAL:O	1:G:67:SER:N	2.32	0.57
1:A:87:TYR:O	1:A:91:ALA:N	2.37	0.57
2:B:113:GLY:HA3	2:B:141:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:ILE:HG21	2:H:134:MET:HE1	1.86	0.57
1:A:671:LYS:HA	1:A:674:GLU:HG2	1.86	0.57
3:C:64:ALA:HB2	3:C:111:LEU:HD21	1.87	0.57
1:G:112:MET:HA	1:G:112:MET:HE2	1.86	0.57
1:M:561:TYR:O	1:M:565:ALA:N	2.33	0.57
1:M:619:MET:HE1	1:M:714:TYR:CB	2.35	0.57
1:G:467:CYS:SG	1:G:509:TRP:CH2	2.95	0.56
3:I:134:VAL:O	3:I:136:ASP:N	2.38	0.56
2:B:155:ARG:HB3	2:B:181:TYR:CE2	2.40	0.56
3:C:93:ILE:O	3:C:95:PHE:N	2.38	0.56
1:G:417:TYR:O	1:G:420:ALA:N	2.39	0.56
3:C:101:ASN:O	3:C:101:ASN:ND2	2.33	0.56
1:G:391:PRO:O	1:G:393:PRO:N	2.38	0.56
1:M:185:GLU:CD	1:M:185:GLU:CB	2.75	0.56
1:G:85:ALA:C	1:G:87:TYR:H	2.14	0.56
3:I:20:THR:O	3:I:23:ALA:HB3	2.05	0.56
1:A:442:LEU:N	1:A:442:LEU:HD12	2.20	0.56
2:H:28:TYR:HB3	2:H:33:TYR:HE1	1.71	0.56
1:A:85:ALA:C	1:A:87:TYR:H	2.14	0.55
2:N:163:HIS:O	2:N:165:TYR:N	2.39	0.55
1:A:324:PHE:CE2	2:B:2:PRO:HG2	2.41	0.55
3:I:36:PHE:N	3:I:36:PHE:C	2.64	0.55
1:G:418:ILE:O	1:G:422:LEU:N	2.39	0.55
1:G:163:TRP:HE1	1:G:176:LEU:HG	1.71	0.55
1:A:115:THR:O	1:A:117:GLU:N	2.40	0.55
2:N:12:ASP:O	2:N:16:MET:CB	2.53	0.55
1:A:321:PRO:HB2	1:A:322:PRO:CD	2.37	0.55
1:A:532:LEU:HD13	1:A:551:ILE:HD11	1.89	0.55
1:G:65:VAL:C	1:G:67:SER:H	2.15	0.55
1:G:510:PHE:O	1:G:514:GLN:N	2.33	0.54
1:G:324:PHE:CE2	2:H:2:PRO:HG2	2.43	0.54
1:A:170:ARG:NH1	1:A:215:CYS:SG	2.75	0.54
1:A:767:LEU:HD13	1:A:801:ILE:HG23	1.87	0.54
2:H:128:GLY:O	2:H:130:ALA:N	2.41	0.54
1:M:245:GLU:CB	1:M:246:PRO:HD3	2.37	0.54
1:M:286:PHE:O	1:M:287:LYS:C	2.50	0.54
1:G:470:VAL:CB	1:G:486:ALA:HB2	2.37	0.54
1:G:532:LEU:HD21	1:G:551:ILE:HG12	1.88	0.54
1:A:575:PHE:O	1:A:579:PHE:N	2.40	0.54
3:I:27:VAL:HG13	3:I:27:VAL:O	2.08	0.54
1:A:177:ALA:HB2	1:A:192:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:O	1:A:252:PHE:N	2.40	0.54
1:G:87:TYR:O	1:G:91:ALA:N	2.41	0.54
1:M:782:LYS:O	1:M:784:VAL:N	2.41	0.54
1:G:404:HIS:C	1:G:406:LEU:H	2.16	0.54
1:M:286:PHE:O	1:M:289:TYR:N	2.27	0.53
1:A:213:SER:O	1:A:215:CYS:N	2.41	0.53
2:B:144:VAL:HG23	2:B:145:HIS:H	1.73	0.53
1:G:177:ALA:HB2	1:G:192:THR:HG23	1.89	0.53
1:M:463:ARG:O	1:M:463:ARG:HG2	2.08	0.53
1:M:711:TYR:O	1:M:713:ASN:N	2.42	0.53
3:I:93:ILE:O	3:I:95:PHE:N	2.42	0.53
1:A:410:ASP:O	1:A:412:PRO:N	2.42	0.53
1:G:321:PRO:O	1:G:322:PRO:C	2.52	0.53
2:H:31:LYS:O	2:H:33:TYR:O	2.26	0.53
1:M:119:LYS:O	1:M:122:ILE:HD12	2.09	0.53
1:A:234:LEU:HD22	1:A:265:LEU:CD1	2.39	0.53
1:A:343:TYR:O	1:A:347:GLN:NE2	2.39	0.53
1:M:134:THR:O	1:M:136:LYS:N	2.42	0.53
3:C:72:GLY:HA2	3:C:98:VAL:HB	1.91	0.53
1:M:234:LEU:O	1:M:238:LEU:N	2.42	0.52
1:G:159:ARG:NE	1:G:175:SER:HB3	2.24	0.52
1:A:391:PRO:O	1:A:393:PRO:N	2.42	0.52
1:G:463:ARG:HB3	1:G:489:PHE:CE2	2.43	0.52
3:C:133:ALA:O	3:C:134:VAL:C	2.53	0.52
2:N:128:GLY:O	2:N:130:ALA:N	2.43	0.52
2:B:149:TYR:CG	2:B:149:TYR:O	2.61	0.52
1:M:262:TYR:HB3	1:M:271:ALA:HB2	1.91	0.52
1:G:254:LEU:O	1:G:256:GLU:N	2.43	0.52
1:G:580:GLU:OE1	1:G:581:ASP:N	2.43	0.52
1:M:193:LEU:O	1:M:196:PHE:N	2.35	0.52
1:M:234:LEU:HD22	1:M:265:LEU:CD1	2.39	0.52
1:M:244:ILE:O	1:M:246:PRO:N	2.43	0.52
1:M:233:LYS:O	1:M:235:GLN:N	2.43	0.52
1:M:515:ALA:HB1	1:M:569:PHE:CE2	2.45	0.52
1:M:547:ILE:O	1:M:551:ILE:HD13	2.10	0.52
1:A:262:TYR:CD2	1:A:270:ASP:O	2.61	0.51
1:G:31:TYR:HA	1:G:32:ASN:C	2.34	0.51
1:M:354:ALA:O	1:M:358:ASN:N	2.43	0.51
1:G:324:PHE:O	1:G:327:LEU:HB3	2.10	0.51
1:M:224:TYR:C	1:M:226:ALA:H	2.17	0.51
3:O:93:ILE:O	3:O:95:PHE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:PHE:HA	1:A:414:ALA:HB3	1.92	0.51
1:A:432:TYR:HB3	1:A:451:ILE:O	2.11	0.51
1:A:556:TRP:O	1:A:559:ARG:N	2.36	0.51
1:A:820:ASP:O	1:A:823:GLY:N	2.42	0.51
2:B:156:GLN:HA	2:B:157:SER:C	2.35	0.51
1:G:574:LYS:O	1:G:578:GLN:N	2.44	0.51
1:A:143:ALA:CB	1:A:159:ARG:HG2	2.40	0.51
1:A:619:MET:CE	1:A:619:MET:CG	2.88	0.51
2:B:24:LEU:HD23	2:B:25:PRO:HD2	1.93	0.51
1:A:217:MET:O	1:A:220:ASN:N	2.44	0.51
1:A:803:ASN:O	1:A:805:SER:N	2.44	0.51
2:B:152:LEU:HD21	2:B:190:MET:HB2	1.93	0.51
1:G:312:LEU:C	1:G:315:PHE:O	2.54	0.51
1:G:398:ASN:HB3	1:G:421:ALA:HB2	1.92	0.51
1:G:573:PRO:O	1:G:576:TYR:N	2.44	0.51
1:M:580:GLU:C	1:M:582:ASP:H	2.18	0.51
1:G:410:ASP:O	1:G:412:PRO:N	2.43	0.51
1:M:215:CYS:SG	1:M:215:CYS:C	2.94	0.51
1:M:255:LEU:HD12	1:M:255:LEU:O	2.11	0.51
1:M:628:GLN:HA	1:M:631:ASP:CB	2.41	0.51
3:C:72:GLY:CA	3:C:98:VAL:HG12	2.41	0.51
3:I:36:PHE:H	3:I:38:ALA:H	1.57	0.51
1:G:279:ILE:O	1:G:283:PRO:N	2.44	0.50
1:M:170:ARG:C	1:M:172:ASN:H	2.18	0.50
1:A:174:THR:O	1:A:178:VAL:N	2.44	0.50
1:A:286:PHE:O	1:A:287:LYS:C	2.54	0.50
1:M:480:ASP:C	1:M:482:ALA:H	2.19	0.50
1:A:815:LYS:N	1:A:816:PHE:HA	2.27	0.50
1:G:344:VAL:O	1:G:345:LEU:C	2.54	0.50
1:M:210:TYR:CZ	1:M:214:GLU:OE1	2.64	0.50
1:M:250:ASP:O	1:M:252:PHE:N	2.45	0.50
3:C:109:SER:CB	7:C:201:ACO:O2A	2.60	0.50
1:G:437:ARG:HD3	5:G:901:G4P:PC	2.52	0.50
1:G:101:SER:O	1:G:104:CYS:N	2.29	0.50
1:A:220:ASN:O	1:A:224:TYR:HB3	2.12	0.50
2:B:28:TYR:HB3	2:B:33:TYR:HE1	1.77	0.50
3:C:24:HIS:ND1	3:C:24:HIS:O	2.45	0.50
1:A:511:ILE:HG23	1:A:568:ARG:HG3	1.94	0.49
1:G:614:MET:HE2	1:G:614:MET:HA	1.93	0.49
1:M:324:PHE:CE2	2:N:2:PRO:HG2	2.46	0.49
1:M:575:PHE:O	1:M:579:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ARG:O	2:B:187:ALA:HA	2.12	0.49
1:G:170:ARG:HG3	1:G:196:PHE:CE2	2.47	0.49
1:G:286:PHE:O	1:G:287:LYS:C	2.55	0.49
1:M:193:LEU:O	1:M:195:GLN:N	2.45	0.49
1:M:324:PHE:O	1:M:327:LEU:HG	2.11	0.49
1:A:781:LYS:HA	1:A:781:LYS:CE	2.41	0.49
1:G:101:SER:O	1:G:102:PRO:C	2.55	0.49
1:A:754:THR:HA	1:A:759:PHE:CD2	2.48	0.49
1:G:170:ARG:C	1:G:172:ASN:H	2.19	0.49
1:G:522:TYR:O	1:G:526:LYS:N	2.43	0.49
2:H:152:LEU:HD11	2:H:190:MET:HB2	1.94	0.49
1:M:215:CYS:SG	1:M:215:CYS:CA	2.98	0.49
1:A:576:TYR:HA	1:A:579:PHE:HB2	1.94	0.49
1:M:172:ASN:O	1:M:174:THR:N	2.38	0.49
1:A:53:LEU:O	1:A:57:ILE:N	2.46	0.49
2:B:138:LEU:O	2:B:141:LEU:N	2.46	0.49
1:A:170:ARG:HG3	1:A:196:PHE:CE1	2.47	0.49
1:A:356:PHE:CD1	1:A:356:PHE:C	2.91	0.49
1:G:515:ALA:C	1:G:517:ALA:N	2.70	0.49
1:M:515:ALA:O	1:M:517:ALA:O	2.31	0.48
1:M:561:TYR:O	1:M:564:LEU:N	2.46	0.48
1:A:619:MET:HA	1:A:710:PHE:HE1	1.78	0.48
1:G:579:PHE:CE1	2:H:30:MET:HG2	2.48	0.48
7:C:201:ACO:H131	7:C:201:ACO:C7P	2.44	0.48
1:G:234:LEU:O	1:G:238:LEU:N	2.46	0.48
1:G:575:PHE:O	1:G:579:PHE:CD1	2.67	0.48
7:I:201:ACO:H72	7:I:201:ACO:CDP	2.39	0.48
2:B:29:MET:CG	2:B:29:MET:CE	2.91	0.48
1:G:56:ALA:O	1:G:59:LYS:N	2.46	0.48
1:G:386:ASP:O	1:G:388:THR:N	2.47	0.48
1:M:573:PRO:O	1:M:576:TYR:N	2.47	0.48
2:B:40:TRP:NE1	2:B:99:LYS:HA	2.29	0.48
1:G:235:GLN:OE1	1:G:265:LEU:HD21	2.13	0.48
1:M:625:LEU:O	1:M:629:MET:HG3	2.13	0.48
2:H:152:LEU:CD1	2:H:190:MET:HB2	2.44	0.48
2:B:149:TYR:O	2:B:149:TYR:CD2	2.67	0.48
2:B:195:LYS:O	2:B:196:LEU:C	2.57	0.48
1:G:250:ASP:O	1:G:252:PHE:N	2.45	0.48
1:A:391:PRO:C	1:A:393:PRO:N	2.72	0.48
1:A:401:LEU:C	1:A:403:GLN:H	2.21	0.48
1:A:510:PHE:O	1:A:514:GLN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:158:ILE:O	3:I:165:GLU:HA	2.14	0.48
1:G:172:ASN:C	1:G:174:THR:H	2.22	0.48
1:M:417:TYR:O	1:M:421:ALA:N	2.44	0.48
2:N:16:MET:O	2:N:18:ASN:N	2.47	0.47
1:A:283:PRO:O	1:A:321:PRO:HG2	2.14	0.47
1:A:782:LYS:O	1:A:784:VAL:N	2.47	0.47
1:M:410:ASP:O	1:M:412:PRO:N	2.46	0.47
1:M:432:TYR:N	1:M:432:TYR:CD1	2.82	0.47
3:O:97:GLY:HA2	7:O:201:ACO:H141	1.96	0.47
1:M:197:GLU:O	1:M:198:LYS:CB	2.62	0.47
1:M:580:GLU:O	1:M:582:ASP:N	2.46	0.47
2:N:13:ILE:HG21	2:N:30:MET:HE1	1.95	0.47
1:M:254:LEU:O	1:M:256:GLU:N	2.48	0.47
1:M:510:PHE:O	1:M:514:GLN:N	2.46	0.47
1:A:185:GLU:HG3	1:A:185:GLU:O	2.15	0.47
1:M:628:GLN:O	1:M:631:ASP:N	2.46	0.47
1:A:522:TYR:C	1:A:524:ASP:H	2.23	0.47
2:B:29:MET:SD	2:B:29:MET:CB	2.97	0.47
1:G:391:PRO:C	1:G:393:PRO:N	2.73	0.47
1:M:690:ASP:O	1:M:693:GLY:N	2.48	0.47
1:A:321:PRO:O	1:A:322:PRO:C	2.57	0.47
1:A:359:VAL:O	1:A:361:PRO:N	2.47	0.47
3:C:72:GLY:HA2	3:C:98:VAL:CB	2.44	0.47
1:G:358:ASN:O	2:H:2:PRO:HG3	2.15	0.47
1:M:51:LEU:O	1:M:55:ASP:N	2.48	0.47
1:M:125:PHE:O	1:M:126:THR:C	2.57	0.47
1:M:101:SER:O	1:M:102:PRO:C	2.57	0.47
1:G:498:GLY:O	1:G:500:LYS:N	2.37	0.47
2:N:36:HIS:CD2	2:N:99:LYS:HB3	2.49	0.47
1:A:356:PHE:HD2	1:A:403:GLN:CB	2.28	0.47
1:A:515:ALA:HB1	1:A:569:PHE:CE2	2.50	0.47
1:A:767:LEU:HB2	1:A:801:ILE:HG23	1.96	0.47
1:M:70:LEU:O	1:M:72:GLY:N	2.48	0.47
1:M:159:ARG:CD	1:M:175:SER:OG	2.63	0.47
1:M:286:PHE:O	1:M:288:TYR:N	2.48	0.47
1:M:430:GLU:CD	1:M:430:GLU:O	2.58	0.47
1:G:274:VAL:O	1:G:278:LEU:N	2.48	0.46
1:M:357:SER:HA	1:M:360:LYS:HB2	1.96	0.46
1:A:398:ASN:HB3	1:A:421:ALA:HB2	1.96	0.46
3:C:103:ARG:CB	7:C:201:ACO:H142	2.46	0.46
1:G:309:TYR:O	1:G:313:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:505:VAL:HG23	1:M:507:ALA:HB2	1.97	0.46
1:A:573:PRO:O	1:A:576:TYR:N	2.48	0.46
2:B:115:ILE:HG21	2:B:134:MET:CE	2.45	0.46
3:C:93:ILE:O	3:C:94:GLU:C	2.58	0.46
1:A:561:TYR:O	1:A:565:ALA:N	2.36	0.46
1:G:556:TRP:O	1:G:558:VAL:N	2.48	0.46
1:A:211:GLU:O	1:A:215:CYS:HB3	2.16	0.46
1:A:614:MET:CE	1:A:614:MET:CG	2.94	0.46
1:G:170:ARG:C	1:G:172:ASN:N	2.74	0.46
1:G:623:SER:O	1:G:626:TYR:N	2.48	0.46
1:M:360:LYS:HB3	1:M:361:PRO:HD3	1.98	0.46
2:N:31:LYS:O	2:N:34:MET:N	2.48	0.46
2:N:179:SER:C	2:N:181:TYR:H	2.23	0.46
1:A:432:TYR:HD2	1:A:455:GLY:CA	2.29	0.46
1:A:811:PHE:CD2	1:A:811:PHE:C	2.93	0.46
1:G:813:GLN:O	1:G:817:GLY:N	2.48	0.46
1:M:401:LEU:CD2	1:M:417:TYR:CD2	2.99	0.46
1:A:143:ALA:HB1	1:A:159:ARG:HG2	1.97	0.46
3:C:21:LYS:O	3:C:23:ALA:O	2.34	0.46
1:A:430:GLU:CD	1:A:430:GLU:O	2.58	0.46
1:G:224:TYR:C	1:G:226:ALA:H	2.24	0.46
1:M:575:PHE:O	1:M:579:PHE:N	2.49	0.46
3:C:98:VAL:HG22	7:C:201:ACO:CEP	2.45	0.46
1:G:811:PHE:C	1:G:811:PHE:CD2	2.93	0.46
1:M:215:CYS:SG	1:M:216:LEU:N	2.89	0.46
1:M:347:GLN:HE21	1:M:355:THR:HA	1.79	0.46
2:B:159:ARG:O	2:B:160:ALA:C	2.59	0.46
2:H:36:HIS:CE1	2:H:99:LYS:HD3	2.50	0.46
1:M:172:ASN:C	1:M:174:THR:H	2.24	0.46
1:M:210:TYR:CE1	1:M:214:GLU:OE1	2.69	0.46
1:A:236:ASN:O	1:A:240:HIS:N	2.39	0.45
3:I:35:PHE:O	3:I:35:PHE:CG	2.69	0.45
3:I:76:ALA:HB2	3:I:93:ILE:HA	1.97	0.45
1:A:76:TYR:C	1:A:78:VAL:H	2.23	0.45
1:A:101:SER:O	1:A:102:PRO:C	2.60	0.45
1:A:134:THR:O	1:A:136:LYS:N	2.49	0.45
1:A:269:LYS:C	1:A:271:ALA:H	2.23	0.45
2:B:179:SER:C	2:B:181:TYR:H	2.24	0.45
1:G:189:ALA:O	1:G:192:THR:HG22	2.16	0.45
1:M:321:PRO:O	1:M:322:PRO:C	2.59	0.45
1:M:804:ASN:HA	1:M:805:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:O	1:A:741:CYS:N	2.48	0.45
1:G:149:ILE:O	1:G:151:ASP:N	2.49	0.45
1:G:711:TYR:C	1:G:713:ASN:H	2.24	0.45
1:M:211:GLU:O	1:M:213:SER:N	2.45	0.45
2:B:112:ASN:CB	2:B:149:TYR:CE1	2.99	0.45
2:N:137:ALA:O	2:N:141:LEU:HB2	2.17	0.45
1:G:406:LEU:HD22	1:G:438:ILE:HG22	1.99	0.45
3:O:76:ALA:CB	3:O:93:ILE:HA	2.47	0.45
1:A:767:LEU:HD12	1:A:768:HIS:CB	2.47	0.45
1:G:386:ASP:C	1:G:388:THR:H	2.24	0.45
1:G:503:HIS:CD2	1:G:682:ALA:HB1	2.52	0.45
3:I:110:LYS:O	3:I:113:LYS:N	2.48	0.45
1:A:503:HIS:CD2	1:A:511:ILE:HD11	2.51	0.45
1:A:610:TYR:HA	1:A:615:TYR:HD2	1.82	0.45
1:G:428:LEU:O	1:G:430:GLU:N	2.49	0.45
1:M:115:THR:O	1:M:117:GLU:N	2.49	0.45
1:M:628:GLN:O	1:M:631:ASP:HB3	2.17	0.45
1:A:619:MET:HG3	1:A:710:PHE:HD1	1.81	0.45
1:G:502:LEU:O	1:G:504:LEU:N	2.50	0.45
2:H:169:LEU:O	2:H:170:ALA:HB3	2.15	0.45
1:M:518:TYR:O	1:M:522:TYR:HB3	2.17	0.45
1:A:56:ALA:O	1:A:59:LYS:HB2	2.16	0.45
3:I:6:CYS:HA	3:I:66:TYR:HA	1.99	0.45
3:I:76:ALA:CB	3:I:93:ILE:HA	2.47	0.45
1:M:27:ALA:O	1:M:30:LYS:N	2.45	0.45
1:M:248:VAL:HG11	1:M:254:LEU:HD22	1.98	0.45
3:O:72:GLY:HA2	3:O:98:VAL:HA	1.99	0.45
1:G:196:PHE:O	1:G:198:LYS:N	2.50	0.45
1:G:625:LEU:O	1:G:629:MET:HG3	2.16	0.45
3:I:119:CYS:O	3:I:124:GLN:N	2.50	0.45
1:M:324:PHE:HE2	2:N:2:PRO:HG2	1.81	0.45
1:M:556:TRP:O	1:M:558:VAL:N	2.50	0.45
3:O:93:ILE:O	3:O:94:GLU:C	2.60	0.45
1:A:503:HIS:NE2	1:A:511:ILE:HD11	2.32	0.44
1:G:437:ARG:O	1:G:441:HIS:N	2.48	0.44
1:G:512:VAL:HG13	1:G:513:GLU:N	2.31	0.44
1:M:726:ILE:HG13	1:M:727:LEU:N	2.32	0.44
1:M:754:THR:HA	1:M:759:PHE:CD2	2.51	0.44
1:M:185:GLU:HG3	1:M:185:GLU:O	2.17	0.44
1:M:391:PRO:C	1:M:393:PRO:N	2.75	0.44
1:G:233:LYS:O	1:G:235:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:ASN:HB3	2:N:5:ILE:O	2.17	0.44
1:M:463:ARG:O	1:M:463:ARG:CG	2.66	0.44
1:M:841:LEU:O	1:M:845:ILE:N	2.49	0.44
1:A:324:PHE:O	1:A:327:LEU:HG	2.18	0.44
1:A:438:ILE:C	1:A:440:LYS:H	2.25	0.44
1:A:824:LEU:O	1:A:825:LEU:C	2.60	0.44
2:B:31:LYS:O	2:B:34:MET:N	2.51	0.44
2:B:179:SER:HA	2:B:185:GLU:O	2.17	0.44
1:M:711:TYR:C	1:M:713:ASN:H	2.25	0.44
1:A:841:LEU:O	1:A:845:ILE:N	2.51	0.44
2:B:144:VAL:HG23	2:B:145:HIS:N	2.32	0.44
1:G:196:PHE:O	1:G:199:LEU:N	2.51	0.44
3:I:16:LEU:CB	3:I:17:GLY:H	2.30	0.44
1:M:576:TYR:HA	1:M:579:PHE:HB2	1.99	0.44
2:N:154:VAL:O	2:N:187:ALA:HB1	2.18	0.44
3:O:95:PHE:HA	7:O:201:ACO:C	2.48	0.44
3:C:155:ASN:O	3:C:156:ASN:C	2.61	0.44
1:G:487:SER:O	1:G:490:THR:N	2.50	0.44
1:A:224:TYR:C	1:A:226:ALA:H	2.26	0.44
1:A:584:LEU:HD23	1:A:584:LEU:C	2.43	0.44
1:A:828:TYR:O	1:A:829:ARG:C	2.58	0.44
1:G:85:ALA:C	1:G:87:TYR:N	2.76	0.44
1:G:518:TYR:HB3	1:G:565:ALA:HB2	1.99	0.44
2:N:131:GLU:O	2:N:133:LEU:N	2.50	0.44
3:O:127:VAL:HG12	3:O:128:PHE:H	1.82	0.44
1:A:252:PHE:C	1:A:254:LEU:H	2.25	0.44
3:C:8:LEU:CB	3:C:64:ALA:HA	2.48	0.44
3:I:99:LEU:HD23	3:I:102:TYR:CE1	2.53	0.44
1:M:432:TYR:HD2	1:M:455:GLY:CA	2.31	0.44
1:M:556:TRP:O	1:M:559:ARG:N	2.39	0.44
1:A:115:THR:C	1:A:117:GLU:H	2.26	0.43
1:A:149:ILE:O	1:A:151:ASP:N	2.46	0.43
1:G:85:ALA:O	1:G:87:TYR:N	2.51	0.43
1:G:282:ASN:O	1:G:283:PRO:C	2.60	0.43
1:G:518:TYR:CB	1:G:565:ALA:HB2	2.48	0.43
1:A:828:TYR:O	1:A:828:TYR:HD1	2.01	0.43
1:A:463:ARG:HD2	1:A:489:PHE:CB	2.48	0.43
1:A:623:SER:C	1:A:625:LEU:H	2.24	0.43
2:B:12:ASP:O	2:B:16:MET:CB	2.62	0.43
1:M:452:LEU:O	1:M:455:GLY:N	2.48	0.43
1:M:56:ALA:O	1:M:59:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:324:PHE:O	1:M:325:ILE:C	2.61	0.43
2:N:24:LEU:HD12	2:N:119:SER:CB	2.49	0.43
1:A:432:TYR:N	1:A:432:TYR:CD1	2.86	0.43
1:A:443:GLY:HA2	1:A:855:HIS:HA	1.99	0.43
3:C:23:ALA:O	3:C:24:HIS:C	2.60	0.43
1:M:189:ALA:O	1:M:192:THR:HG22	2.18	0.43
1:M:193:LEU:C	1:M:195:GLN:H	2.27	0.43
1:A:405:PHE:O	1:A:414:ALA:HB2	2.19	0.43
3:C:101:ASN:C	3:C:101:ASN:ND2	2.77	0.43
1:G:711:TYR:O	1:G:713:ASN:N	2.52	0.43
1:M:312:LEU:O	1:M:315:PHE:N	2.52	0.43
1:A:118:TYR:O	1:A:119:LYS:C	2.62	0.43
1:A:472:TYR:C	1:A:474:LEU:H	2.27	0.43
1:G:115:THR:O	1:G:117:GLU:N	2.52	0.43
2:H:36:HIS:CE1	2:H:99:LYS:HB3	2.54	0.43
3:I:104:HIS:O	7:I:201:ACO:C4A	2.67	0.43
1:M:193:LEU:HD12	1:M:194:SER:N	2.33	0.43
1:A:398:ASN:CB	1:A:421:ALA:HB2	2.47	0.43
1:G:78:VAL:O	1:G:80:GLU:N	2.49	0.43
1:M:279:ILE:O	1:M:283:PRO:N	2.52	0.43
1:M:404:HIS:C	1:M:406:LEU:H	2.27	0.43
1:M:528:LYS:O	1:M:532:LEU:HD12	2.19	0.43
1:A:162:TYR:O	1:A:164:GLU:N	2.52	0.43
1:M:308:LEU:O	1:M:312:LEU:HB2	2.19	0.43
1:A:235:GLN:O	1:A:239:LYS:N	2.47	0.42
1:A:579:PHE:CE2	2:B:30:MET:HG2	2.54	0.42
1:G:472:TYR:C	1:G:474:LEU:H	2.27	0.42
1:A:196:PHE:O	1:A:198:LYS:N	2.52	0.42
1:A:234:LEU:O	1:A:238:LEU:N	2.48	0.42
1:A:324:PHE:O	1:A:325:ILE:C	2.62	0.42
1:G:764:ILE:O	1:G:766:LEU:N	2.52	0.42
2:H:5:ILE:HA	2:H:47:ALA:HB2	2.00	0.42
2:H:35:TYR:O	2:H:39:SER:OG	2.33	0.42
1:M:233:LYS:HA	1:M:236:ASN:ND2	2.34	0.42
2:B:100:MET:HE2	2:B:141:LEU:HG	2.02	0.42
1:G:514:GLN:OE1	1:G:568:ARG:NH1	2.53	0.42
2:B:97:LEU:HA	2:B:97:LEU:HD23	1.83	0.42
2:B:100:MET:O	2:B:102:ASP:N	2.52	0.42
1:G:514:GLN:O	1:G:514:GLN:HG2	2.20	0.42
3:I:16:LEU:CB	3:I:17:GLY:N	2.82	0.42
3:O:109:SER:HA	7:O:201:ACO:O2A	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LEU:CD2	1:A:551:ILE:HG12	2.49	0.42
1:M:250:ASP:O	1:M:251:LYS:C	2.61	0.42
1:M:463:ARG:HG3	1:M:489:PHE:CZ	2.53	0.42
1:M:583:GLN:HB2	1:M:602:MET:HE3	2.00	0.42
1:M:828:TYR:O	1:M:829:ARG:C	2.60	0.42
3:O:74:LEU:CB	3:O:111:LEU:HD21	2.50	0.42
3:C:76:ALA:CB	3:C:93:ILE:HA	2.49	0.42
1:G:250:ASP:HA	2:H:143:GLU:OE2	2.20	0.42
1:G:359:VAL:O	1:G:361:PRO:N	2.53	0.42
1:M:517:ALA:O	1:M:519:TYR:N	2.52	0.42
1:A:148:GLN:O	1:A:150:GLY:N	2.45	0.42
2:B:141:LEU:HD23	2:B:141:LEU:O	2.19	0.42
2:B:155:ARG:HA	2:B:187:ALA:CB	2.49	0.42
1:G:690:ASP:O	1:G:693:GLY:N	2.53	0.42
1:G:711:TYR:OH	1:G:728:ASP:HB2	2.19	0.42
1:M:76:TYR:C	1:M:78:VAL:H	2.27	0.42
1:A:435:LYS:O	1:A:438:ILE:O	2.37	0.42
1:A:610:TYR:HA	1:A:615:TYR:CD2	2.55	0.42
3:C:71:VAL:HA	3:C:99:LEU:HD21	2.02	0.42
3:C:98:VAL:H	7:C:201:ACO:H141	1.85	0.42
1:M:95:ILE:N	1:M:96:GLU:OE1	2.52	0.42
1:A:312:LEU:O	1:A:314:GLN:N	2.52	0.42
2:B:152:LEU:CD2	2:B:190:MET:HB2	2.49	0.42
1:G:417:TYR:O	1:G:418:ILE:C	2.62	0.42
1:A:155:ALA:O	1:A:159:ARG:HB2	2.19	0.42
1:M:428:LEU:O	1:M:430:GLU:N	2.53	0.42
1:M:599:TYR:CD1	1:M:599:TYR:C	2.97	0.42
2:N:179:SER:HA	2:N:185:GLU:O	2.20	0.42
1:A:101:SER:O	1:A:103:ILE:N	2.53	0.41
1:A:270:ASP:CA	1:A:273:ILE:HG22	2.50	0.41
1:G:267:GLN:O	1:G:271:ALA:HB2	2.20	0.41
1:M:367:LYS:HG2	1:M:368:SER:H	1.85	0.41
1:A:782:LYS:O	1:A:783:VAL:C	2.63	0.41
1:M:515:ALA:C	1:M:517:ALA:O	2.63	0.41
1:M:800:GLU:O	1:M:802:SER:N	2.45	0.41
3:O:24:HIS:O	3:O:25:VAL:CB	2.66	0.41
3:O:119:CYS:O	3:O:124:GLN:N	2.53	0.41
1:A:227:ALA:O	1:A:229:ASP:N	2.53	0.41
1:G:464:PHE:HD2	2:H:122:ARG:CB	2.34	0.41
2:N:31:LYS:C	2:N:33:TYR:N	2.78	0.41
1:A:233:LYS:O	1:A:235:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:O	1:G:313:GLU:C	2.63	0.41
1:M:113:ARG:CB	1:M:145:LEU:HD21	2.50	0.41
1:M:378:VAL:O	1:M:381:TYR:N	2.46	0.41
1:G:282:ASN:O	1:G:282:ASN:ND2	2.54	0.41
1:M:85:ALA:C	1:M:87:TYR:H	2.28	0.41
1:A:524:ASP:C	1:A:527:LYS:H	2.29	0.41
1:A:561:TYR:O	1:A:564:LEU:N	2.54	0.41
1:A:825:LEU:O	1:A:826:PHE:C	2.63	0.41
2:B:40:TRP:CZ2	2:B:99:LYS:HB2	2.55	0.41
1:G:463:ARG:HD3	2:H:24:LEU:C	2.45	0.41
1:G:726:ILE:C	1:G:728:ASP:H	2.29	0.41
2:N:159:ARG:O	2:N:160:ALA:C	2.64	0.41
1:A:528:LYS:C	1:A:530:ASP:H	2.29	0.41
3:C:61:THR:HA	3:C:75:VAL:HA	2.03	0.41
1:M:159:ARG:NE	1:M:175:SER:OG	2.53	0.41
2:N:138:LEU:O	2:N:141:LEU:N	2.48	0.41
3:O:95:PHE:HA	7:O:201:ACO:O	2.20	0.41
1:A:521:LEU:O	1:A:561:TYR:HD2	2.03	0.41
1:G:532:LEU:CG	1:G:551:ILE:HD11	2.50	0.41
2:H:8:ALA:HB3	2:H:44:SER:O	2.21	0.41
1:A:324:PHE:HE2	2:B:2:PRO:HG2	1.82	0.41
1:A:567:LYS:NZ	1:A:688:ASP:OD1	2.53	0.41
1:A:808:TRP:CD1	1:A:808:TRP:H	2.38	0.41
1:M:316:TYR:HA	1:M:317:PRO:HD3	1.95	0.41
2:N:16:MET:HB2	2:N:16:MET:HE3	1.92	0.41
2:N:168:THR:OG1	2:N:169:LEU:N	2.54	0.41
1:G:502:LEU:HD22	1:G:510:PHE:CD2	2.56	0.41
2:H:45:PHE:O	2:H:96:VAL:N	2.54	0.41
1:M:498:GLY:O	1:M:500:LYS:N	2.51	0.41
1:A:125:PHE:C	1:A:127:ALA:N	2.79	0.40
1:G:561:TYR:O	1:G:564:LEU:N	2.53	0.40
2:H:179:SER:HA	2:H:185:GLU:O	2.21	0.40
3:O:35:PHE:O	3:O:38:ALA:HB3	2.21	0.40
1:A:344:VAL:O	1:A:345:LEU:C	2.63	0.40
1:G:197:GLU:O	1:G:198:LYS:CB	2.68	0.40
1:G:443:GLY:C	1:G:445:MET:N	2.79	0.40
1:G:826:PHE:O	1:G:828:TYR:O	2.38	0.40
1:M:825:LEU:O	1:M:826:PHE:C	2.64	0.40
2:N:97:LEU:HD12	2:N:97:LEU:O	2.21	0.40
1:G:172:ASN:O	1:G:174:THR:N	2.53	0.40
1:G:418:ILE:HA	1:G:421:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:117:ASP:O	3:I:119:CYS:N	2.54	0.40
1:M:74:ASP:O	1:M:77:SER:C	2.63	0.40
1:M:193:LEU:C	1:M:195:GLN:N	2.79	0.40
2:B:31:LYS:O	2:B:33:TYR:N	2.55	0.40
1:G:210:TYR:CE1	1:G:214:GLU:CD	3.00	0.40
2:H:12:ASP:O	2:H:16:MET:N	2.51	0.40
1:M:344:VAL:C	1:M:346:PRO:N	2.79	0.40
1:M:628:GLN:O	1:M:631:ASP:CB	2.69	0.40
1:A:170:ARG:C	1:A:172:ASN:H	2.26	0.40
1:G:66:ASP:HA	1:G:104:CYS:CB	2.52	0.40
1:G:386:ASP:O	1:G:389:GLN:N	2.49	0.40
1:G:532:LEU:HG	1:G:551:ILE:HD11	2.02	0.40
1:M:292:LEU:HA	1:M:295:SER:CB	2.52	0.40
1:M:824:LEU:O	1:M:825:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	751/854 (88%)	487 (65%)	185 (25%)	79 (10%)	0	7
1	G	754/854 (88%)	494 (66%)	179 (24%)	81 (11%)	0	6
1	M	753/854 (88%)	504 (67%)	173 (23%)	76 (10%)	0	8
2	B	158/238 (66%)	94 (60%)	39 (25%)	25 (16%)	0	3
2	H	158/238 (66%)	91 (58%)	49 (31%)	18 (11%)	0	5
2	N	158/238 (66%)	93 (59%)	42 (27%)	23 (15%)	0	3
3	C	150/176 (85%)	94 (63%)	35 (23%)	21 (14%)	0	3
3	I	149/176 (85%)	89 (60%)	37 (25%)	23 (15%)	0	3
3	O	147/176 (84%)	90 (61%)	41 (28%)	16 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	4/8 (50%)	4 (100%)	0	0	100	100
4	K	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
4	Q	4/8 (50%)	4 (100%)	0	0	100	100
All	All	3190/3828 (83%)	2047 (64%)	781 (24%)	362 (11%)	0	5

All (362) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	101	SER
1	A	116	LYS
1	A	135	ASN
1	A	163	TRP
1	A	198	LYS
1	A	215	CYS
1	A	245	GLU
1	A	251	LYS
1	A	256	GLU
1	A	317	PRO
1	A	320	GLU
1	A	350	ARG
1	A	360	LYS
1	A	361	PRO
1	A	368	SER
1	A	371	SER
1	A	372	PRO
1	A	392	ILE
1	A	393	PRO
1	A	411	PHE
1	A	444	LEU
1	A	499	ILE
1	A	523	LEU
1	A	547	ILE
1	A	712	ASN
1	A	797	PRO
1	A	804	ASN
2	B	101	ASN
2	B	111	PRO
2	B	150	VAL
2	B	155	ARG
2	B	166	ARG

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Mol	Chain	Res	Type
2	B	172	GLU
2	B	173	VAL
2	B	199	LEU
3	C	4	ASP
3	C	16	LEU
3	C	25	VAL
3	C	80	PRO
3	C	87	SER
3	C	104	HIS
3	C	135	ASP
3	C	155	ASN
3	C	162	ASN
1	G	60	LYS
1	G	78	VAL
1	G	116	LYS
1	G	135	ASN
1	G	164	GLU
1	G	198	LYS
1	G	206	ASP
1	G	245	GLU
1	G	256	GLU
1	G	283	PRO
1	G	312	LEU
1	G	313	GLU
1	G	360	LYS
1	G	361	PRO
1	G	368	SER
1	G	371	SER
1	G	372	PRO
1	G	392	ILE
1	G	393	PRO
1	G	411	PHE
1	G	444	LEU
1	G	480	ASP
1	G	557	LEU
1	G	674	GLU
1	G	691	VAL
1	G	702	PRO
1	G	722	GLU
1	G	797	PRO
1	G	805	SER
2	H	96	VAL

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Mol	Chain	Res	Type
2	H	101	ASN
2	H	110	PRO
2	H	111	PRO
2	H	124	TYR
2	H	132	ASN
2	H	164	LEU
2	H	165	TYR
3	I	16	LEU
3	I	35	PHE
3	I	67	SER
3	I	80	PRO
3	I	88	LEU
3	I	104	HIS
3	I	135	ASP
3	I	158	ILE
3	I	162	ASN
1	M	60	LYS
1	M	116	LYS
1	M	135	ASN
1	M	163	TRP
1	M	198	LYS
1	M	245	GLU
1	M	283	PRO
1	M	287	LYS
1	M	345	LEU
1	M	350	ARG
1	M	368	SER
1	M	371	SER
1	M	411	PHE
1	M	444	LEU
1	M	446	ASP
1	M	447	THR
1	M	557	LEU
1	M	674	GLU
1	M	691	VAL
1	M	712	ASN
1	M	722	GLU
1	M	797	PRO
1	M	801	ILE
2	N	8	ALA
2	N	29	MET
2	N	102	ASP

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Mol	Chain	Res	Type
2	N	110	PRO
2	N	111	PRO
2	N	129	ILE
2	N	165	TYR
2	N	172	GLU
2	N	173	VAL
3	O	4	ASP
3	O	25	VAL
3	O	80	PRO
3	O	110	LYS
3	O	135	ASP
3	O	162	ASN
1	A	78	VAL
1	A	86	SER
1	A	95	ILE
1	A	173	TRP
1	A	228	SER
1	A	259	ALA
1	A	287	LYS
1	A	312	LEU
1	A	480	ASP
1	A	722	GLU
1	A	780	LEU
1	A	783	VAL
2	B	8	ALA
2	B	21	LEU
2	B	49	THR
2	B	110	PRO
2	B	124	TYR
2	B	157	SER
2	B	162	LEU
2	B	196	LEU
3	C	94	GLU
1	G	65	VAL
1	G	80	GLU
1	G	86	SER
1	G	95	ILE
1	G	101	SER
1	G	150	GLY
1	G	173	TRP
1	G	197	GLU
1	G	228	SER

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Mol	Chain	Res	Type
1	G	287	LYS
1	G	317	PRO
1	G	318	ARG
1	G	320	GLU
1	G	333	LYS
1	G	390	ASP
1	G	429	VAL
1	G	462	ASP
1	G	499	ILE
1	G	520	ARG
1	G	621	GLU
1	G	766	LEU
1	G	783	VAL
2	H	20	ASN
2	H	129	ILE
2	H	183	ASP
3	I	4	ASP
3	I	17	GLY
3	I	36	PHE
3	I	75	VAL
3	I	87	SER
3	I	94	GLU
3	I	119	CYS
1	M	78	VAL
1	M	150	GLY
1	M	151	ASP
1	M	173	TRP
1	M	215	CYS
1	M	256	GLU
1	M	259	ALA
1	M	273	ILE
1	M	317	PRO
1	M	332	ASP
1	M	372	PRO
1	M	393	PRO
1	M	632	ASP
1	M	783	VAL
1	M	808	TRP
1	M	833	ASP
2	N	96	VAL
2	N	124	TYR
2	N	131	GLU

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Mol	Chain	Res	Type
2	N	144	VAL
3	O	16	LEU
3	O	34	ALA
3	O	71	VAL
3	O	86	LEU
1	A	172	ASN
1	A	197	GLU
1	A	255	LEU
1	A	284	ASP
1	A	500	LYS
1	A	506	GLU
1	A	546	GLN
1	A	573	PRO
1	A	574	LYS
1	A	624	LYS
1	A	700	SER
1	A	862	GLN
2	B	129	ILE
2	B	156	GLN
2	B	165	TYR
3	C	62	GLN
3	C	68	GLU
1	G	166	PHE
1	G	233	LYS
1	G	250	ASP
1	G	255	LEU
1	G	463	ARG
1	G	497	ASN
1	G	506	GLU
1	G	608	ALA
1	G	765	VAL
1	G	819	ASN
1	G	829	ARG
2	H	49	THR
2	H	131	GLU
2	H	152	LEU
2	H	167	ASP
3	I	8	LEU
3	I	105	LYS
1	M	71	LYS
1	M	171	ALA
1	M	194	SER

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Mol	Chain	Res	Type
1	M	225	LYS
1	M	228	SER
1	M	233	LYS
1	M	234	LEU
1	M	251	LYS
1	M	297	GLY
1	M	391	PRO
1	M	480	ASP
1	M	506	GLU
1	M	581	ASP
1	M	596	PRO
2	N	17	GLN
2	N	49	THR
2	N	132	ASN
2	N	167	ASP
3	O	94	GLU
3	O	109	SER
1	A	30	LYS
1	A	150	GLY
1	A	200	ALA
1	A	234	LEU
1	A	344	VAL
1	A	391	PRO
1	A	429	VAL
1	A	625	LEU
1	A	634	LEU
1	A	691	VAL
1	A	737	LYS
3	C	71	VAL
3	C	154	VAL
1	G	171	ALA
1	G	321	PRO
1	G	387	PRO
1	G	502	LEU
1	G	516	GLU
1	G	573	PRO
1	G	596	PRO
1	G	791	GLU
2	H	24	LEU
3	I	71	VAL
3	I	123	HIS
1	M	218	TYR

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Mol	Chain	Res	Type
1	M	333	LYS
1	M	367	LYS
1	M	392	ILE
1	M	463	ARG
1	M	497	ASN
1	M	573	PRO
1	M	782	LYS
2	N	16	MET
2	N	32	TYR
2	N	174	LEU
3	O	93	ILE
3	O	123	HIS
1	A	233	LYS
1	A	313	GLU
1	A	403	GLN
1	A	497	ASN
1	A	632	ASP
1	A	701	THR
2	B	96	VAL
2	B	164	LEU
3	C	15	ASN
3	C	31	TYR
3	C	123	HIS
3	C	171	LEU
1	G	316	TYR
1	G	366	ARG
1	G	367	LYS
1	G	583	GLN
1	G	712	ASN
1	G	750	LYS
2	H	35	TYR
3	I	68	GLU
1	M	255	LEU
1	M	271	ALA
1	M	282	ASN
1	M	318	ARG
1	M	321	PRO
1	M	344	VAL
1	M	499	ILE
1	M	805	SER
2	N	24	LEU
2	N	196	LEU

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Mol	Chain	Res	Type
3	O	169	ILE
1	A	66	ASP
1	A	367	LYS
1	A	796	PHE
2	B	32	TYR
2	B	116	THR
1	G	212	HIS
1	G	282	ASN
3	I	169	ILE
1	M	429	VAL
1	M	796	PHE
2	N	199	LEU
3	O	15	ASN
1	A	102	PRO
1	A	321	PRO
1	A	345	LEU
1	A	616	VAL
3	C	75	VAL
3	C	93	ILE
1	G	149	ILE
2	H	144	VAL
3	I	129	VAL
1	A	149	ILE
2	B	144	VAL
1	G	418	ILE
1	M	95	ILE
1	M	702	PRO
1	A	596	PRO
2	B	24	LEU
3	C	129	VAL
1	M	149	ILE
1	M	485	VAL
1	A	322	PRO
1	G	322	PRO
1	M	101	SER

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	186/759 (24%)	150 (81%)	36 (19%)	1	9
1	G	189/759 (25%)	144 (76%)	45 (24%)	1	5
1	M	188/759 (25%)	155 (82%)	33 (18%)	2	12
2	B	51/216 (24%)	45 (88%)	6 (12%)	5	21
2	H	51/216 (24%)	40 (78%)	11 (22%)	1	6
2	N	51/216 (24%)	43 (84%)	8 (16%)	2	15
3	C	29/153 (19%)	22 (76%)	7 (24%)	1	5
3	I	28/153 (18%)	25 (89%)	3 (11%)	6	24
3	O	25/153 (16%)	23 (92%)	2 (8%)	11	35
All	All	798/3384 (24%)	647 (81%)	151 (19%)	1	10

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	77	SER
1	A	93	ARG
1	A	159	ARG
1	A	170	ARG
1	A	194	SER
1	A	214	GLU
1	A	224	TYR
1	A	236	ASN
1	A	252	PHE
1	A	254	LEU
1	A	273	ILE
1	A	285	ASN
1	A	312	LEU
1	A	328	THR
1	A	338	LYS
1	A	345	LEU
1	A	407	PHE
1	A	430	GLU
1	A	442	LEU
1	A	506	GLU
1	A	511	ILE
1	A	520	ARG
1	A	522	TYR

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Mol	Chain	Res	Type
1	A	532	LEU
1	A	578	GLN
1	A	585	ASP
1	A	688	ASP
1	A	708	THR
1	A	709	GLU
1	A	710	PHE
1	A	728	ASP
1	A	733	TYR
1	A	808	TRP
1	A	815	LYS
1	A	832	ASP
2	B	22	HIS
2	B	35	TYR
2	B	100	MET
2	B	148	GLU
2	B	163	HIS
2	B	192	LYS
3	C	36	PHE
3	C	86	LEU
3	C	95	PHE
3	C	99	LEU
3	C	101	ASN
3	C	104	HIS
3	C	171	LEU
1	G	48	LYS
1	G	76	TYR
1	G	106	HIS
1	G	117	GLU
1	G	135	ASN
1	G	148	GLN
1	G	159	ARG
1	G	163	TRP
1	G	170	ARG
1	G	188	GLN
1	G	196	PHE
1	G	214	GLU
1	G	224	TYR
1	G	236	ASN
1	G	251	LYS
1	G	252	PHE
1	G	254	LEU

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Mol	Chain	Res	Type
1	G	255	LEU
1	G	262	TYR
1	G	265	LEU
1	G	272	SER
1	G	273	ILE
1	G	328	THR
1	G	332	ASP
1	G	334	GLU
1	G	398	ASN
1	G	407	PHE
1	G	430	GLU
1	G	431	PHE
1	G	437	ARG
1	G	463	ARG
1	G	489	PHE
1	G	502	LEU
1	G	506	GLU
1	G	522	TYR
1	G	532	LEU
1	G	580	GLU
1	G	584	LEU
1	G	585	ASP
1	G	626	TYR
1	G	633	ARG
1	G	705	ASP
1	G	708	THR
1	G	733	TYR
1	G	832	ASP
2	H	10	ILE
2	H	16	MET
2	H	22	HIS
2	H	24	LEU
2	H	29	MET
2	H	35	TYR
2	H	40	TRP
2	H	117	SER
2	H	152	LEU
2	H	163	HIS
2	H	200	GLN
3	I	95	PHE
3	I	113	LYS
3	I	157	PHE

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Mol	Chain	Res	Type
1	M	48	LYS
1	M	55	ASP
1	M	74	ASP
1	M	96	GLU
1	M	117	GLU
1	M	196	PHE
1	M	215	CYS
1	M	224	TYR
1	M	236	ASN
1	M	254	LEU
1	M	273	ILE
1	M	291	LEU
1	M	312	LEU
1	M	330	LEU
1	M	338	LYS
1	M	339	LYS
1	M	407	PHE
1	M	429	VAL
1	M	447	THR
1	M	464	PHE
1	M	468	LYS
1	M	489	PHE
1	M	522	TYR
1	M	532	LEU
1	M	551	ILE
1	M	599	TYR
1	M	626	TYR
1	M	628	GLN
1	M	710	PHE
1	M	726	ILE
1	M	728	ASP
1	M	808	TRP
1	M	832	ASP
2	N	10	ILE
2	N	22	HIS
2	N	24	LEU
2	N	28	TYR
2	N	29	MET
2	N	35	TYR
2	N	40	TRP
2	N	153	HIS
3	O	95	PHE

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Mol	Chain	Res	Type
3	O	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	HIS
1	G	188	GLN
1	G	282	ASN
2	H	114	HIS
1	M	135	ASN
1	M	236	ASN
1	M	347	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
5	G4P	A	901	-	36,38,38	1.58	5 (13%)	56,61,61	1.70	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CMC	H	301	-	51,53,54	1.12	5 (9%)	72,78,80	1.69	13 (18%)
6	CMC	N	301	-	51,53,54	1.13	5 (9%)	72,78,80	1.71	15 (20%)
7	ACO	O	201	-	51,53,53	1.37	6 (11%)	73,79,79	1.79	11 (15%)
5	G4P	G	901	-	36,38,38	3.96	8 (22%)	56,61,61	2.17	17 (30%)
7	ACO	C	201	-	51,53,53	1.27	4 (7%)	73,79,79	2.14	18 (24%)
5	G4P	M	901	-	36,38,38	1.47	4 (11%)	56,61,61	1.82	9 (16%)
7	ACO	I	201	-	51,53,53	1.59	8 (15%)	73,79,79	2.22	25 (34%)
6	CMC	B	301	-	51,53,54	1.13	6 (11%)	72,78,80	1.69	14 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G4P	A	901	-	-	7/27/43/43	0/3/3/3
6	CMC	H	301	-	-	2/50/67/68	0/3/3/3
6	CMC	N	301	-	-	3/50/67/68	0/3/3/3
7	ACO	O	201	-	-	18/51/67/67	0/3/3/3
5	G4P	G	901	-	-	4/27/43/43	0/3/3/3
7	ACO	C	201	-	-	22/51/67/67	0/3/3/3
5	G4P	M	901	-	-	8/27/43/43	0/3/3/3
7	ACO	I	201	-	-	24/51/67/67	0/3/3/3
6	CMC	B	301	-	-	3/50/67/68	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	901	G4P	PC-O3C	20.03	1.81	1.59
5	G	901	G4P	PA-O3A	7.30	1.67	1.59
7	I	201	ACO	C5A-C4A	6.12	1.50	1.39
5	G	901	G4P	PD-O1D	5.17	1.66	1.50
5	A	901	G4P	PC-O3C	5.03	1.64	1.59
7	O	201	ACO	C5A-C4A	4.95	1.47	1.39
7	C	201	ACO	C5A-C4A	4.92	1.47	1.39
5	M	901	G4P	PC-O3C	4.69	1.64	1.59
5	G	901	G4P	O3'-C3'	4.08	1.58	1.44
7	I	201	ACO	C5A-C6A	3.93	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	G4P	PA-O3A	3.62	1.63	1.59
5	G	901	G4P	C5-C4	3.51	1.48	1.38
5	M	901	G4P	C5-C4	3.51	1.48	1.38
7	I	201	ACO	C5P-N4P	3.51	1.41	1.33
7	O	201	ACO	P1A-O3A	3.38	1.63	1.59
5	A	901	G4P	C5-C4	3.33	1.47	1.38
7	C	201	ACO	C5A-C6A	3.12	1.49	1.41
6	N	301	CMC	C9P-N8P	-3.09	1.26	1.33
6	B	301	CMC	C9P-N8P	-3.04	1.26	1.33
6	H	301	CMC	C9P-N8P	-3.03	1.26	1.33
7	O	201	ACO	C5A-C6A	3.01	1.49	1.41
6	N	301	CMC	C5P-N4P	-2.98	1.26	1.33
6	H	301	CMC	C5P-N4P	-2.97	1.26	1.33
6	B	301	CMC	C5P-N4P	-2.94	1.26	1.33
6	H	301	CMC	C5A-C6A	2.85	1.48	1.41
6	B	301	CMC	C5A-C6A	2.84	1.48	1.41
6	N	301	CMC	C5A-C6A	2.83	1.48	1.41
7	I	201	ACO	C4A-N3A	2.73	1.39	1.34
5	A	901	G4P	PC-O3'	2.66	1.67	1.59
7	I	201	ACO	P2A-O3A	2.60	1.62	1.59
5	M	901	G4P	PC-O3'	2.56	1.67	1.59
5	G	901	G4P	PB-O1B	2.54	1.58	1.50
7	I	201	ACO	O5P-C5P	2.51	1.28	1.23
5	G	901	G4P	PD-O3D	2.45	1.63	1.54
7	I	201	ACO	P3B-O7A	2.44	1.58	1.50
7	I	201	ACO	P3B-O3B	2.43	1.63	1.59
7	O	201	ACO	C8A-N7A	2.43	1.36	1.31
7	O	201	ACO	C5A-N7A	-2.41	1.34	1.39
7	C	201	ACO	C8A-N7A	2.39	1.36	1.31
5	M	901	G4P	PA-O3A	2.37	1.62	1.59
5	G	901	G4P	O6-C6	2.18	1.27	1.23
6	N	301	CMC	C5A-N7A	-2.18	1.35	1.39
6	B	301	CMC	C5A-N7A	-2.15	1.35	1.39
6	H	301	CMC	C8A-N7A	2.14	1.35	1.31
6	H	301	CMC	C5A-N7A	-2.12	1.35	1.39
7	C	201	ACO	C5A-N7A	-2.11	1.35	1.39
7	O	201	ACO	P2A-O3A	2.09	1.61	1.59
6	B	301	CMC	C8A-N7A	2.09	1.35	1.31
6	N	301	CMC	C8A-N7A	2.07	1.35	1.31
6	B	301	CMC	P1A-O3A	2.04	1.61	1.59
5	A	901	G4P	C6-N1	-2.04	1.35	1.38

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	201	ACO	C5A-C4A-N3A	-7.12	116.91	126.72
7	C	201	ACO	C5A-C4A-N3A	-6.89	117.23	126.72
7	C	201	ACO	O3A-P2A-O4A	-6.21	92.04	110.70
5	M	901	G4P	C5-C4-N3	-5.88	119.03	128.39
7	I	201	ACO	CAP-C9P-N8P	5.74	127.39	116.48
7	O	201	ACO	N3A-C4A-N9A	5.72	136.90	127.17
7	I	201	ACO	N3A-C4A-N9A	5.72	136.89	127.17
5	G	901	G4P	C5-C4-N3	-5.66	119.39	128.39
7	C	201	ACO	N3A-C4A-N9A	5.51	136.54	127.17
7	I	201	ACO	C5A-C4A-N3A	-5.49	119.15	126.72
6	N	301	CMC	C5A-C4A-N3A	-5.41	119.27	126.72
5	M	901	G4P	C2-N3-C4	5.31	121.44	112.30
6	B	301	CMC	C5A-C4A-N3A	-5.30	119.42	126.72
6	H	301	CMC	C5A-C4A-N3A	-5.27	119.46	126.72
5	G	901	G4P	C2-N3-C4	5.04	120.97	112.30
5	A	901	G4P	C5-C4-N3	-4.99	120.44	128.39
6	B	301	CMC	C2P-S1P-C1	4.83	109.68	101.72
5	G	901	G4P	O3D-PD-O2D	4.69	125.40	107.80
6	H	301	CMC	C2P-S1P-C1	4.68	109.43	101.72
5	G	901	G4P	N9-C4-N3	4.67	135.28	125.95
5	M	901	G4P	N9-C4-N3	4.64	135.22	125.95
5	A	901	G4P	C2-N3-C4	4.62	120.26	112.30
5	A	901	G4P	N9-C4-N3	4.56	135.08	125.95
6	N	301	CMC	C2P-S1P-C1	4.53	109.19	101.72
7	I	201	ACO	C6P-C7P-N8P	4.45	121.46	112.00
7	O	201	ACO	C2A-N3A-C4A	4.31	122.37	111.83
7	I	201	ACO	N3A-C2A-N1A	-4.26	122.13	128.58
7	I	201	ACO	C2A-N3A-C4A	4.23	122.16	111.83
7	C	201	ACO	C2A-N3A-C4A	4.23	122.15	111.83
7	C	201	ACO	CAP-C9P-N8P	4.01	124.10	116.48
6	H	301	CMC	N3A-C2A-N1A	-4.01	122.51	128.58
6	B	301	CMC	N3A-C2A-N1A	-4.00	122.52	128.58
6	N	301	CMC	N3A-C2A-N1A	-3.98	122.56	128.58
5	G	901	G4P	O3'-PC-O1C	-3.96	97.14	109.81
7	C	201	ACO	C4A-C5A-N7A	-3.96	106.06	110.58
6	N	301	CMC	C2A-N3A-C4A	3.93	121.44	111.83
6	H	301	CMC	C2A-N3A-C4A	3.91	121.37	111.83
6	B	301	CMC	C2A-N3A-C4A	3.90	121.36	111.83
7	O	201	ACO	C4A-C5A-N7A	-3.89	106.14	110.58
7	O	201	ACO	N3A-C2A-N1A	-3.80	122.84	128.58
7	I	201	ACO	O9P-C9P-N8P	-3.74	115.07	122.98
6	H	301	CMC	C2P-C3P-N4P	-3.69	104.72	112.41
5	G	901	G4P	O3C-PC-O1C	-3.69	99.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	901	G4P	O3D-PD-O1D	-3.68	96.51	110.83
5	G	901	G4P	C5'-C4'-C3'	-3.67	102.14	114.38
6	N	301	CMC	C2P-C3P-N4P	-3.66	104.77	112.41
7	C	201	ACO	C5A-N7A-C8A	3.63	109.16	103.45
7	O	201	ACO	C5A-N7A-C8A	3.62	109.14	103.45
7	C	201	ACO	N3A-C2A-N1A	-3.61	123.12	128.58
6	N	301	CMC	N3A-C4A-N9A	3.61	133.30	127.17
7	C	201	ACO	O9P-C9P-N8P	-3.54	115.50	122.98
5	A	901	G4P	C6-C5-N7	3.52	136.69	130.29
7	I	201	ACO	O5P-C5P-C6P	-3.51	115.65	122.02
5	G	901	G4P	O4'-C4'-C5'	3.50	120.54	109.33
6	B	301	CMC	N3A-C4A-N9A	3.48	133.09	127.17
6	H	301	CMC	N9A-C8A-N7A	-3.48	109.00	113.94
6	B	301	CMC	C2P-C3P-N4P	-3.46	105.19	112.41
6	B	301	CMC	N9A-C8A-N7A	-3.44	109.06	113.94
6	H	301	CMC	N3A-C4A-N9A	3.43	133.00	127.17
5	M	901	G4P	C6-C5-N7	3.43	136.53	130.29
6	N	301	CMC	C6P-C7P-N8P	-3.42	104.72	112.00
7	I	201	ACO	CEP-CBP-CAP	3.40	114.57	108.77
6	H	301	CMC	C6P-C7P-N8P	-3.37	104.82	112.00
7	I	201	ACO	C4A-N9A-C8A	3.35	109.26	105.74
6	N	301	CMC	N9A-C8A-N7A	-3.34	109.19	113.94
6	B	301	CMC	C6P-C7P-N8P	-3.23	105.13	112.00
5	G	901	G4P	C6-C5-N7	3.19	136.09	130.29
5	M	901	G4P	O4'-C1'-N9	3.15	115.50	108.36
7	C	201	ACO	CDP-CBP-CAP	3.05	113.97	108.77
5	M	901	G4P	O3B-PB-O2B	2.92	118.76	107.80
7	I	201	ACO	P3B-O3B-C3B	2.90	131.18	123.43
7	I	201	ACO	OAP-CAP-CBP	-2.89	103.49	110.18
7	C	201	ACO	O2A-P1A-O3A	-2.89	99.47	107.27
7	I	201	ACO	O5A-P2A-O4A	2.86	125.77	112.44
7	I	201	ACO	O6A-P2A-O4A	-2.81	97.82	108.94
7	C	201	ACO	C6P-C7P-N8P	2.80	117.96	112.00
5	A	901	G4P	O3D-PD-O2D	2.77	118.19	107.80
7	C	201	ACO	N9A-C8A-N7A	-2.77	110.01	113.94
7	I	201	ACO	C2P-C3P-N4P	-2.73	106.71	112.41
7	C	201	ACO	O5A-P2A-O4A	2.73	125.13	112.44
7	C	201	ACO	C2P-C3P-N4P	-2.71	106.75	112.41
6	H	301	CMC	C7P-N8P-C9P	2.71	127.42	122.55
7	C	201	ACO	C4A-N9A-C8A	2.68	108.55	105.74
5	M	901	G4P	C4-C5-N7	-2.64	106.49	110.67
5	G	901	G4P	O5'-C5'-C4'	2.62	117.92	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	CMC	C7P-N8P-C9P	2.61	127.24	122.55
7	O	201	ACO	N9A-C8A-N7A	-2.60	110.25	113.94
6	B	301	CMC	C3P-N4P-C5P	2.57	127.61	122.82
6	N	301	CMC	C7P-N8P-C9P	2.55	127.12	122.55
6	H	301	CMC	C4A-N9A-C8A	2.54	108.40	105.74
6	N	301	CMC	C3P-N4P-C5P	2.53	127.53	122.82
7	I	201	ACO	C2P-S1P-C	2.52	113.53	101.42
6	B	301	CMC	C4A-N9A-C8A	2.51	108.37	105.74
5	G	901	G4P	O2C-PC-O3'	2.51	116.91	106.70
6	H	301	CMC	C4A-C5A-N7A	-2.50	107.72	110.58
6	N	301	CMC	C4A-N9A-C8A	2.50	108.36	105.74
6	B	301	CMC	C4A-C5A-N7A	-2.49	107.73	110.58
6	B	301	CMC	C5A-N7A-C8A	2.48	107.34	103.45
6	H	301	CMC	C5A-N7A-C8A	2.47	107.34	103.45
5	G	901	G4P	O3'-C3'-C2'	-2.46	102.84	111.68
7	O	201	ACO	C7P-C6P-C5P	2.46	116.49	112.39
6	N	301	CMC	C4A-C5A-N7A	-2.46	107.77	110.58
7	O	201	ACO	C7P-N8P-C9P	2.45	126.94	122.55
7	I	201	ACO	C6A-C5A-N7A	2.44	136.78	132.09
7	O	201	ACO	C4A-N9A-C8A	2.42	108.28	105.74
6	N	301	CMC	C5A-N7A-C8A	2.42	107.25	103.45
6	H	301	CMC	C3P-N4P-C5P	2.40	127.29	122.82
5	A	901	G4P	C6-C5-C4	-2.37	115.26	118.83
5	G	901	G4P	O2C-PC-O3C	2.36	113.66	107.27
7	I	201	ACO	C3B-C2B-C1B	2.36	105.08	99.89
7	I	201	ACO	CEP-CBP-CCP	2.35	112.11	108.22
5	A	901	G4P	O2A-PA-O3A	-2.35	100.92	107.27
5	M	901	G4P	O2'-C2'-C1'	2.32	118.08	110.10
5	G	901	G4P	C4-C5-N7	-2.29	107.04	110.67
5	A	901	G4P	C5-C6-N1	2.26	119.01	113.25
5	A	901	G4P	O3B-PB-O2B	2.20	116.03	107.80
6	N	301	CMC	C3B-C2B-C1B	2.19	104.70	99.89
5	M	901	G4P	C2'-C1'-N9	2.18	119.31	113.25
7	I	201	ACO	C2A-N1A-C6A	2.18	122.31	118.73
5	A	901	G4P	C8-N9-C4	2.17	110.10	106.03
6	N	301	CMC	O6A-CCP-CBP	-2.16	107.07	110.55
6	B	301	CMC	C3B-C2B-C1B	2.15	104.62	99.89
7	I	201	ACO	O4B-C4B-C3B	2.12	109.40	104.92
7	C	201	ACO	O2A-P1A-O1A	2.11	122.25	112.44
5	G	901	G4P	O2A-PA-O1A	2.10	122.22	112.44
7	O	201	ACO	N6A-C6A-N1A	2.10	123.05	118.38
7	I	201	ACO	CEP-CBP-CDP	-2.09	105.03	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	201	ACO	O2B-C2B-C3B	2.08	117.00	111.19
7	I	201	ACO	O3B-P3B-O7A	-2.07	101.96	109.33
5	G	901	G4P	O3A-PA-O1A	-2.06	104.51	110.70
5	A	901	G4P	O2A-PA-O1A	2.04	121.96	112.44
5	A	901	G4P	O4'-C1'-N9	2.04	112.98	108.36
7	I	201	ACO	O5P-C5P-N4P	2.02	127.00	123.03
7	C	201	ACO	O5P-C5P-C6P	-2.01	118.38	122.02

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	G4P	O4'-C4'-C5'-O5'
5	A	901	G4P	C3'-C4'-C5'-O5'
5	G	901	G4P	C4'-C3'-O3'-PC
5	G	901	G4P	O4'-C1'-N9-C8
5	G	901	G4P	O4'-C1'-N9-C4
5	M	901	G4P	C2'-C3'-O3'-PC
6	B	301	CMC	C5B-O5B-P1A-O1A
6	B	301	CMC	C5B-O5B-P1A-O2A
6	B	301	CMC	C5B-O5B-P1A-O3A
6	N	301	CMC	C5B-O5B-P1A-O1A
6	N	301	CMC	C5B-O5B-P1A-O2A
6	N	301	CMC	C5B-O5B-P1A-O3A
7	C	201	ACO	C5B-O5B-P1A-O2A
7	C	201	ACO	N8P-C9P-CAP-OAP
7	C	201	ACO	CAP-C9P-N8P-C7P
7	C	201	ACO	O-C-S1P-C2P
7	C	201	ACO	CH3-C-S1P-C2P
7	I	201	ACO	C2B-C1B-N9A-C8A
7	I	201	ACO	CDP-CBP-CCP-O6A
7	I	201	ACO	CEP-CBP-CCP-O6A
7	I	201	ACO	CAP-CBP-CCP-O6A
7	I	201	ACO	C9P-CAP-CBP-CCP
7	I	201	ACO	C9P-CAP-CBP-CDP
7	I	201	ACO	C9P-CAP-CBP-CEP
7	I	201	ACO	O9P-C9P-CAP-CBP
7	I	201	ACO	N8P-C9P-CAP-CBP
7	I	201	ACO	O9P-C9P-CAP-OAP
7	I	201	ACO	N8P-C9P-CAP-OAP
7	I	201	ACO	CAP-C9P-N8P-C7P
7	I	201	ACO	C3P-C2P-S1P-C

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Mol	Chain	Res	Type	Atoms
7	I	201	ACO	O-C-S1P-C2P
7	I	201	ACO	CH3-C-S1P-C2P
7	O	201	ACO	C5B-O5B-P1A-O1A
7	O	201	ACO	C5B-O5B-P1A-O3A
7	O	201	ACO	O9P-C9P-CAP-CBP
7	O	201	ACO	N8P-C9P-CAP-CBP
7	O	201	ACO	O9P-C9P-CAP-OAP
7	O	201	ACO	N8P-C9P-CAP-OAP
7	O	201	ACO	C3P-C2P-S1P-C
7	O	201	ACO	O-C-S1P-C2P
7	O	201	ACO	CH3-C-S1P-C2P
7	I	201	ACO	O9P-C9P-N8P-C7P
7	C	201	ACO	O9P-C9P-N8P-C7P
5	A	901	G4P	C2'-C3'-O3'-PC
5	M	901	G4P	C4'-C3'-O3'-PC
7	I	201	ACO	C4B-C3B-O3B-P3B
5	A	901	G4P	O4'-C1'-N9-C4
7	I	201	ACO	C2B-C1B-N9A-C4A
5	A	901	G4P	C4'-C3'-O3'-PC
7	I	201	ACO	C2B-C3B-O3B-P3B
5	A	901	G4P	O4'-C1'-N9-C8
5	M	901	G4P	O4'-C1'-N9-C8
5	M	901	G4P	O4'-C1'-N9-C4
5	A	901	G4P	C4'-C5'-O5'-PA
7	C	201	ACO	O9P-C9P-CAP-OAP
7	C	201	ACO	C2B-C1B-N9A-C8A
7	I	201	ACO	OAP-CAP-CBP-CEP
7	I	201	ACO	C3B-O3B-P3B-O9A
5	G	901	G4P	C4'-C5'-O5'-PA
5	M	901	G4P	C4'-C5'-O5'-PA
7	O	201	ACO	C2B-C1B-N9A-C8A
5	M	901	G4P	C3'-O3'-PC-O1C
6	H	301	CMC	P1A-O3A-P2A-O4A
7	I	201	ACO	O5P-C5P-C6P-C7P
7	C	201	ACO	C9P-CAP-CBP-CCP
7	C	201	ACO	C3P-C2P-S1P-C
7	C	201	ACO	C5B-O5B-P1A-O1A
7	C	201	ACO	C5B-O5B-P1A-O3A
7	O	201	ACO	C5B-O5B-P1A-O2A
7	O	201	ACO	CCP-O6A-P2A-O3A
7	O	201	ACO	CCP-O6A-P2A-O4A
7	O	201	ACO	CCP-O6A-P2A-O5A

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Mol	Chain	Res	Type	Atoms
7	I	201	ACO	N4P-C5P-C6P-C7P
7	I	201	ACO	OAP-CAP-CBP-CDP
7	C	201	ACO	C2B-C1B-N9A-C4A
7	O	201	ACO	C2B-C1B-N9A-C4A
5	M	901	G4P	C3'-C4'-C5'-O5'
7	C	201	ACO	S1P-C2P-C3P-N4P
7	C	201	ACO	N8P-C9P-CAP-CBP
5	M	901	G4P	O4'-C4'-C5'-O5'
7	O	201	ACO	O4B-C1B-N9A-C8A
7	C	201	ACO	C9P-CAP-CBP-CDP
7	C	201	ACO	C9P-CAP-CBP-CEP
6	H	301	CMC	P1A-O3A-P2A-O5A
7	C	201	ACO	P2A-O3A-P1A-O1A
7	O	201	ACO	P1A-O3A-P2A-O4A
7	O	201	ACO	P1A-O3A-P2A-O5A
7	C	201	ACO	O9P-C9P-CAP-CBP
7	C	201	ACO	O5P-C5P-C6P-C7P
7	C	201	ACO	O4B-C1B-N9A-C8A
7	C	201	ACO	P2A-O3A-P1A-O2A

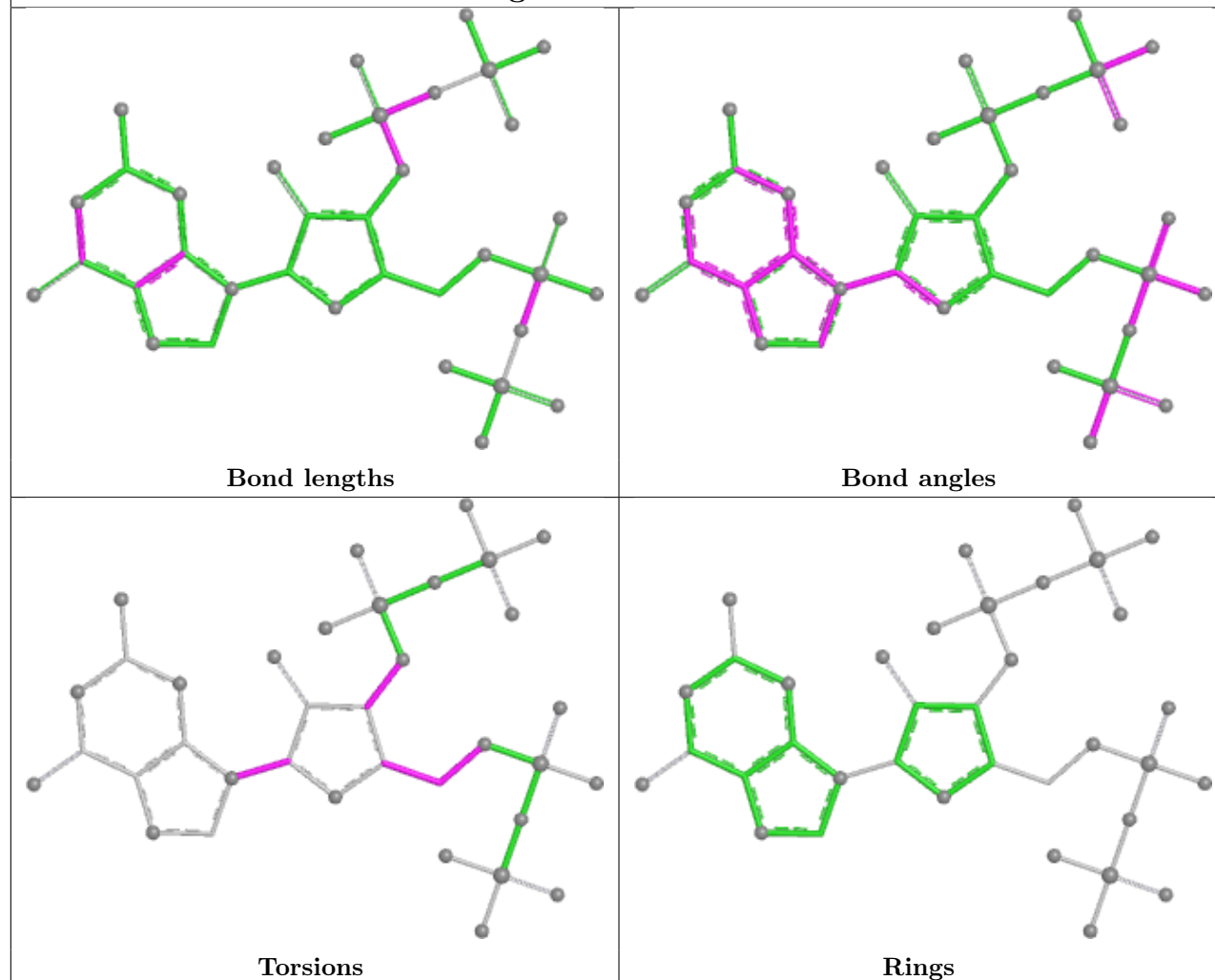
There are no ring outliers.

5 monomers are involved in 28 short contacts:

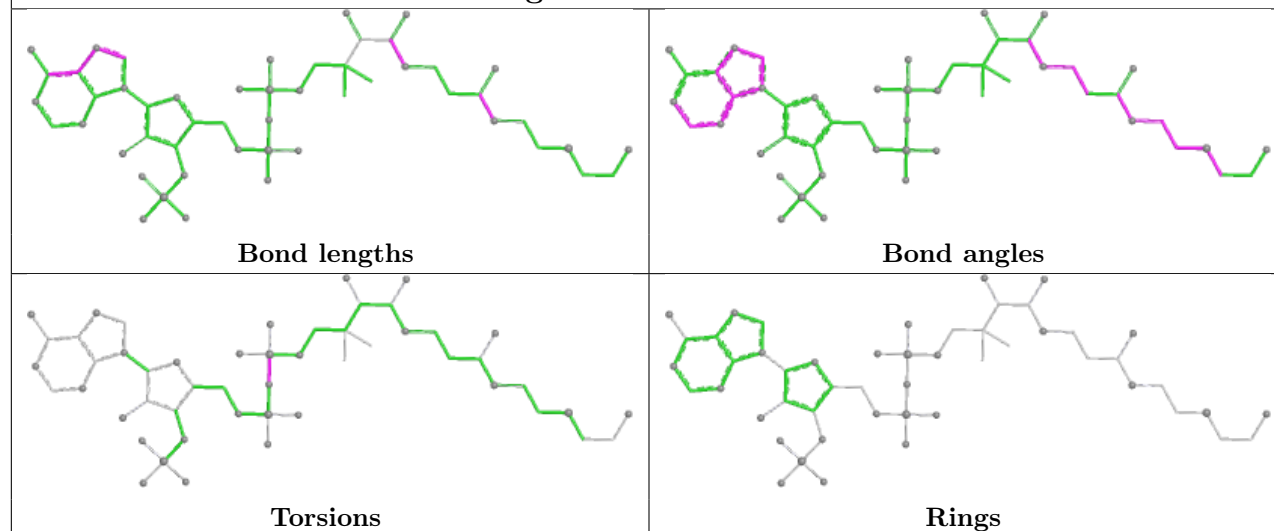
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	G4P	1	0
7	O	201	ACO	5	0
5	G	901	G4P	3	0
7	C	201	ACO	10	0
7	I	201	ACO	9	0

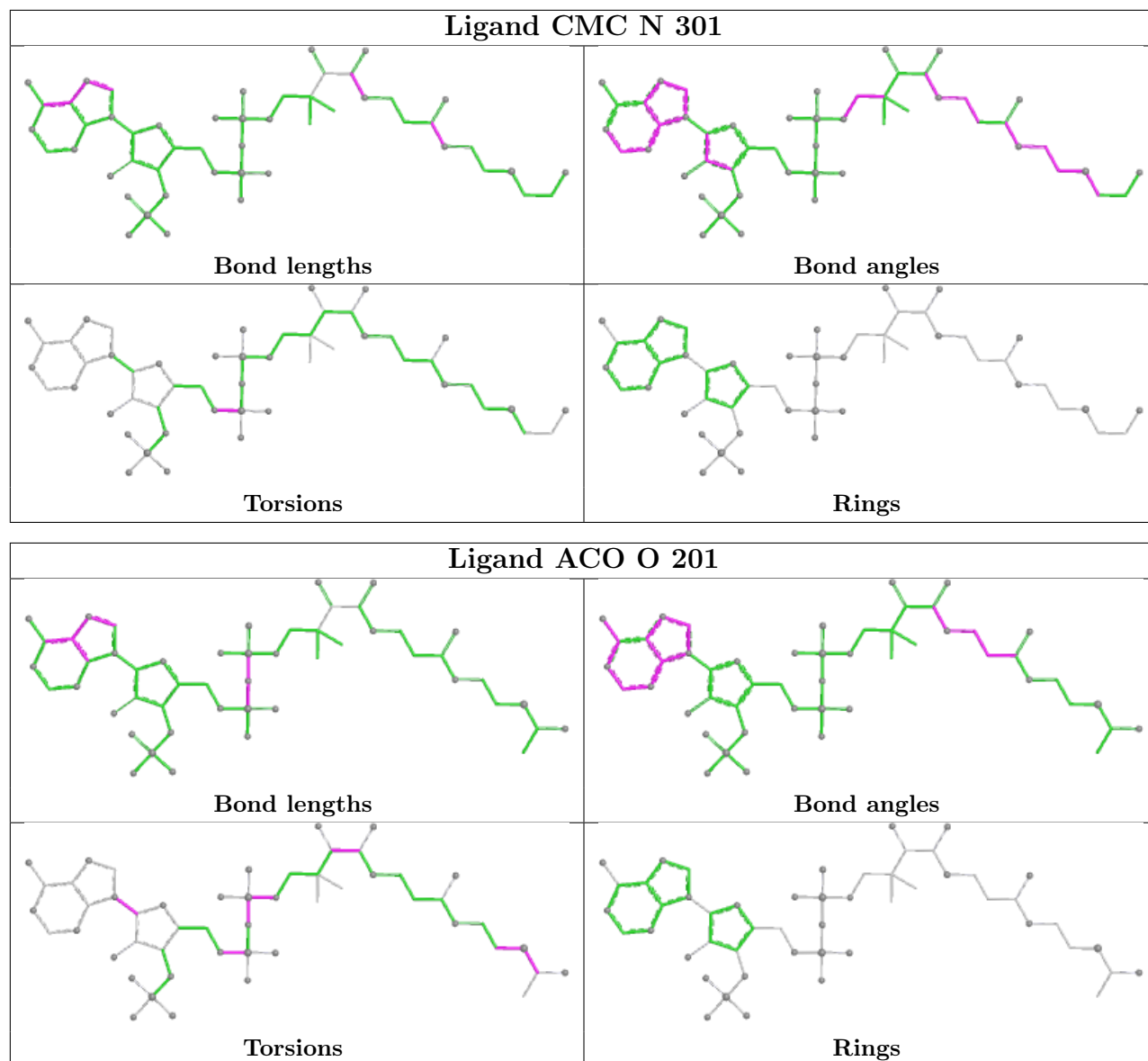
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 G4P A 901

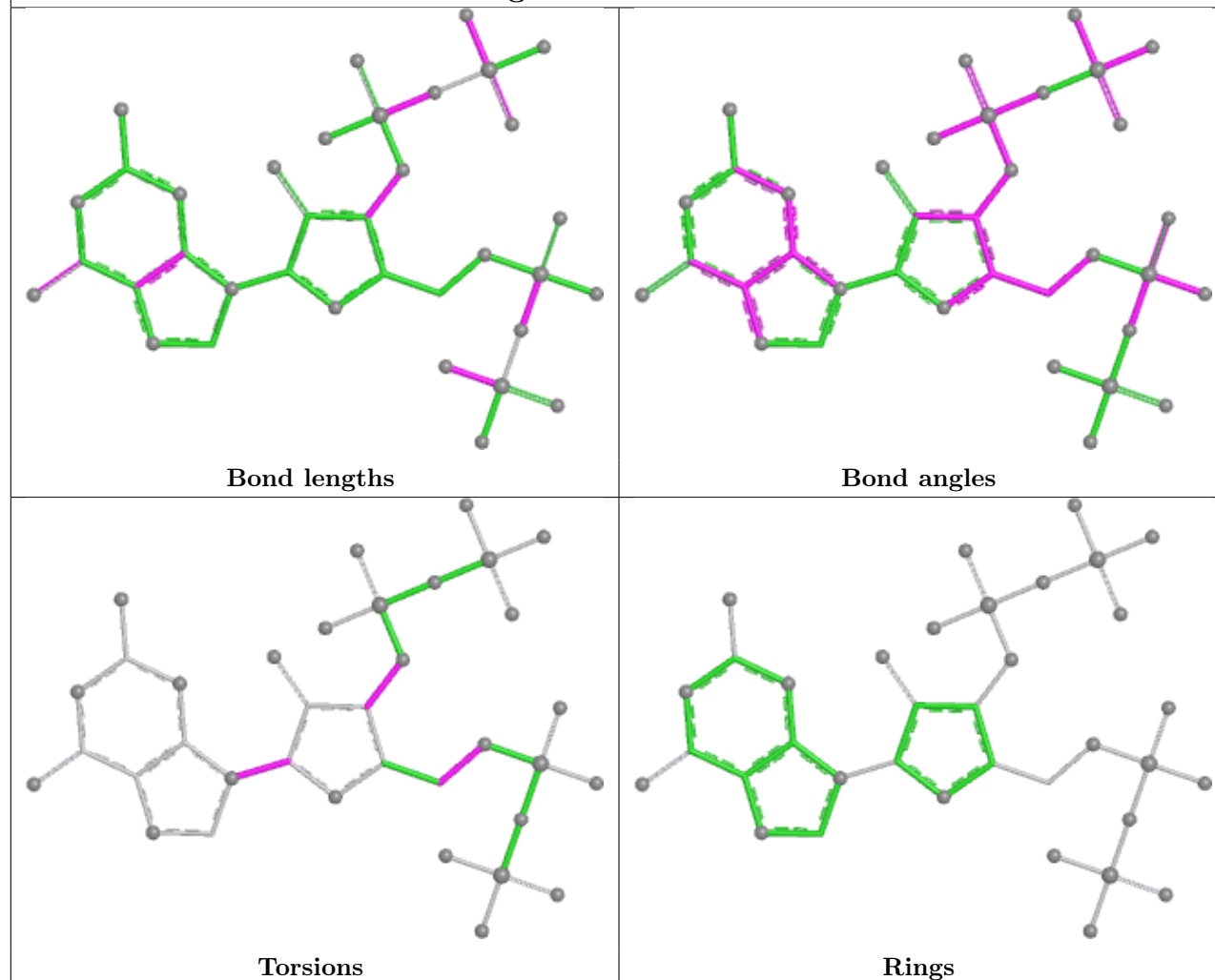


Ligand CMC H 301

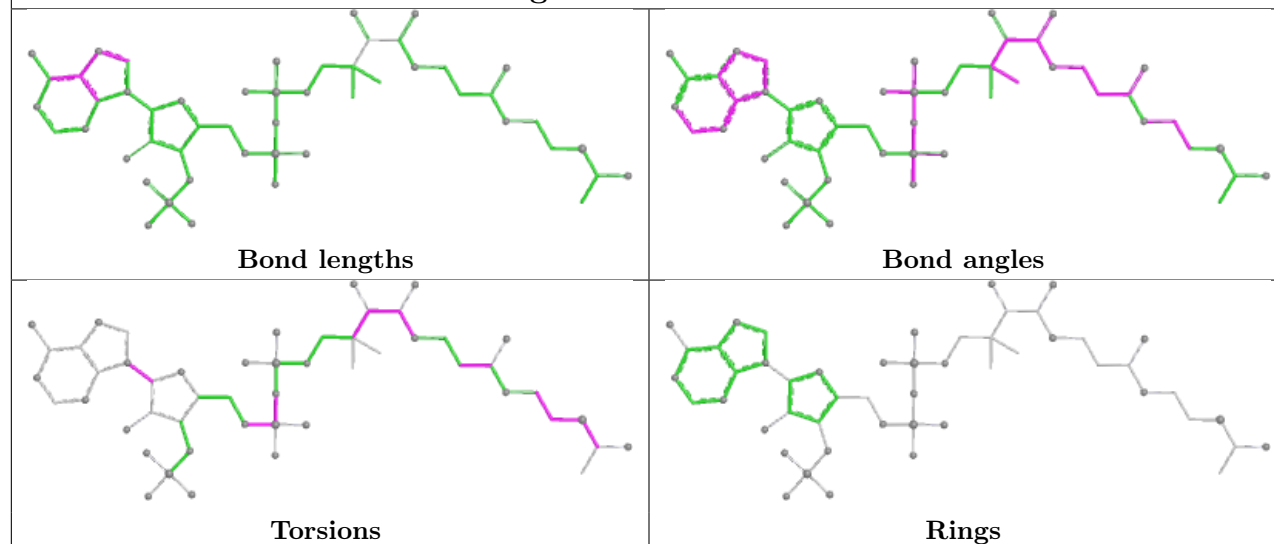




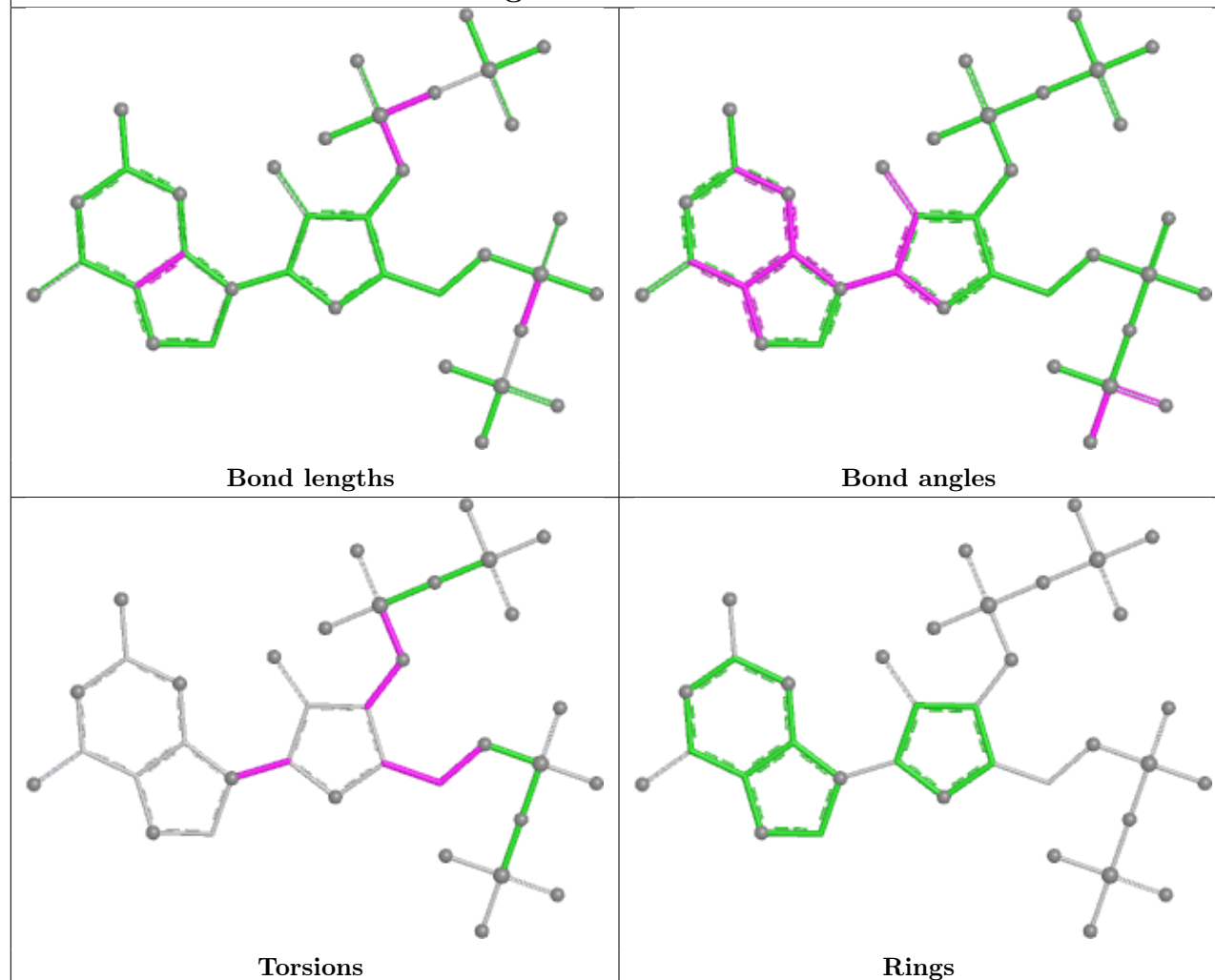
Ligand G4P G 901



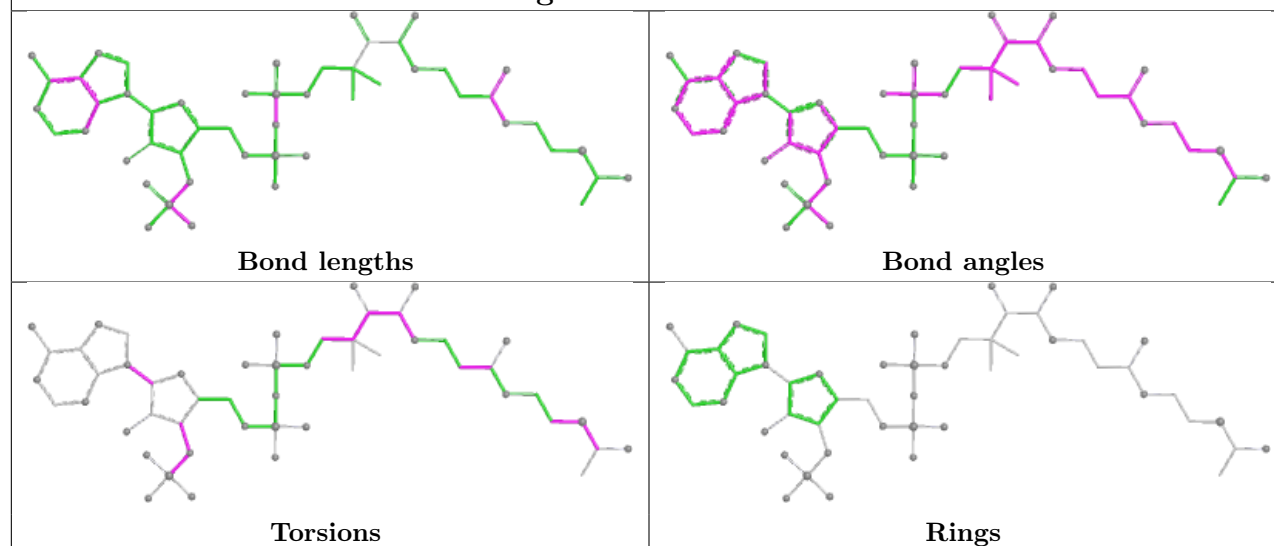
Ligand ACO C 201

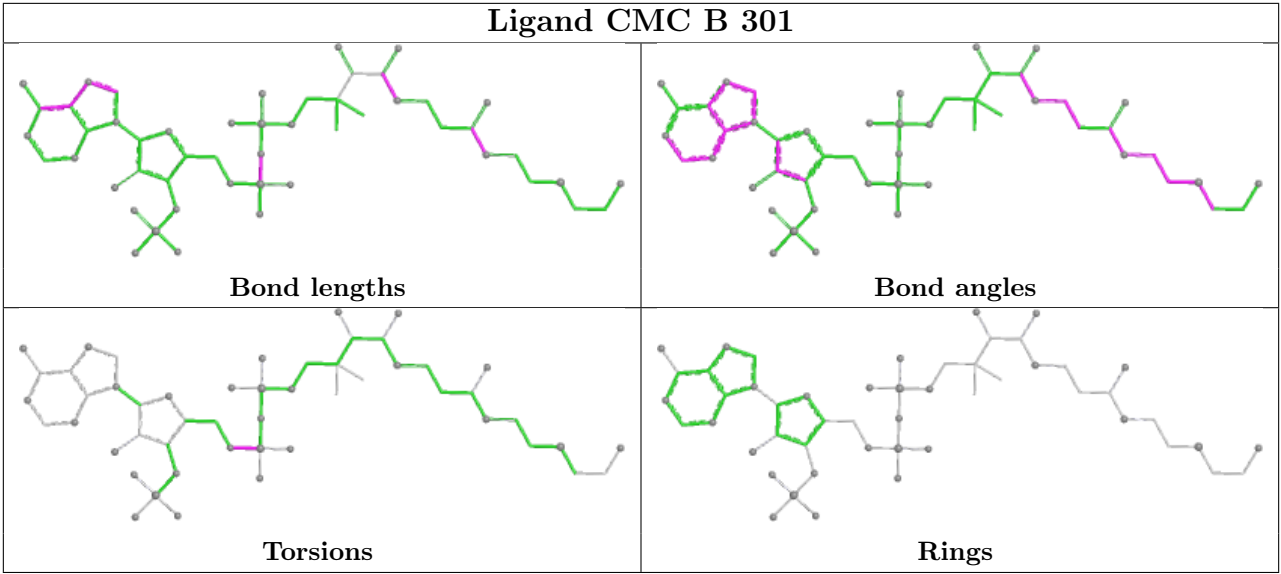


Ligand G4P M 901



Ligand ACO I 201





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	35:PHE	C	36:PHE	N	0.90

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	769/854 (90%)	1.67	234 (30%)  	83, 86, 91, 94	0
1	G	770/854 (90%)	1.72	268 (34%)  	73, 85, 88, 88	0
1	M	769/854 (90%)	1.68	244 (31%)  	84, 86, 90, 92	0
2	B	164/238 (68%)	1.90	55 (33%)  	48, 84, 86, 88	0
2	H	164/238 (68%)	1.78	62 (37%)  	84, 85, 86, 87	0
2	N	164/238 (68%)	1.78	52 (31%)  	54, 86, 87, 88	0
3	C	156/176 (88%)	1.60	43 (27%)  	62, 86, 88, 88	2 (1%)
3	I	155/176 (88%)	1.74	55 (35%)  	68, 87, 89, 90	2 (1%)
3	O	154/176 (87%)	1.60	42 (27%)  	64, 90, 93, 93	2 (1%)
4	E	6/8 (75%)	1.85	2 (33%)  	83, 83, 84, 84	0
4	K	6/8 (75%)	1.87	2 (33%)  	84, 84, 85, 85	0
4	Q	6/8 (75%)	1.62	2 (33%)  	85, 85, 85, 85	0
All	All	3283/3828 (85%)	1.70	1061 (32%)  	48, 86, 90, 94	6 (0%)

All (1061) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	GLU	12.2
2	B	166	ARG	9.7
2	B	148	GLU	9.5
1	G	332	ASP	8.2
1	A	676	GLU	8.2
1	A	673	LYS	7.8
1	G	775	PRO	7.6
2	B	200	GLN	7.3
2	N	131	GLU	7.2
1	G	349	GLU	6.9
1	G	64	HIS	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	356	PHE	6.7
1	A	64	HIS	6.5
1	G	509	TRP	6.4
1	M	221	ASP	6.4
3	C	174	HIS	6.3
1	M	206	ASP	6.3
1	A	674	GLU	6.3
3	C	102	TYR	6.3
3	C	101	ASN	6.2
1	M	110	ILE	6.2
2	B	131	GLU	6.0
1	M	732	ASN	5.9
3	I	102	TYR	5.9
3	O	109	SER	5.9
2	N	169	LEU	5.9
1	G	437	ARG	5.9
1	M	807	ASP	5.9
1	M	337	SER	5.9
1	M	307	ALA	5.8
3	O	24	HIS	5.8
1	A	307	ALA	5.8
1	M	250	ASP	5.7
3	O	23	ALA	5.7
1	M	114	ASN	5.7
2	N	102	ASP	5.6
1	M	480	ASP	5.6
1	A	250	ASP	5.4
1	G	683	TYR	5.4
2	N	165	TYR	5.4
1	G	446	ASP	5.4
1	M	188	GLN	5.4
1	A	560	LYS	5.3
1	A	221	ASP	5.3
2	B	165	TYR	5.2
1	G	582	ASP	5.2
2	H	34	MET	5.2
1	G	110	ILE	5.1
1	A	275	TYR	5.1
2	H	148	GLU	5.0
1	M	243	ASP	5.0
1	A	323	LYS	5.0
2	H	183	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
2	H	202	SER	4.9
2	H	133	LEU	4.9
1	A	503	HIS	4.9
1	G	384	GLY	4.9
1	A	524	ASP	4.8
1	M	56	ALA	4.8
1	M	305	LYS	4.8
1	G	803	ASN	4.8
1	G	825	LEU	4.8
1	M	560	LYS	4.8
1	A	126	THR	4.7
1	A	556	TRP	4.7
1	G	519	TYR	4.7
1	M	259	ALA	4.7
1	G	114	ASN	4.7
2	B	102	ASP	4.7
1	G	709	GLU	4.7
3	C	24	HIS	4.7
3	O	138	THR	4.7
1	A	704	GLU	4.7
2	H	165	TYR	4.7
1	M	825	LEU	4.6
2	B	183	ASP	4.6
1	G	250	ASP	4.6
1	M	181	ASP	4.6
1	A	825	LEU	4.6
1	M	124	TRP	4.6
1	M	487	SER	4.6
2	B	202	SER	4.6
1	M	582	ASP	4.5
1	A	767	LEU	4.5
1	A	259	ALA	4.5
1	A	305	LYS	4.5
1	A	557	LEU	4.5
1	A	582	ASP	4.4
1	A	110	ILE	4.4
3	O	104	HIS	4.4
1	G	679	SER	4.4
2	N	202	SER	4.4
1	A	499	ILE	4.4
1	G	295	SER	4.4
2	N	51	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	614	MET	4.4
1	A	284	ASP	4.4
1	G	337	SER	4.4
1	G	503	HIS	4.4
1	M	106	HIS	4.4
1	M	503	HIS	4.4
1	M	791	GLU	4.4
1	A	281	ARG	4.4
1	G	348	LEU	4.4
1	A	716	MET	4.3
1	M	96	GLU	4.3
1	A	801	ILE	4.3
1	G	223	MET	4.3
1	A	517	ALA	4.3
1	A	337	SER	4.3
1	M	556	TRP	4.2
1	G	731	PHE	4.2
1	M	489	PHE	4.2
1	A	671	LYS	4.2
1	G	56	ALA	4.2
2	B	145	HIS	4.2
3	O	174	HIS	4.2
1	G	363	TYR	4.2
1	A	403	GLN	4.2
1	A	670	ASN	4.2
1	A	732	ASN	4.2
3	I	151	GLY	4.1
1	G	727	LEU	4.1
1	A	791	GLU	4.1
1	M	210	TYR	4.1
2	H	9	THR	4.1
3	I	72	GLY	4.1
1	G	24	ALA	4.1
1	G	517	ALA	4.1
1	A	614	MET	4.1
2	H	7	ARG	4.1
3	I	174	HIS	4.1
2	N	130	ALA	4.1
1	A	56	ALA	4.1
1	G	103	ILE	4.1
3	O	152	GLU	4.0
2	N	148	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	124	TRP	4.0
1	G	284	ASP	4.0
1	A	124	TRP	4.0
2	H	158	ASN	4.0
1	G	555	GLN	4.0
1	G	305	LYS	3.9
1	G	487	SER	3.9
1	A	832	ASP	3.9
1	A	346	PRO	3.9
3	I	100	PRO	3.9
1	M	185	GLU	3.9
1	M	557	LEU	3.9
1	A	588	SER	3.9
2	H	166	ARG	3.9
1	M	284	ASP	3.9
1	M	400	TYR	3.9
1	A	611	THR	3.9
1	M	384	GLY	3.9
2	N	145	HIS	3.9
1	G	680	VAL	3.8
2	H	144	VAL	3.8
1	A	243	ASP	3.8
1	G	27	ALA	3.8
3	I	104	HIS	3.8
2	B	38	LEU	3.8
1	M	55	ASP	3.8
3	C	104	HIS	3.8
1	G	791	GLU	3.8
1	M	137	GLN	3.8
1	G	785	THR	3.8
1	A	185	GLU	3.8
1	M	262	TYR	3.8
1	M	339	LYS	3.8
1	M	559	ARG	3.8
1	G	221	ASP	3.8
2	B	161	ALA	3.8
2	N	116	THR	3.8
1	G	106	HIS	3.8
1	A	511	ILE	3.8
1	A	114	ASN	3.8
1	G	811	PHE	3.8
3	I	164	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	560	LYS	3.8
1	G	612	LYS	3.8
1	M	363	TYR	3.8
1	M	591	MET	3.7
1	A	840	ASN	3.7
1	M	851	PRO	3.7
2	B	143	GLU	3.7
2	N	7	ARG	3.7
1	G	466	ASN	3.7
2	H	130	ALA	3.7
1	A	59	LYS	3.7
1	G	462	ASP	3.7
1	G	344	VAL	3.7
1	A	728	ASP	3.7
2	B	97	LEU	3.7
3	C	171	LEU	3.7
3	C	138	THR	3.7
3	I	127	VAL	3.7
1	A	363	TYR	3.7
1	G	96	GLU	3.7
1	G	556	TRP	3.7
1	G	381	TYR	3.7
1	G	407	PHE	3.7
1	A	502	LEU	3.7
1	G	423	ASP	3.7
2	B	133	LEU	3.7
3	C	151	GLY	3.6
1	G	314	GLN	3.6
1	M	519	TYR	3.6
1	M	103	ILE	3.6
1	G	105	CYS	3.6
1	G	595	THR	3.6
2	B	51	THR	3.6
3	C	111	LEU	3.6
1	M	141	ASP	3.6
1	A	701	THR	3.6
1	M	32	ASN	3.6
2	B	136	GLN	3.6
1	G	32	ASN	3.6
3	C	152	GLU	3.6
1	A	384	GLY	3.6
1	M	345	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	498	GLY	3.6
1	A	332	ASP	3.6
1	A	558	VAL	3.6
1	A	721	ASP	3.6
1	M	107	VAL	3.6
1	M	77	SER	3.6
3	O	101	ASN	3.6
1	G	316	TYR	3.6
2	N	136	GLN	3.5
1	M	48	LYS	3.5
1	M	707	ALA	3.5
1	M	466	ASN	3.5
1	M	467	CYS	3.5
3	I	93	ILE	3.5
1	G	172	ASN	3.5
1	M	64	HIS	3.5
1	M	728	ASP	3.5
1	G	796	PHE	3.5
1	M	275	TYR	3.5
1	A	595	THR	3.5
1	G	390	ASP	3.5
1	A	709	GLU	3.5
1	G	334	GLU	3.5
2	N	53	ASP	3.5
1	A	381	TYR	3.5
1	A	334	GLU	3.5
1	G	732	ASN	3.5
1	G	55	ASP	3.4
3	O	173	LYS	3.4
1	A	520	ARG	3.4
1	A	172	ASN	3.4
1	M	326	PRO	3.4
1	G	670	ASN	3.4
1	M	670	ASN	3.4
1	A	106	HIS	3.4
1	G	259	ALA	3.4
1	A	63	SER	3.4
1	M	105	CYS	3.4
2	B	18	ASN	3.4
1	M	332	ASP	3.4
2	H	200	GLN	3.4
2	N	164	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	412	PRO	3.4
1	M	346	PRO	3.4
1	G	819	ASN	3.4
1	M	381	TYR	3.4
1	A	498	GLY	3.4
3	I	20	THR	3.4
2	H	89	GLY	3.3
1	G	428	LEU	3.3
1	G	721	ASP	3.3
1	G	393	PRO	3.3
1	G	262	TYR	3.3
4	E	2	TYR	3.3
1	M	388	THR	3.3
3	O	76	ALA	3.3
1	M	811	PHE	3.3
1	A	207	SER	3.3
1	A	741	CYS	3.3
2	H	51	THR	3.3
1	G	716	MET	3.3
1	M	435	LYS	3.3
3	C	103	ARG	3.3
1	M	172	ASN	3.3
1	A	76	TYR	3.3
1	M	578	GLN	3.3
1	M	612	LYS	3.3
1	G	741	CYS	3.3
1	M	590	CYS	3.3
1	G	742	PHE	3.2
1	G	301	ASP	3.2
1	G	358	ASN	3.2
1	A	262	TYR	3.2
1	A	100	ALA	3.2
1	A	107	VAL	3.2
1	A	141	ASP	3.2
1	M	66	ASP	3.2
3	O	157	PHE	3.2
1	A	276	ARG	3.2
1	G	207	SER	3.2
1	A	55	ASP	3.2
1	A	462	ASP	3.2
3	I	138	THR	3.2
1	G	249	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	315	PHE	3.2
2	B	180	TYR	3.2
1	M	743	ALA	3.2
1	M	207	SER	3.2
3	O	98	VAL	3.2
1	G	233	LYS	3.2
2	B	195	LYS	3.2
1	G	480	ASP	3.2
2	N	183	ASP	3.2
1	M	76	TYR	3.2
1	M	709	GLU	3.2
1	G	737	LYS	3.2
1	G	708	THR	3.2
1	M	723	ARG	3.2
1	M	795	ASN	3.2
1	A	480	ASP	3.2
1	G	711	TYR	3.2
1	M	316	TYR	3.2
3	I	23	ALA	3.2
1	G	278	LEU	3.2
3	I	91	ILE	3.1
1	A	559	ARG	3.1
1	G	137	GLN	3.1
3	C	155	ASN	3.1
2	B	53	ASP	3.1
3	C	136	ASP	3.1
1	A	103	ILE	3.1
2	H	135	ARG	3.1
1	G	144	THR	3.1
1	G	567	LYS	3.1
2	H	116	THR	3.1
1	M	803	ASN	3.1
3	I	126	ASN	3.1
1	G	275	TYR	3.1
1	M	864	TYR	3.1
1	A	105	CYS	3.1
1	M	334	GLU	3.1
2	B	144	VAL	3.1
1	G	416	GLU	3.1
1	M	200	ALA	3.1
1	G	356	PHE	3.1
1	M	280	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	768	HIS	3.1
4	K	6	HIS	3.1
1	M	328	THR	3.1
1	M	63	SER	3.1
1	M	242	ASN	3.1
2	N	144	VAL	3.1
1	M	499	ILE	3.1
3	I	36	PHE	3.1
1	A	693	GLY	3.1
1	G	523	LEU	3.1
1	A	483	VAL	3.1
1	G	78	VAL	3.1
1	A	812	TYR	3.1
1	M	24	ALA	3.1
3	I	87	SER	3.1
2	N	180	TYR	3.1
1	A	372	PRO	3.1
2	N	52	LEU	3.1
1	G	299	GLN	3.0
1	A	272	SER	3.0
1	G	623	SER	3.0
1	M	715	SER	3.0
2	H	161	ALA	3.0
1	G	309	TYR	3.0
2	B	124	TYR	3.0
1	A	391	PRO	3.0
1	G	614	MET	3.0
1	A	766	LEU	3.0
3	C	132	PRO	3.0
1	M	546	GLN	3.0
1	M	595	THR	3.0
1	G	588	SER	3.0
1	G	191	ASN	3.0
2	H	18	ASN	3.0
1	G	780	LEU	3.0
1	A	390	ASP	3.0
1	G	498	GLY	3.0
2	B	186	ASP	3.0
2	H	53	ASP	3.0
3	O	151	GLY	3.0
1	A	567	LYS	3.0
3	I	173	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	O	106	SER	3.0
1	A	677	ALA	3.0
1	M	276	ARG	3.0
2	B	34	MET	3.0
1	G	607	LYS	3.0
1	A	744	SER	3.0
1	G	766	LEU	3.0
2	H	138	LEU	3.0
4	Q	6	HIS	3.0
1	G	185	GLU	3.0
1	G	704	GLU	3.0
1	M	320	GLU	3.0
1	A	596	PRO	3.0
3	I	113	LYS	3.0
1	M	232	ASP	3.0
1	M	254	LEU	3.0
1	M	278	LEU	3.0
2	H	102	ASP	3.0
2	N	4	ASN	3.0
1	A	255	LEU	3.0
1	M	611	THR	3.0
3	O	86	LEU	3.0
3	I	154	VAL	3.0
1	A	435	LYS	2.9
1	G	90	ASN	2.9
1	A	278	LEU	2.9
1	G	557	LEU	2.9
1	M	450	GLY	2.9
1	A	555	GLN	2.9
2	B	130	ALA	2.9
2	B	140	ALA	2.9
2	N	161	ALA	2.9
1	A	519	TYR	2.9
2	N	28	TYR	2.9
1	G	254	LEU	2.9
1	M	401	LEU	2.9
3	I	128	PHE	2.9
1	A	319	CYS	2.9
3	I	38	ALA	2.9
1	G	820	ASP	2.9
1	M	74	ASP	2.9
2	N	133	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	214	GLU	2.9
2	N	143	GLU	2.9
4	E	5	GLU	2.9
1	M	78	VAL	2.9
3	O	158	ILE	2.9
1	A	523	LEU	2.9
1	G	439	LEU	2.9
1	G	832	ASP	2.9
3	I	33	ASP	2.9
1	A	720	GLU	2.9
1	M	716	MET	2.9
1	M	157	VAL	2.9
1	A	280	LYS	2.9
1	M	126	THR	2.9
1	A	27	ALA	2.9
2	N	19	ALA	2.9
1	G	53	LEU	2.9
3	I	96	LEU	2.9
1	A	196	PHE	2.9
1	G	125	PHE	2.9
1	G	692	PHE	2.9
3	I	101	ASN	2.9
1	A	65	VAL	2.9
1	M	461	GLN	2.9
2	H	19	ALA	2.9
1	M	600	LEU	2.9
1	G	792	TYR	2.9
3	C	29	ASN	2.9
1	A	66	ASP	2.8
1	M	438	ILE	2.8
3	I	92	GLN	2.8
1	G	391	PRO	2.8
2	B	26	GLU	2.8
2	H	128	GLY	2.8
2	H	134	MET	2.8
1	G	559	ARG	2.8
1	A	54	LEU	2.8
1	G	77	SER	2.8
1	G	616	VAL	2.8
3	O	67	SER	2.8
2	N	132	ASN	2.8
2	N	198	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	I	152	GLU	2.8
1	G	693	GLY	2.8
1	M	488	LEU	2.8
1	G	31	TYR	2.8
2	H	136	GLN	2.8
3	I	76	ALA	2.8
1	G	431	PHE	2.8
3	O	36	PHE	2.8
1	A	49	LYS	2.8
1	G	435	LYS	2.8
3	I	105	LYS	2.8
1	A	838	SER	2.8
3	C	31	TYR	2.8
3	C	130	TYR	2.8
1	A	154	ASN	2.8
3	I	145	HIS	2.8
1	G	255	LEU	2.8
1	M	70	LEU	2.8
1	G	438	ILE	2.8
1	A	137	GLN	2.8
1	A	546	GLN	2.8
2	B	109	GLU	2.8
3	C	59	HIS	2.7
2	H	164	LEU	2.7
1	A	690	ASP	2.7
1	M	423	ASP	2.7
1	M	501	ASP	2.7
1	M	686	ASP	2.7
1	M	558	VAL	2.7
1	G	280	LYS	2.7
1	M	335	GLU	2.7
3	C	116	GLU	2.7
1	A	439	LEU	2.7
1	A	630	HIS	2.7
1	G	181	ASP	2.7
1	M	462	ASP	2.7
2	N	39	SER	2.7
1	M	263	MET	2.7
3	I	98	VAL	2.7
1	M	361	PRO	2.7
1	M	372	PRO	2.7
3	C	56	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	830	TYR	2.7
1	M	314	GLN	2.7
2	H	180	TYR	2.7
1	M	469	THR	2.7
1	M	780	LEU	2.7
2	B	164	LEU	2.7
2	H	125	ARG	2.7
1	A	232	ASP	2.7
1	G	483	VAL	2.7
1	M	483	VAL	2.7
1	G	578	GLN	2.7
1	M	523	LEU	2.7
2	H	196	LEU	2.7
3	I	17	GLY	2.7
3	O	111	LEU	2.7
2	N	140	ALA	2.7
1	A	388	THR	2.7
1	G	430	GLU	2.7
1	M	840	ASN	2.7
1	A	181	ASP	2.7
1	A	206	ASP	2.7
1	M	301	ASP	2.7
3	O	33	ASP	2.7
1	M	246	PRO	2.7
1	G	618	ALA	2.7
2	H	124	TYR	2.7
3	I	158	ILE	2.7
1	G	126	THR	2.7
1	G	840	ASN	2.7
1	A	121	SER	2.7
1	G	63	SER	2.7
1	M	405	PHE	2.7
2	H	145	HIS	2.7
1	A	157	VAL	2.7
3	O	127	VAL	2.7
1	G	243	ASP	2.7
1	G	797	PRO	2.7
1	A	364	GLN	2.7
1	A	72	GLY	2.7
1	G	522	TYR	2.7
1	M	792	TYR	2.7
1	A	256	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	195	LYS	2.7
1	M	356	PHE	2.7
1	A	357	SER	2.7
1	A	679	SER	2.7
1	A	798	LEU	2.7
1	G	67	SER	2.7
1	G	596	PRO	2.6
1	G	380	ASP	2.6
2	B	103	ASP	2.6
3	O	41	ALA	2.6
2	B	35	TYR	2.6
2	H	28	TYR	2.6
3	I	130	TYR	2.6
1	M	570	ASN	2.6
1	M	744	SER	2.6
2	N	193	VAL	2.6
1	A	563	GLY	2.6
1	G	269	LYS	2.6
2	B	93	VAL	2.6
1	M	244	ILE	2.6
1	A	468	LYS	2.6
1	G	461	GLN	2.6
1	G	707	ALA	2.6
1	G	619	MET	2.6
1	M	439	LEU	2.6
1	M	490	THR	2.6
2	H	186	ASP	2.6
3	C	33	ASP	2.6
1	M	819	ASN	2.6
2	B	101	ASN	2.6
1	G	359	VAL	2.6
1	A	412	PRO	2.6
1	A	414	ALA	2.6
2	B	19	ALA	2.6
2	N	147	ALA	2.6
3	C	76	ALA	2.6
3	I	123	HIS	2.6
1	A	217	MET	2.6
1	A	731	PHE	2.6
1	M	721	ASP	2.6
1	A	799	ASN	2.6
1	G	131	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	302	ASN	2.6
1	M	95	ILE	2.6
2	B	132	ASN	2.6
2	N	203	ASN	2.6
1	A	251	LYS	2.6
1	A	299	GLN	2.6
1	M	555	GLN	2.6
1	M	731	PHE	2.6
2	H	90	GLU	2.6
1	A	501	ASP	2.6
1	G	807	ASP	2.6
1	M	459	ASP	2.6
1	G	450	GLY	2.6
1	M	125	PHE	2.6
1	M	693	GLY	2.6
1	A	392	ILE	2.5
1	M	309	TYR	2.5
2	N	188	TYR	2.5
3	I	31	TYR	2.5
1	A	580	GLU	2.5
1	G	66	ASP	2.5
1	G	570	ASN	2.5
1	M	390	ASP	2.5
1	M	446	ASP	2.5
1	M	832	ASP	2.5
3	O	164	ASP	2.5
1	M	73	LEU	2.5
1	M	327	LEU	2.5
1	A	692	PHE	2.5
1	G	608	ALA	2.5
1	G	763	ALA	2.5
2	H	156	GLN	2.5
3	O	100	PRO	2.5
1	G	563	GLY	2.5
1	A	31	TYR	2.5
2	N	166	ARG	2.5
1	A	32	ASN	2.5
1	G	689	ASN	2.5
1	A	394	PHE	2.5
1	A	295	SER	2.5
3	I	67	SER	2.5
3	I	106	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	603	LEU	2.5
2	H	98	VAL	2.5
2	H	162	LEU	2.5
3	C	127	VAL	2.5
1	G	746	ASN	2.5
2	N	18	ASN	2.5
1	G	728	ASP	2.5
1	G	200	ALA	2.5
1	G	682	ALA	2.5
1	A	333	LYS	2.5
1	A	781	LYS	2.5
1	G	95	ILE	2.5
3	C	108	GLY	2.5
1	G	276	ARG	2.5
1	G	611	THR	2.5
1	M	561	TYR	2.5
1	M	714	TYR	2.5
1	G	157	VAL	2.5
1	G	211	GLU	2.5
1	A	249	PHE	2.5
1	A	816	PHE	2.5
1	A	52	LYS	2.5
1	A	301	ASP	2.5
1	G	74	ASP	2.5
1	M	563	GLY	2.5
2	H	38	LEU	2.5
2	H	155	ARG	2.5
1	G	432	TYR	2.5
1	M	217	MET	2.5
2	B	188	TYR	2.5
3	C	58	VAL	2.5
1	M	407	PHE	2.5
3	C	36	PHE	2.5
1	A	135	ASN	2.5
1	M	131	ASN	2.5
1	A	318	ARG	2.5
1	G	590	CYS	2.5
2	N	186	ASP	2.5
1	M	699	THR	2.5
1	M	588	SER	2.5
1	M	375	GLU	2.4
1	M	726	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	415	GLN	2.4
3	C	41	ALA	2.4
1	A	623	SER	2.4
1	M	344	VAL	2.4
1	G	394	PHE	2.4
1	G	405	PHE	2.4
1	M	333	LYS	2.4
1	M	599	TYR	2.4
1	M	692	PHE	2.4
1	M	796	PHE	2.4
3	O	31	TYR	2.4
1	M	547	ILE	2.4
2	H	201	ILE	2.4
2	N	90	GLU	2.4
2	H	101	ASN	2.4
1	G	121	SER	2.4
1	G	793	SER	2.4
2	B	9	THR	2.4
1	G	107	VAL	2.4
1	A	309	TYR	2.4
1	G	256	GLU	2.4
1	G	345	LEU	2.4
1	G	424	HIS	2.4
1	G	580	GLU	2.4
1	G	621	GLU	2.4
1	M	154	ASN	2.4
2	N	23	ASN	2.4
1	M	391	PRO	2.4
1	G	455	GLY	2.4
1	G	48	LYS	2.4
1	G	232	ASP	2.4
1	A	162	TYR	2.4
1	G	76	TYR	2.4
1	M	610	TYR	2.4
1	G	319	CYS	2.4
1	M	211	GLU	2.4
2	H	36	HIS	2.4
1	A	128	ALA	2.4
1	M	364	GLN	2.4
1	G	154	ASN	2.4
1	M	130	ASN	2.4
1	M	810	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	132	ASN	2.4
1	A	253	GLY	2.4
1	G	744	SER	2.4
1	M	196	PHE	2.4
1	G	511	ILE	2.4
2	H	13	ILE	2.4
1	G	459	ASP	2.4
1	G	864	TYR	2.4
1	A	159	ARG	2.4
1	A	314	GLN	2.4
1	G	307	ALA	2.4
1	M	517	ALA	2.4
1	A	607	LYS	2.4
1	A	131	ASN	2.4
1	G	317	PRO	2.4
1	G	398	ASN	2.4
1	M	713	ASN	2.4
1	M	144	THR	2.4
1	M	248	VAL	2.4
2	N	168	THR	2.4
1	G	584	LEU	2.4
1	G	841	LEU	2.4
3	O	143	ILE	2.4
2	H	143	GLU	2.4
1	M	306	LYS	2.4
1	A	202	GLY	2.3
1	A	450	GLY	2.3
1	A	590	CYS	2.3
1	G	702	PRO	2.3
1	G	392	ILE	2.3
1	G	547	ILE	2.3
1	G	856	SER	2.3
1	M	394	PHE	2.3
1	M	398	ASN	2.3
1	M	57	ILE	2.3
2	B	141	LEU	2.3
2	N	38	LEU	2.3
2	B	99	LYS	2.3
1	G	789	GLU	2.3
1	M	214	GLU	2.3
1	M	299	GLN	2.3
2	H	131	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	116	GLU	2.3
1	A	238	LEU	2.3
3	C	145	HIS	2.3
1	G	50	SER	2.3
1	G	805	SER	2.3
1	A	819	ASN	2.3
1	G	469	THR	2.3
1	M	319	CYS	2.3
3	C	6	CYS	2.3
3	O	153	THR	2.3
1	G	263	MET	2.3
2	N	135	ARG	2.3
1	A	730	GLU	2.3
3	O	4	ASP	2.3
1	A	279	ILE	2.3
1	M	357	SER	2.3
1	M	424	HIS	2.3
1	M	793	SER	2.3
2	B	89	GLY	2.3
1	M	281	ARG	2.3
2	H	15	CYS	2.3
1	G	218	TYR	2.3
1	A	428	LEU	2.3
1	A	95	ILE	2.3
1	A	188	GLN	2.3
1	A	600	LEU	2.3
1	G	70	LEU	2.3
1	G	292	LEU	2.3
1	M	100	ALA	2.3
1	M	725	TYR	2.3
1	A	430	GLU	2.3
3	C	143	ILE	2.3
3	I	143	ILE	2.3
3	O	93	ILE	2.3
1	G	501	ASP	2.3
1	M	295	SER	2.3
1	G	297	GLY	2.3
1	A	178	VAL	2.3
3	I	24	HIS	2.3
1	G	795	ASN	2.3
1	G	799	ASN	2.3
2	H	4	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	23	ASN	2.3
2	N	9	THR	2.3
1	A	163	TRP	2.3
1	A	269	LYS	2.3
1	A	762	MET	2.3
2	N	125	ARG	2.3
1	A	830	TYR	2.3
1	M	128	ALA	2.3
1	M	763	ALA	2.3
2	B	8	ALA	2.3
2	N	171	PHE	2.3
1	A	553	GLU	2.3
1	G	117	GLU	2.3
1	M	245	GLU	2.3
2	B	90	GLU	2.3
2	H	109	GLU	2.3
1	A	793	SER	2.3
1	M	623	SER	2.3
2	N	117	SER	2.3
1	A	297	GLY	2.3
1	M	596	PRO	2.3
2	B	128	GLY	2.3
2	N	89	GLY	2.3
1	M	689	ASN	2.3
2	H	20	ASN	2.3
3	I	141	TRP	2.3
1	M	329	PHE	2.3
1	A	763	ALA	2.3
2	B	170	ALA	2.3
1	G	722	GLU	2.3
1	G	65	VAL	2.3
1	G	326	PRO	2.3
1	G	558	VAL	2.3
1	G	690	ASP	2.3
1	M	524	ASP	2.3
1	A	795	ASN	2.2
1	A	327	LEU	2.2
1	M	841	LEU	2.2
2	B	162	LEU	2.2
3	C	115	ALA	2.2
3	O	144	ALA	2.2
1	M	432	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	181	TYR	2.2
2	N	33	TYR	2.2
1	M	272	SER	2.2
1	G	720	GLU	2.2
1	M	722	GLU	2.2
1	G	488	LEU	2.2
1	M	411	PHE	2.2
3	O	91	ILE	2.2
1	M	163	TRP	2.2
1	A	682	ALA	2.2
1	G	421	ALA	2.2
3	O	168	ALA	2.2
1	M	31	TYR	2.2
2	H	99	LYS	2.2
2	H	179	SER	2.2
1	M	580	GLU	2.2
1	G	408	LEU	2.2
1	M	382	LEU	2.2
2	H	169	LEU	2.2
3	I	132	PRO	2.2
3	O	20	THR	2.2
1	A	125	PHE	2.2
1	A	688	ASP	2.2
1	A	713	ASN	2.2
1	G	411	PHE	2.2
2	N	20	ASN	2.2
3	C	4	ASP	2.2
1	G	112	MET	2.2
1	G	175	SER	2.2
1	M	522	TYR	2.2
2	H	117	SER	2.2
2	N	124	TYR	2.2
1	A	182	VAL	2.2
1	A	274	VAL	2.2
1	G	313	GLU	2.2
1	G	429	VAL	2.2
3	I	88	LEU	2.2
1	M	297	GLY	2.2
3	O	97	GLY	2.2
1	A	144	THR	2.2
1	A	697	ILE	2.2
1	A	386	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	810	ASN	2.2
2	B	20	ASN	2.2
2	B	23	ASN	2.2
1	M	198	LYS	2.2
2	H	195	LYS	2.2
1	G	546	GLN	2.2
1	A	241	LEU	2.2
1	A	522	TYR	2.2
1	G	406	LEU	2.2
1	G	502	LEU	2.2
1	M	359	VAL	2.2
1	A	317	PRO	2.2
1	G	516	GLU	2.2
1	M	253	GLY	2.2
3	I	108	GLY	2.2
1	G	499	ILE	2.2
2	H	14	ILE	2.2
3	C	107	ILE	2.2
1	A	796	PHE	2.2
1	M	236	ASN	2.2
1	A	263	MET	2.2
1	G	739	ALA	2.2
1	G	749	ALA	2.2
1	G	768	HIS	2.2
1	M	99	SER	2.2
1	M	312	LEU	2.2
1	A	218	TYR	2.2
1	G	310	GLY	2.2
2	H	37	ILE	2.2
1	M	416	GLU	2.2
1	A	145	LEU	2.2
1	A	448	ALA	2.1
1	G	128	ALA	2.1
1	M	630	HIS	2.1
1	A	47	TYR	2.1
1	A	344	VAL	2.1
1	A	409	LYS	2.1
1	A	823	GLY	2.1
1	G	300	GLY	2.1
1	G	346	PRO	2.1
1	G	443	GLY	2.1
1	A	843	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	28	LEU	2.1
3	O	112	LEU	2.1
1	A	746	ASN	2.1
1	G	100	ALA	2.1
1	G	436	ALA	2.1
1	G	810	ASN	2.1
1	M	171	ALA	2.1
1	M	302	ASN	2.1
3	O	156	ASN	2.1
1	A	848	SER	2.1
1	M	175	SER	2.1
2	B	12	ASP	2.1
3	C	91	ILE	2.1
1	A	405	PHE	2.1
3	C	172	LYS	2.1
3	I	157	PHE	2.1
3	O	130	TYR	2.1
1	A	201	GLU	2.1
1	A	827	LEU	2.1
1	A	404	HIS	2.1
1	A	491	LYS	2.1
1	G	718	VAL	2.1
1	G	757	GLY	2.1
3	I	122	CYS	2.1
1	G	199	LEU	2.1
1	M	444	LEU	2.1
3	I	22	LEU	2.1
1	M	511	ILE	2.1
2	B	203	ASN	2.1
3	I	37	SER	2.1
4	K	1	SER	2.1
1	G	489	PHE	2.1
3	O	145	HIS	2.1
1	A	432	TYR	2.1
1	A	561	TYR	2.1
3	O	146	GLY	2.1
3	I	26	THR	2.1
3	I	94	GLU	2.1
2	B	159	ARG	2.1
1	A	200	ALA	2.1
1	G	271	ALA	2.1
1	G	433	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	13	ILE	2.1
2	B	201	ILE	2.1
2	H	160	ALA	2.1
1	G	838	SER	2.1
2	B	4	ASN	2.1
2	B	156	GLN	2.1
1	M	255	LEU	2.1
1	M	502	LEU	2.1
1	M	827	LEU	2.1
1	G	404	HIS	2.1
1	G	253	GLY	2.1
4	Q	4	MET	2.1
1	M	684	PRO	2.1
3	I	4	ASP	2.1
1	A	513	GLU	2.1
1	M	720	GLU	2.1
3	I	165	GLU	2.1
3	O	61	THR	2.1
3	C	110	LYS	2.1
3	I	110	LYS	2.1
1	A	155	ALA	2.1
1	A	533	ALA	2.1
1	A	715	SER	2.1
1	A	805	SER	2.1
3	I	41	ALA	2.1
3	I	109	SER	2.1
1	A	378	VAL	2.1
1	G	382	LEU	2.1
1	M	308	LEU	2.1
1	A	733	TYR	2.0
1	A	694	GLU	2.0
3	C	3	ARG	2.0
3	C	61	THR	2.0
1	G	251	LYS	2.0
1	M	52	LYS	2.0
2	N	5	ILE	2.0
1	G	715	SER	2.0
1	M	618	ALA	2.0
2	N	43	ALA	2.0
1	A	70	LEU	2.0
1	G	401	LEU	2.0
1	G	467	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	145	LEU	2.0
1	M	740	LEU	2.0
2	B	15	CYS	2.0
1	G	712	ASN	2.0
1	G	591	MET	2.0
1	M	606	GLY	2.0
1	G	561	TYR	2.0
1	M	322	PRO	2.0
3	C	65	TYR	2.0
1	G	468	LYS	2.0
1	M	737	LYS	2.0
3	I	59	HIS	2.0
1	A	699	THR	2.0
1	G	260	THR	2.0
1	A	722	GLU	2.0
1	G	524	ASP	2.0
1	A	608	ALA	2.0
1	G	787	SER	2.0
1	M	448	ALA	2.0
2	N	139	PHE	2.0
1	G	331	GLN	2.0
1	M	470	VAL	2.0
1	G	762	MET	2.0
1	M	619	MET	2.0
1	A	466	ASN	2.0
3	C	72	GLY	2.0
1	M	589	TYR	2.0
3	O	132	PRO	2.0
1	A	260	THR	2.0
1	A	424	HIS	2.0
1	A	74	ASP	2.0
1	G	141	ASP	2.0
1	G	603	LEU	2.0
1	A	856	SER	2.0
1	G	213	SER	2.0
1	M	85	ALA	2.0
1	M	121	SER	2.0
2	H	137	ALA	2.0
3	C	117	ASP	2.0
3	C	157	PHE	2.0
1	M	680	VAL	2.0
3	C	27	VAL	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

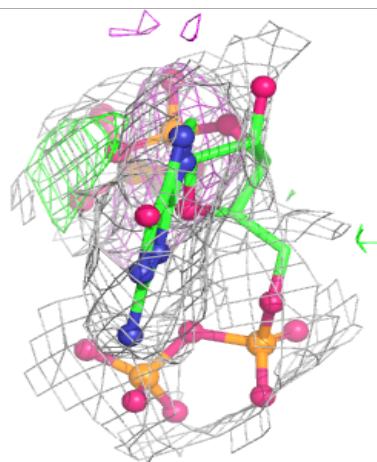
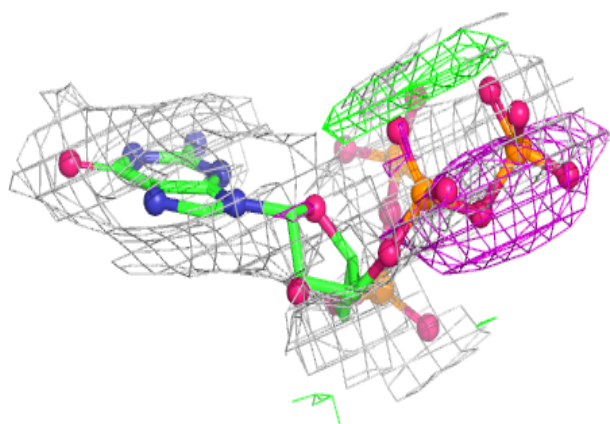
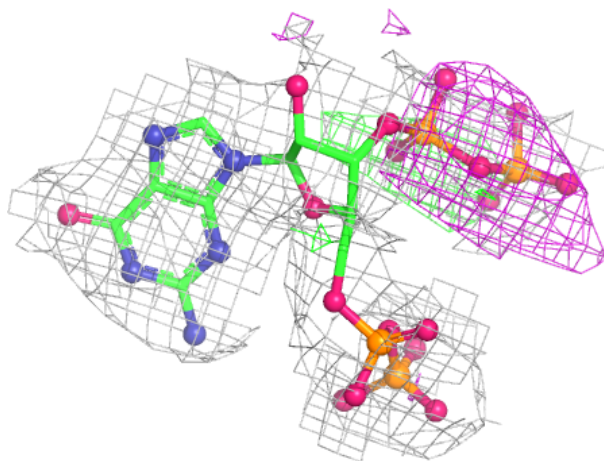
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	G4P	G	901	36/36	0.64	0.24	83,83,84,84	0
7	ACO	C	201	51/51	0.78	0.23	86,87,88,89	0
5	G4P	A	901	36/36	0.80	0.19	85,86,87,87	0
6	CMC	B	301	51/52	-	-	20,20,20,20	51
6	CMC	H	301	51/52	-	-	20,20,20,20	51
6	CMC	N	301	51/52	-	-	20,20,20,20	51
7	ACO	I	201	51/51	0.80	0.23	85,86,87,87	0
5	G4P	M	901	36/36	0.81	0.20	85,86,86,86	0
7	ACO	O	201	51/51	0.81	0.23	89,90,92,92	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.

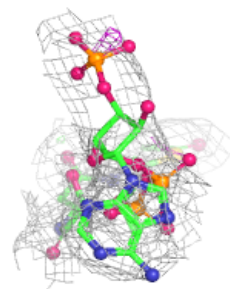
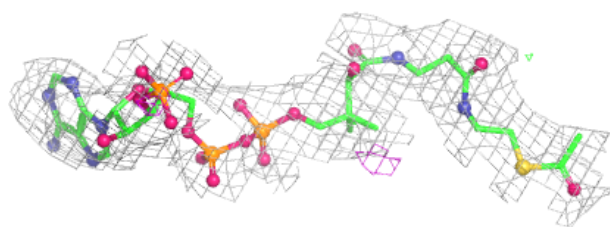
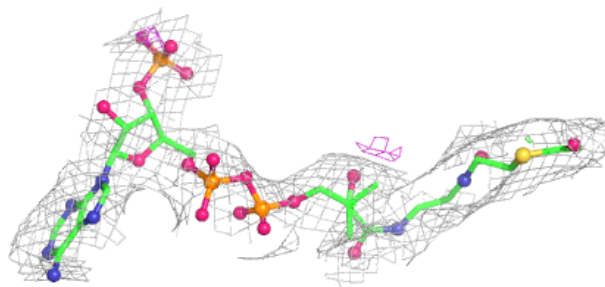
Electron density around G4P G 901:

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

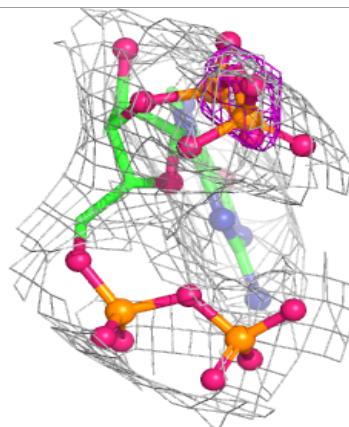
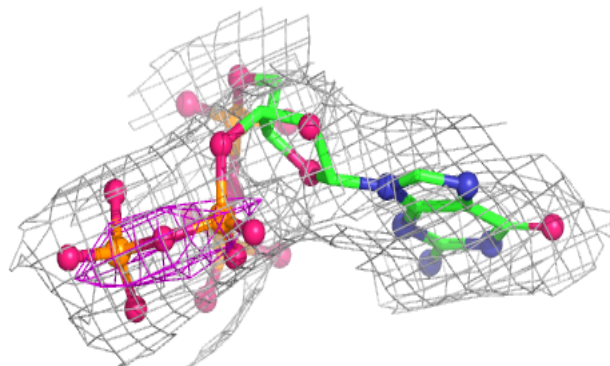
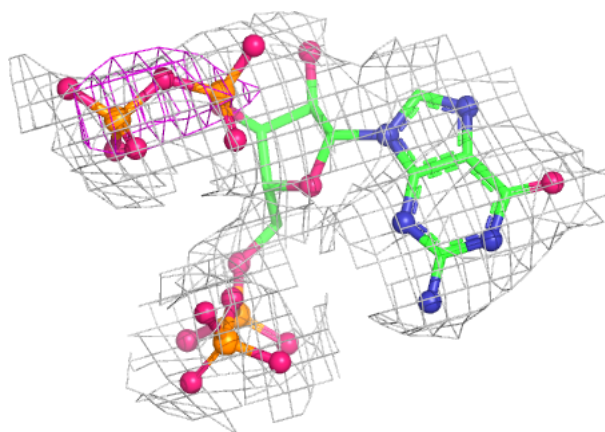


Electron density around ACO C 201:

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

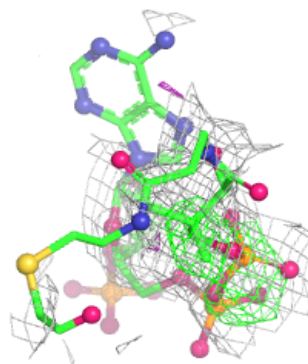
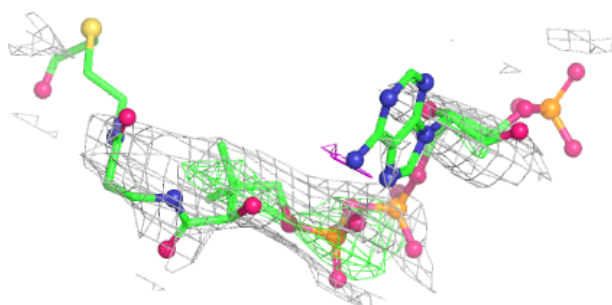
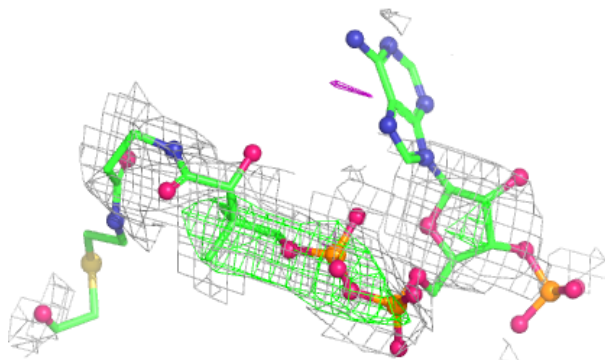
**Electron density around G4P A 901:**

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

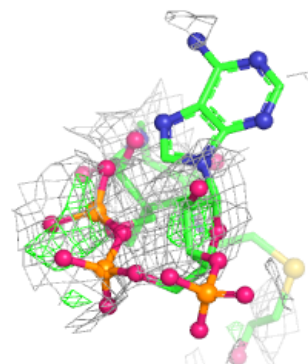
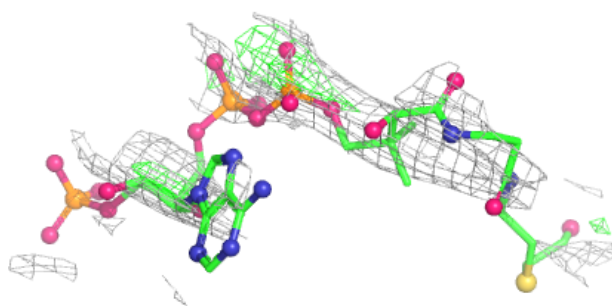
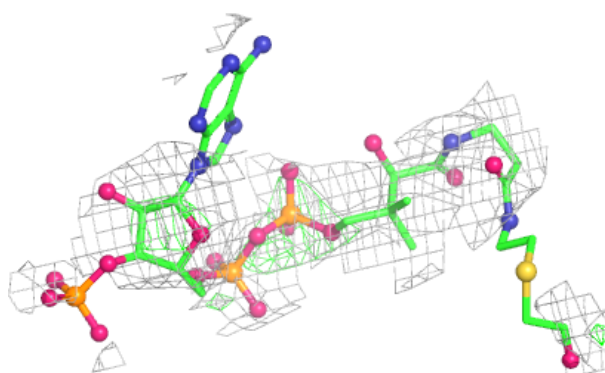


Electron density around CMC B 301:

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

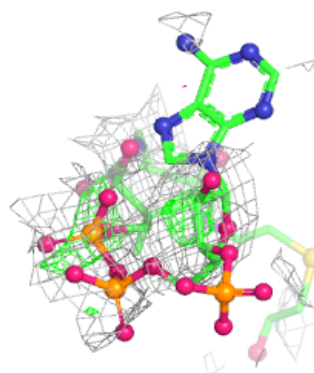
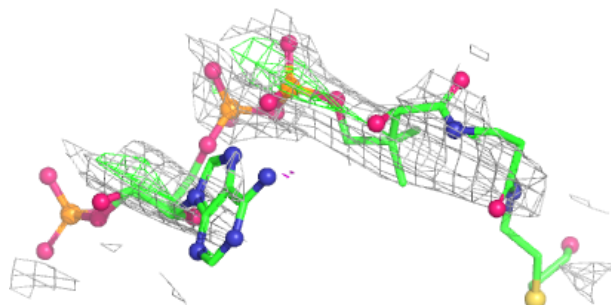
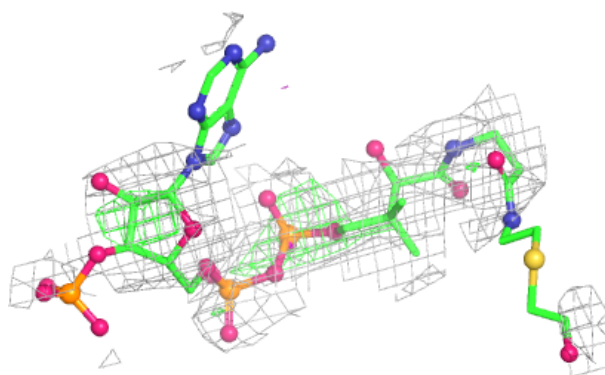
**Electron density around CMC H 301:**

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

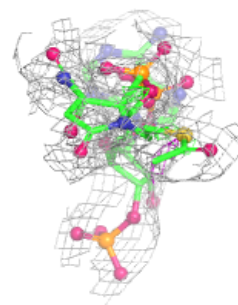
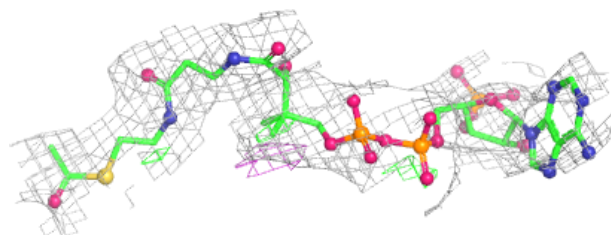
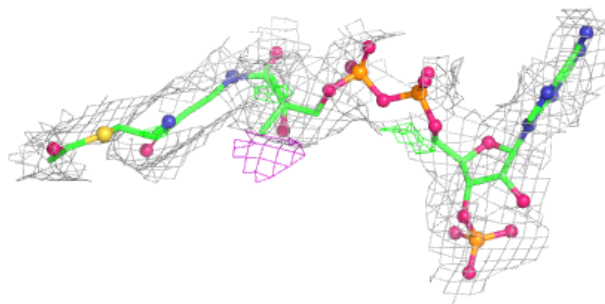


Electron density around CMC N 301:

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

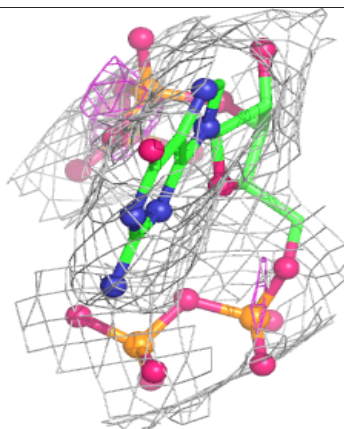
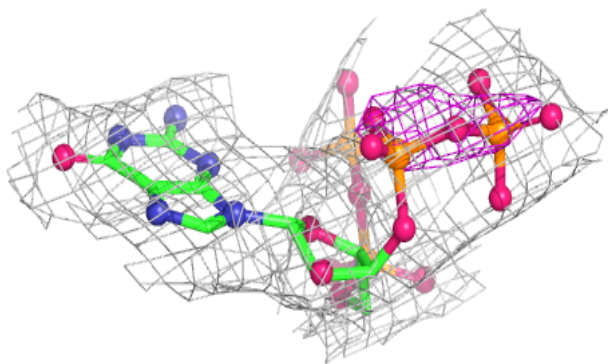
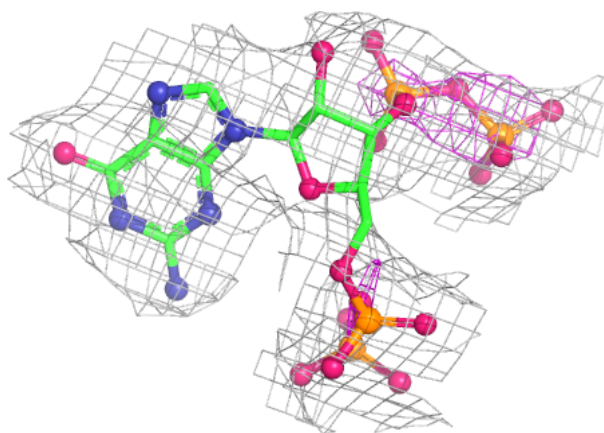
**Electron density around ACO I 201:**

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

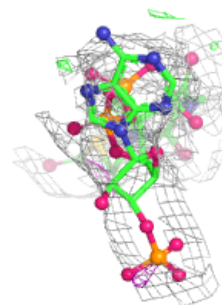
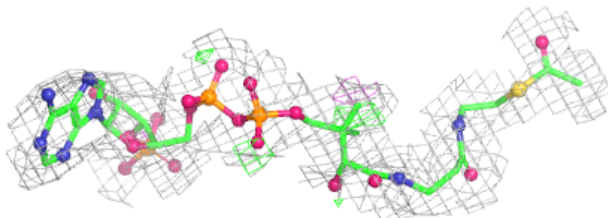
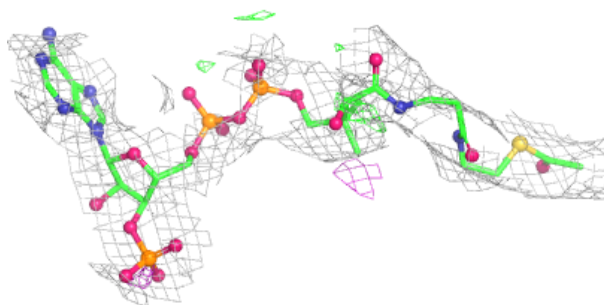


Electron density around G4P M 901:

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

**Electron density around ACO O 201:**

$2mF_o-DF_c$ (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.