Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 11:11 AM EST

PDB ID	:	4Y49
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:

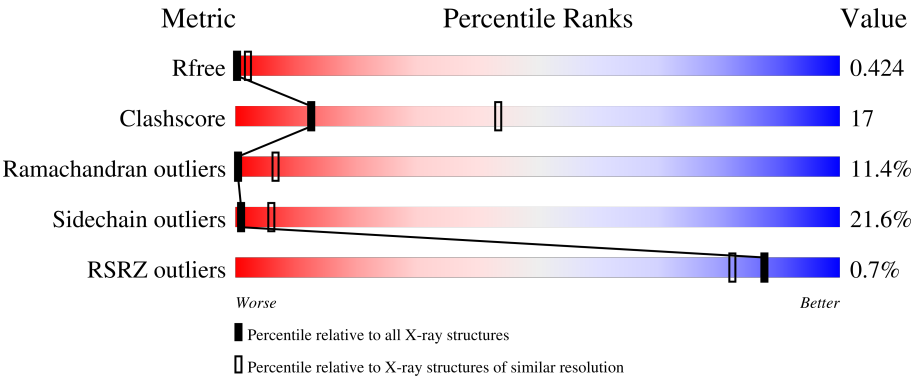
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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 <=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	60% 23% 6% • 10%
1	G	854	60% 23% 7% • 10%
1	M	854	60% 23% 6% • 10%
2	B	238	40% 22% 6% • 31%
2	H	238	44% 21% • • 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	238	42% 23% 31%
3	C	176	% 63% 19% 6% 11%
3	I	176	58% 23% 6% 12%
3	O	176	66% 18% 13%
4	E	8	75% 25%
4	K	8	12% 75% 25%
4	Q	8	75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	G4P	G	901	-	-	-	X

2 Entry composition (i)

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			

Continued on next page...

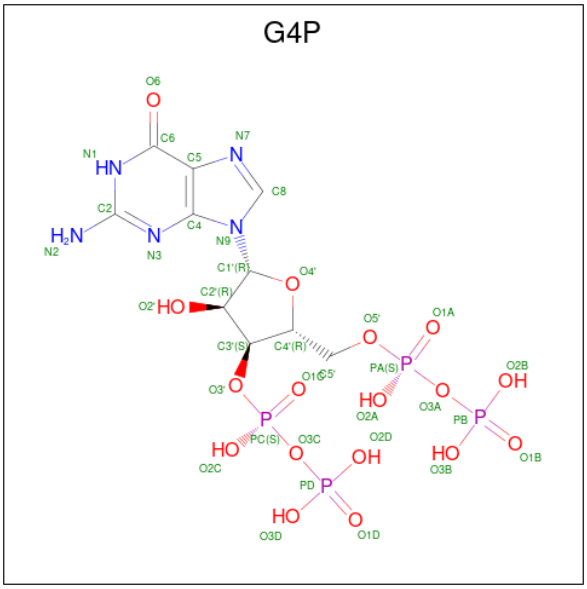
Continued from previous page...

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.

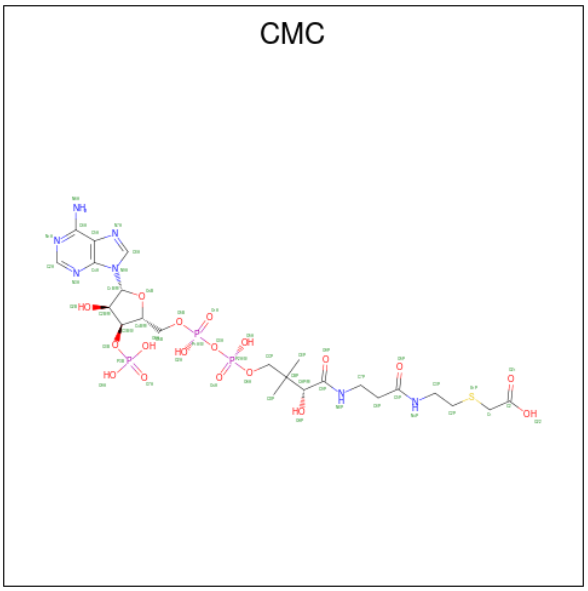
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	0	0	0
			30	18	6	6			
4	K	6	Total	C	N	O	0	0	0
			30	18	6	6			
4	Q	6	Total	C	N	O	0	0	0
			30	18	6	6			

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



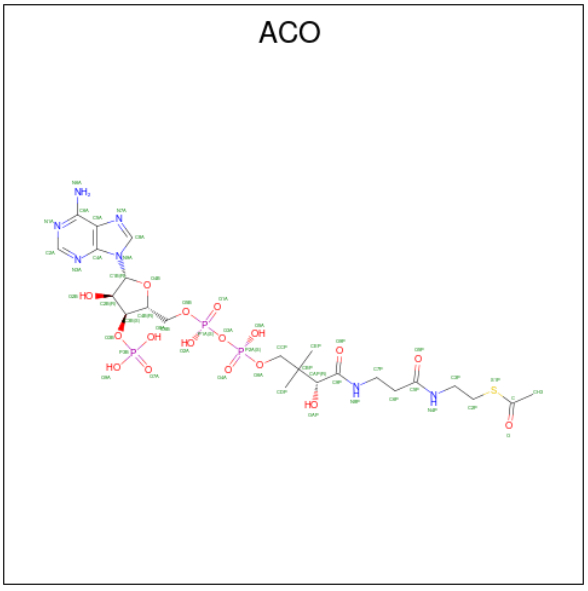
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	G	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	M	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 6 is CARBOXYMETHYL COENZYME *A (three-letter code: 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 (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



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

Continued on next page...

Continued from previous page...

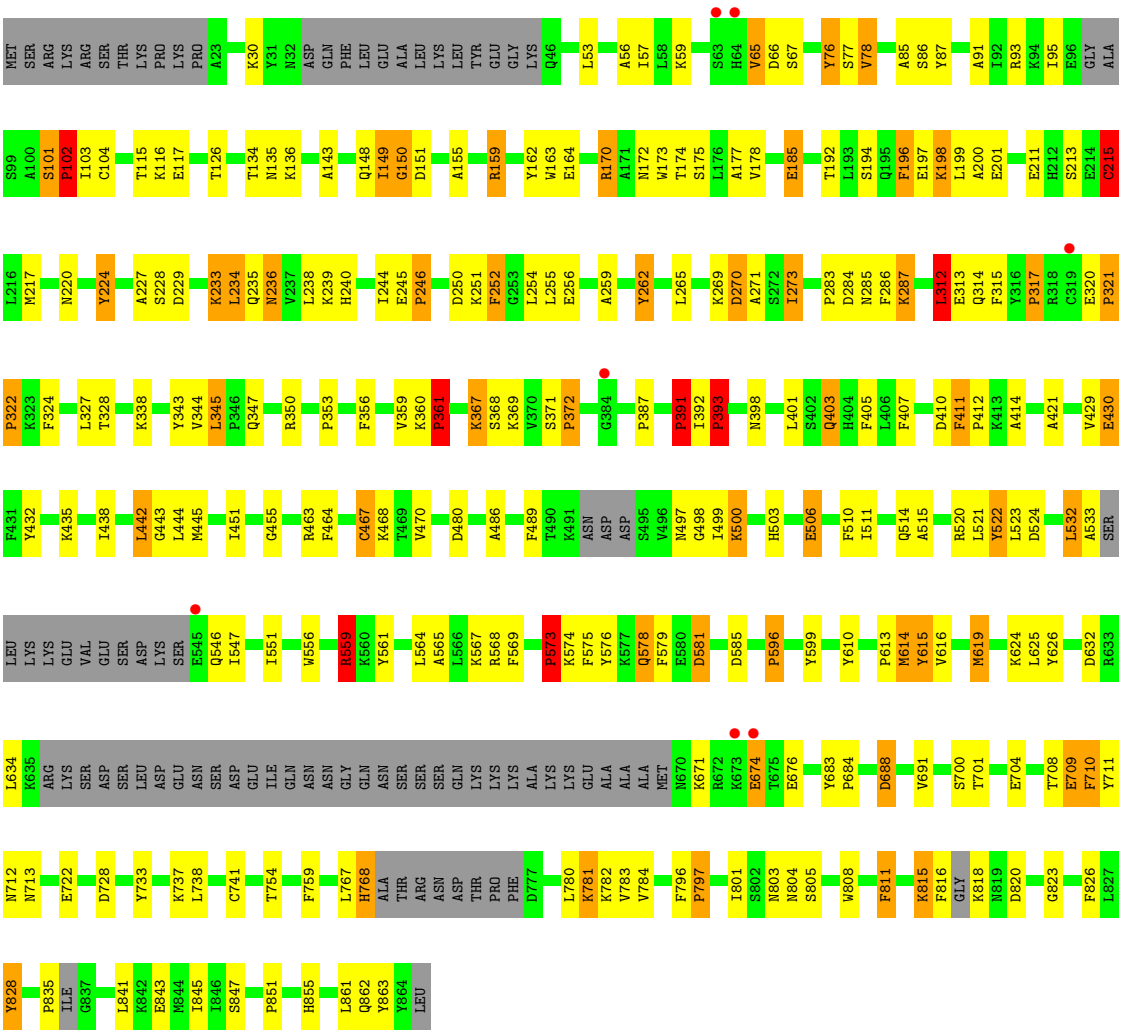
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
7	O	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

3 Residue-property plots (i)

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

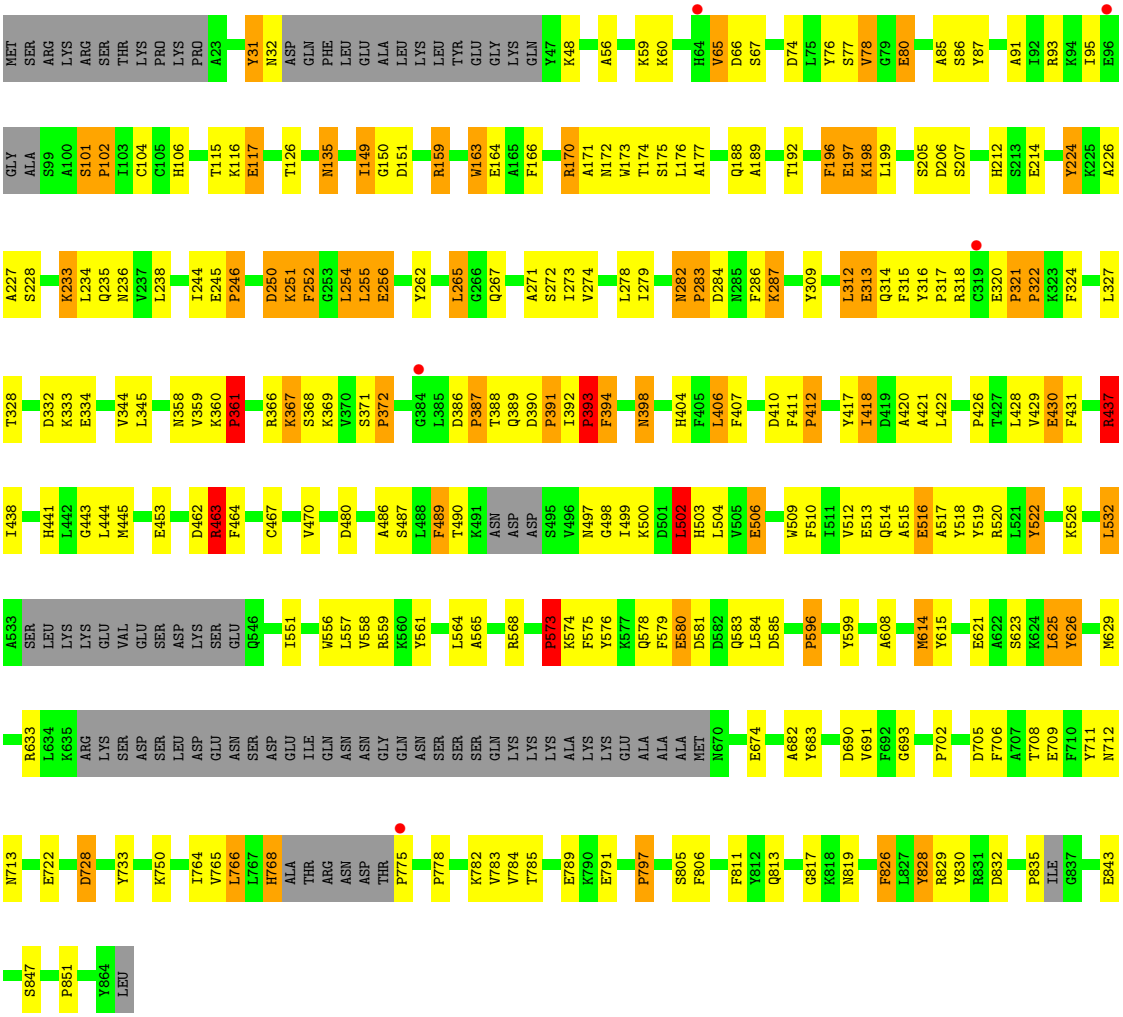
• Molecule 1: N-terminal acetyltransferase A complex subunit NAT1

Chain A:



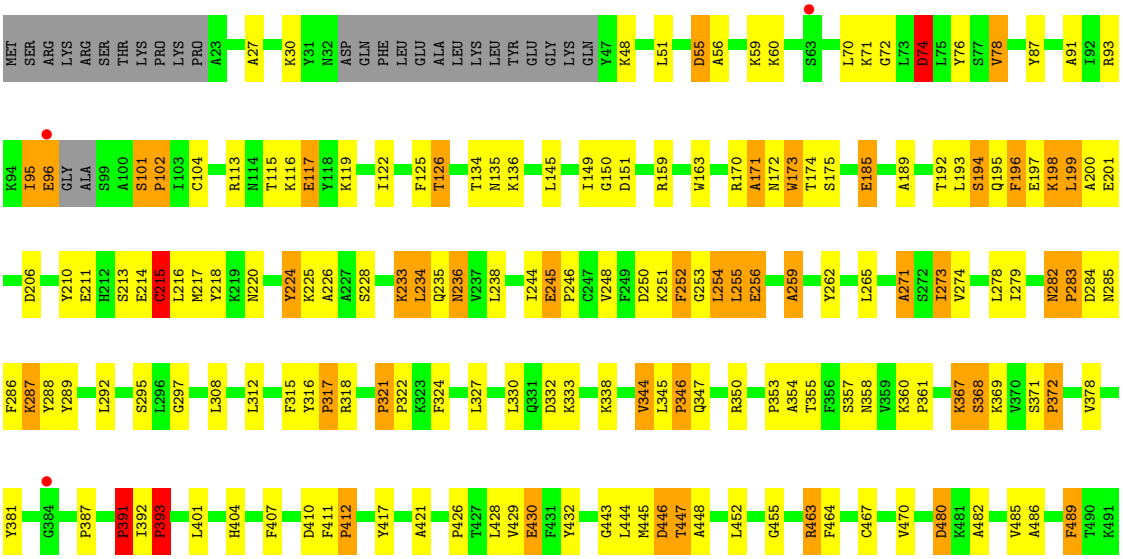
• Molecule 1: N-terminal acetyltransferase A complex subunit NAT1

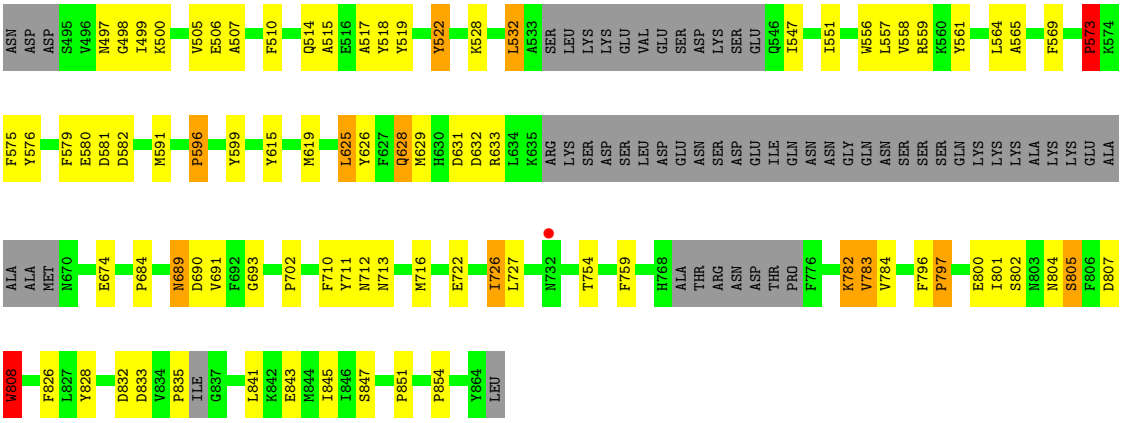
Chain G:



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

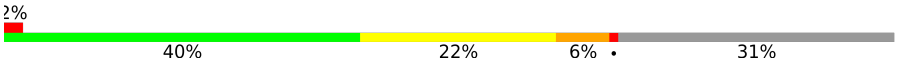
Chain M:

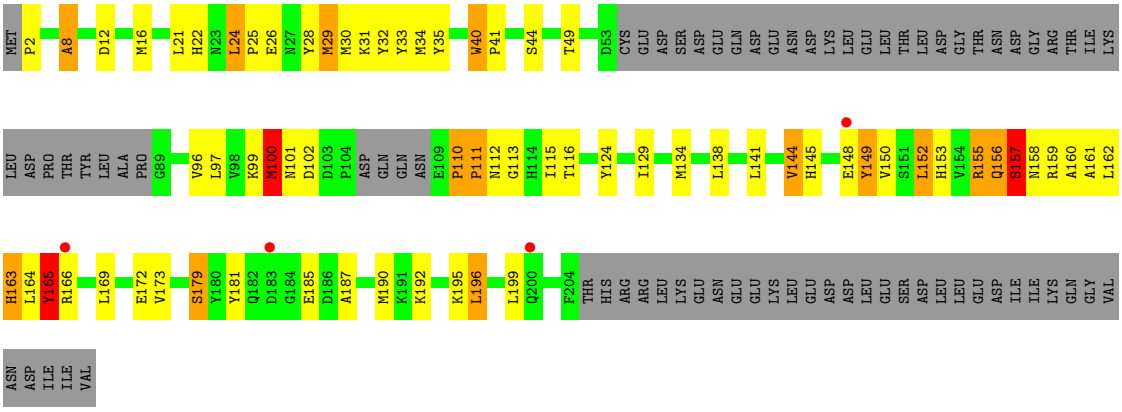




• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1

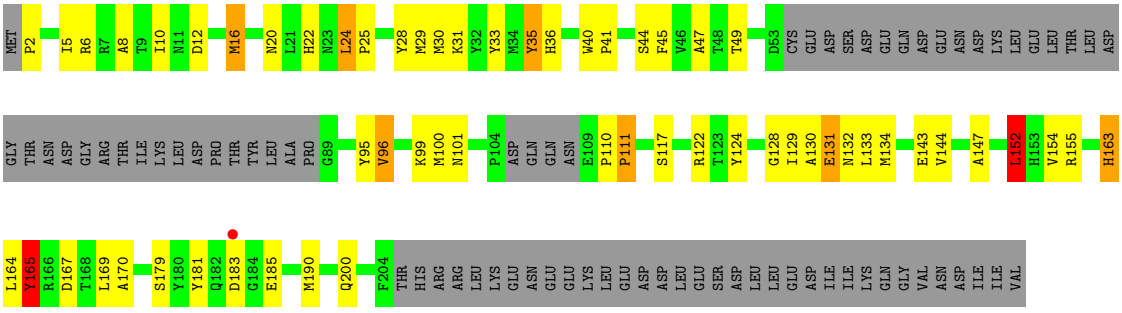
Chain B:





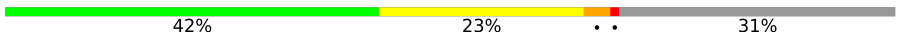
• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1

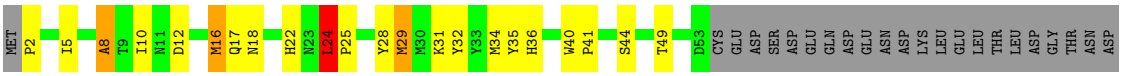
Chain H:

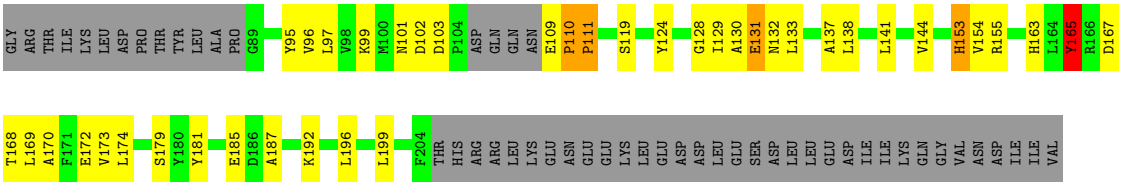


• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1

Chain N:

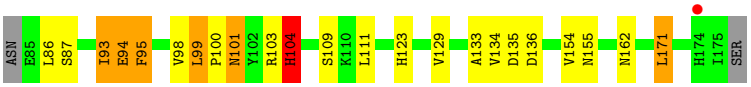






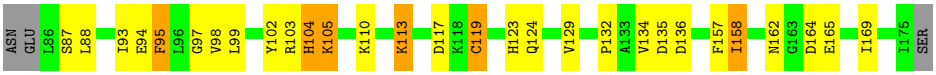
• Molecule 3: N-terminal acetyltransferase A complex subunit NAT5

Chain C:



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

Chain I:



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

Chain O:

• Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA

Chain E:

• 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 (i)

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
$< I/\sigma(I) >$ [1]	5.03 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.355 , 0.421 0.366 , 0.424	Depositor DCC
R_{free} test set	1799 reflections (4.99%)	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)	0.14 , 112.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACO, G4P, CMC

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	1.26	19/4701 (0.4%)	0.90	20/6458 (0.3%)
1	G	1.04	13/4725 (0.3%)	0.95	21/6500 (0.3%)
1	M	0.95	10/4689 (0.2%)	0.90	22/6453 (0.3%)
2	B	1.13	7/1040 (0.7%)	1.06	7/1424 (0.5%)
2	H	0.93	2/1041 (0.2%)	0.99	5/1424 (0.4%)
2	N	0.79	1/1040 (0.1%)	0.92	5/1423 (0.4%)
3	C	1.30	4/900 (0.4%)	1.06	6/1243 (0.5%)
3	I	1.23	5/889 (0.6%)	1.09	9/1224 (0.7%)
3	O	0.70	0/870	0.86	5/1197 (0.4%)
4	E	1.17	0/29	1.07	0/39
4	K	1.18	0/29	0.99	0/39
4	Q	1.24	0/29	0.66	0/39
All	All	1.08	61/19982 (0.3%)	0.94	100/27463 (0.4%)

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

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

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	768	HIS	C-O	33.82	1.87	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	CYS	CB-SG	32.14	2.36	1.82
1	A	709	GLU	CD-OE1	28.81	1.57	1.25
1	A	768	HIS	C-O	26.80	1.74	1.23
1	A	709	GLU	CD-OE2	22.47	1.50	1.25
1	M	185	GLU	CG-CD	21.48	1.84	1.51
1	A	676	GLU	CD-OE1	21.02	1.48	1.25
3	C	36	PHE	C-O	20.91	1.63	1.23
3	I	36	PHE	N-CA	20.49	1.87	1.46
3	C	35	PHE	C-N	-19.07	0.90	1.34
1	M	185	GLU	CD-OE2	18.73	1.46	1.25
1	A	467	CYS	CB-SG	15.83	2.09	1.82
1	M	215	CYS	CB-SG	15.36	2.08	1.82
3	C	36	PHE	CA-CB	-15.24	1.20	1.53
2	B	29	MET	CG-SD	13.23	2.15	1.81
1	G	453	GLU	CD-OE1	11.07	1.37	1.25
3	I	16	LEU	CA-C	11.02	1.81	1.52
1	A	533	ALA	C-O	11.00	1.44	1.23
1	G	709	GLU	CD-OE2	9.61	1.36	1.25
1	A	704	GLU	CG-CD	8.99	1.65	1.51
1	A	619	MET	SD-CE	8.95	2.27	1.77
1	G	614	MET	SD-CE	8.62	2.26	1.77
1	G	614	MET	CB-CG	8.14	1.77	1.51
1	A	614	MET	SD-CE	8.06	2.23	1.77
1	A	709	GLU	CG-CD	7.87	1.63	1.51
1	A	185	GLU	CD-OE1	7.84	1.34	1.25
1	A	185	GLU	CD-OE2	7.83	1.34	1.25
2	B	26	GLU	CD-OE1	7.82	1.34	1.25
1	M	689	ASN	C-O	7.68	1.38	1.23
1	M	126	THR	C-O	7.61	1.37	1.23
2	B	149	TYR	CG-CD1	-7.48	1.29	1.39
1	A	704	GLU	CD-OE2	7.47	1.33	1.25
3	I	97	GLY	C-O	7.46	1.35	1.23
3	I	164	ASP	CG-OD2	7.44	1.42	1.25
2	H	134	MET	CG-SD	7.41	2.00	1.81
1	A	674	GLU	CD-OE2	7.40	1.33	1.25
1	M	591	MET	CG-SD	7.30	2.00	1.81
1	G	437	ARG	CZ-NH1	7.09	1.42	1.33
1	G	614	MET	CG-SD	7.04	1.99	1.81
1	G	709	GLU	CD-OE1	7.00	1.33	1.25
1	M	206	ASP	CB-CG	6.86	1.66	1.51
3	I	36	PHE	CA-CB	6.47	1.68	1.53
1	M	467	CYS	CB-SG	6.24	1.92	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	683	TYR	CG-CD2	6.22	1.47	1.39
1	G	126	THR	C-O	6.00	1.34	1.23
2	B	149	TYR	CE1-CZ	-5.97	1.30	1.38
1	M	619	MET	CG-SD	5.87	1.96	1.81
1	G	516	GLU	CD-OE1	5.61	1.31	1.25
1	G	775	PRO	C-N	5.55	1.46	1.34
1	M	199	LEU	C-O	5.50	1.33	1.23
2	N	109	GLU	C-N	5.43	1.44	1.34
2	B	100	MET	CG-SD	5.41	1.95	1.81
2	B	149	TYR	CE2-CZ	-5.36	1.31	1.38
3	C	19	LEU	C-O	5.35	1.33	1.23
1	G	683	TYR	CE1-CZ	5.33	1.45	1.38
1	A	126	THR	C-O	5.22	1.33	1.23
2	B	179	SER	CB-OG	5.22	1.49	1.42
1	A	619	MET	CG-SD	5.21	1.94	1.81
1	A	683	TYR	C-O	5.19	1.33	1.23
1	A	674	GLU	CD-OE1	5.15	1.31	1.25
2	H	165	TYR	CE1-CZ	5.10	1.45	1.38

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	35	PHE	O-C-N	-16.32	96.58	122.70
3	I	36	PHE	N-CA-CB	13.10	134.18	110.60
3	C	35	PHE	CA-C-N	11.87	143.30	117.20
3	C	36	PHE	O-C-N	-9.46	107.57	122.70
2	H	134	MET	CG-SD-CE	-9.31	85.31	100.20
3	I	164	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	A	619	MET	CG-SD-CE	-8.97	85.85	100.20
1	A	709	GLU	OE1-CD-OE2	8.27	133.22	123.30
2	B	26	GLU	OE1-CD-OE2	7.56	132.37	123.30
1	A	215	CYS	CA-CB-SG	-7.39	100.69	114.00
3	I	16	LEU	CA-C-N	-7.39	101.43	116.20
1	A	573	PRO	N-CA-CB	7.32	112.08	103.30
1	M	573	PRO	N-CA-CB	7.24	111.99	103.30
1	G	768	HIS	CA-C-O	-7.19	105.00	120.10
3	I	35	PHE	C-N-CA	-7.19	103.73	121.70
2	N	170	ALA	N-CA-CB	7.02	119.93	110.10
1	G	851	PRO	N-CA-CB	6.71	111.35	103.30
3	O	28	PRO	N-CA-CB	6.66	111.30	103.30
2	B	111	PRO	N-CA-CB	6.59	111.20	103.30
3	I	132	PRO	N-CA-CB	6.58	111.20	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	851	PRO	N-CA-CB	6.58	111.20	103.30
2	H	111	PRO	N-CA-CB	6.56	111.17	103.30
3	C	28	PRO	N-CA-CB	6.42	111.01	103.30
2	N	111	PRO	N-CA-CB	6.39	110.97	103.30
1	M	596	PRO	N-CA-CB	6.38	110.95	103.30
2	H	25	PRO	N-CA-CB	6.36	110.94	103.30
1	A	851	PRO	N-CA-CB	6.33	110.90	103.30
2	B	100	MET	CG-SD-CE	-6.19	90.29	100.20
1	A	317	PRO	N-CA-CB	6.19	110.72	103.30
1	G	393	PRO	N-CA-CB	6.18	110.72	103.30
1	M	854	PRO	N-CA-CB	6.14	110.66	103.30
1	A	387	PRO	N-CA-CB	6.13	110.66	103.30
1	G	596	PRO	N-CA-CB	6.12	110.65	103.30
2	N	25	PRO	N-CA-CB	6.12	110.64	103.30
1	G	573	PRO	N-CA-CB	6.10	110.62	103.30
1	M	102	PRO	N-CA-CB	6.09	110.60	103.30
1	A	835	PRO	N-CA-CB	6.08	110.59	103.30
1	M	835	PRO	N-CA-CB	6.05	110.56	103.30
1	M	797	PRO	N-CA-CB	6.05	110.56	103.30
1	M	185	GLU	CG-CD-OE2	6.01	130.33	118.30
1	A	684	PRO	N-CA-CB	6.01	110.51	103.30
2	B	29	MET	CG-SD-CE	-6.01	90.59	100.20
2	B	41	PRO	N-CA-CB	5.99	110.49	103.30
1	M	689	ASN	O-C-N	5.98	132.26	122.70
1	G	102	PRO	N-CA-CB	5.96	110.45	103.30
1	A	797	PRO	N-CA-CB	5.95	110.44	103.30
1	M	625	LEU	CA-CB-CG	5.91	128.90	115.30
1	G	391	PRO	N-CA-CB	5.91	110.39	103.30
1	A	391	PRO	N-CA-CB	5.89	110.37	103.30
1	M	391	PRO	N-CA-CB	5.87	110.35	103.30
1	G	372	PRO	N-CA-CB	5.86	110.33	103.30
1	M	387	PRO	N-CA-CB	5.83	110.30	103.30
1	G	797	PRO	N-CA-CB	5.81	110.27	103.30
1	A	393	PRO	N-CA-CB	5.80	110.26	103.30
2	N	41	PRO	N-CA-CB	5.76	110.21	103.30
1	A	246	PRO	N-CA-CB	5.73	110.18	103.30
1	M	372	PRO	N-CA-CB	5.69	110.13	103.30
1	G	426	PRO	N-CA-CB	5.69	110.13	103.30
1	A	372	PRO	N-CA-CB	5.69	110.12	103.30
1	G	625	LEU	CA-CB-CG	5.68	128.37	115.30
1	M	684	PRO	N-CA-CB	5.68	110.12	103.30
1	G	387	PRO	N-CA-CB	5.68	110.12	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	437	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	H	41	PRO	N-CA-CB	5.66	110.09	103.30
1	G	835	PRO	N-CA-CB	5.64	110.07	103.30
1	A	361	PRO	N-CA-CB	5.63	110.05	103.30
2	N	110	PRO	N-CA-CB	5.61	110.03	103.30
2	B	157	SER	N-CA-C	5.60	126.13	111.00
1	M	346	PRO	N-CA-CB	5.60	110.02	103.30
1	G	406	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	G	778	PRO	N-CA-CB	5.58	110.00	103.30
1	M	353	PRO	N-CA-CB	5.58	110.00	103.30
3	I	70	PRO	N-CA-CB	5.58	109.99	103.30
3	I	80	PRO	N-CA-CB	5.57	109.98	103.30
1	G	246	PRO	N-CA-CB	5.56	109.97	103.30
3	C	100	PRO	N-CA-CB	5.56	109.97	103.30
3	O	80	PRO	N-CA-CB	5.56	109.97	103.30
3	I	28	PRO	N-CA-CB	5.54	109.95	103.30
3	C	80	PRO	N-CA-CB	5.54	109.95	103.30
3	O	100	PRO	N-CA-CB	5.54	109.94	103.30
1	M	93	ARG	NE-CZ-NH1	5.53	123.06	120.30
3	O	132	PRO	N-CA-CB	5.49	109.89	103.30
1	A	559	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	M	412	PRO	N-CA-CB	5.43	109.82	103.30
1	A	353	PRO	N-CA-CB	5.41	109.80	103.30
1	G	394	PHE	CB-CG-CD1	5.39	124.57	120.80
2	B	110	PRO	N-CA-CB	5.28	109.63	103.30
1	G	361	PRO	N-CA-CB	5.26	109.62	103.30
1	A	613	PRO	N-CA-CB	5.25	109.59	103.30
1	G	93	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	M	393	PRO	N-CA-CB	5.19	109.53	103.30
1	M	426	PRO	N-CA-CB	5.19	109.53	103.30
1	A	614	MET	CG-SD-CE	-5.17	91.92	100.20
1	M	74	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	M	716	MET	CG-SD-CE	-5.15	91.96	100.20
1	A	102	PRO	N-CA-CB	5.11	109.43	103.30
1	G	412	PRO	N-CA-CB	5.11	109.43	103.30
2	H	6	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	O	8	LEU	CA-CB-CG	5.05	126.91	115.30
3	I	36	PHE	N-CA-C	-5.02	97.45	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4636	0	2969	127	0
1	G	4656	0	2966	129	0
1	M	4624	0	2960	137	0
2	B	1024	0	710	41	0
2	H	1025	0	695	25	0
2	N	1025	0	699	24	0
3	C	888	0	539	26	0
3	I	879	0	527	32	0
3	O	861	0	511	16	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	548	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 17.

All (548) 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	1.44
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:614:MET:SD	1:A:614:MET:CE	2.23	1.27
1:A:768:HIS:O	1:A:768:HIS:C	1.74	1.24
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:A:215:CYS:CB	1:A:215:CYS:SG	2.36	1.13
1:G:768:HIS:O	1:G:768:HIS:C	1.87	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: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
1:A:816:PHE:C	1:A:818:LYS:N	2.31	0.84
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:PHE:CE1	1:M:278:LEU:HD11	2.24	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
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
3:C:103:ARG:C	7:C:201:ACO:O4A	2.33	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:M:532:LEU:HG	1:M:551:ILE:HD11	1.83	0.60
1:A:843:GLU:O	1:A:847:SER:N	2.34	0.60
1:G:515:ALA:C	1:G:517:ALA:H	2.04	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
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
2:N:153:HIS:O	2:N:181:TYR:OH	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ALA:HB3	2:B:44:SER:O	2.03	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
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:M:561:TYR:O	1:M:565:ALA:N	2.33	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
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
2:N:163:HIS:O	2:N:165:TYR:N	2.39	0.55
1:G:250:ASP:O	1:G:251:LYS:C	2.44	0.55
1:A:324:PHE:CE2	2:B:2:PRO:HG2	2.41	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: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:G:470:VAL:CB	1:G:486:ALA:HB2	2.37	0.54
3:C:101:ASN:HD22	3:C:101:ASN:C	2.09	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:532:LEU:HD21	1:G:551:ILE:HG12	1.88	0.54
3:I:103:ARG:C	7:I:201:ACO:O1A	2.44	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
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: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
1:M:782:LYS:O	1:M:783:VAL:C	2.47	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
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
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:185:GLU:CD	1:M:185:GLU:CB	2.75	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:85:ALA:C	1:G:87:TYR:H	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:93:ILE:O	3:O:95:PHE:N	2.44	0.51
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
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:85:ALA:C	1:A:87:TYR:H	2.14	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: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:G:410:ASP:O	1:G:412:PRO:N	2.43	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:A:174:THR:O	1:A:178:VAL:N	2.44	0.50
3:I:36:PHE:N	3:I:36:PHE:C	2.64	0.50
1:A:815:LYS:N	1:A:816:PHE:HA	2.27	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:65:VAL:C	1:G:67:SER:H	2.15	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: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
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:M:193:LEU:O	1:M:195:GLN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:324:PHE:O	1:M:327:LEU:HG	2.11	0.49
1:M:286:PHE:O	1:M:287:LYS:C	2.50	0.49
1:A:781:LYS:HA	1:A:781:LYS:CE	2.41	0.49
1:A:754:THR:HA	1:A:759:PHE:CD2	2.48	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:G:404:HIS:C	1:G:406:LEU:H	2.16	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: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:321:PRO:O	1:G:322:PRO:C	2.52	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
1:G:250:ASP:O	1:G:252:PHE:N	2.45	0.48
1:A:510:PHE:O	1:A:514:GLN:N	2.47	0.48
3:I:158:ILE:O	3:I:165:GLU:HA	2.14	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
3:C:133:ALA:O	3:C:134:VAL:C	2.53	0.47
2:H:100:MET:HE3	2:H:147:ALA:HB2	1.95	0.47
1:M:410:ASP:O	1:M:412:PRO:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:29:MET:SD	2:B:29:MET:CB	2.97	0.47
1:M:690:ASP:O	1:M:693:GLY:N	2.48	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: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:G:274:VAL:O	1:G:278:LEU:N	2.48	0.46
1:M:224:TYR:C	1:M:226:ALA:H	2.17	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
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
1:G:31:TYR:HA	1:G:32:ASN:C	2.34	0.46
1:A:561:TYR:O	1:A:565:ALA:N	2.36	0.46
2:B:156:GLN:HA	2:B:157:SER:C	2.35	0.46
1:G:556:TRP:O	1:G:558:VAL:N	2.48	0.46
1:M:215:CYS:SG	1:M:215:CYS:C	2.94	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: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
1:M:580:GLU:C	1:M:582:ASP:H	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:31:LYS:O	2:N:34:MET:N	2.48	0.46
1:A:432:TYR:HD2	1:A:455:GLY:CA	2.29	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:M:575:PHE:O	1:M:579:PHE:N	2.49	0.46
1:A:286:PHE:O	1:A:287:LYS:C	2.54	0.46
3:C:98:VAL:HG22	7:C:201:ACO:CEP	2.45	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:H:36:HIS:CE1	2:H:99:LYS:HD3	2.50	0.46
1:M:210:TYR:CE1	1:M:214:GLU:OE1	2.69	0.46
1:M:480:ASP:C	1:M:482:ALA:H	2.19	0.46
1:A:236:ASN:O	1:A:240:HIS:N	2.39	0.45
1:G:344:VAL:O	1:G:345:LEU:C	2.54	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:134:THR:O	1:A:136:LYS:N	2.49	0.45
1:G:101:SER:O	1:G:102:PRO:C	2.55	0.45
1:G:189:ALA:O	1:G:192:THR:HG22	2.16	0.45
1:M:804:ASN:HA	1:M:805:SER:O	2.16	0.45
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:312:LEU:C	1:G:315:PHE:O	2.54	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
1:M:170:ARG:C	1:M:172:ASN:H	2.18	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: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:286:PHE:O	1:G:287:LYS:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:515:ALA:C	1:G:517:ALA:N	2.70	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
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:G:170:ARG:C	1:G:172:ASN:H	2.19	0.44
1:M:185:GLU:HG3	1:M:185:GLU:O	2.17	0.44
1:G:233:LYS:O	1:G:235:GLN:N	2.50	0.44
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
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
2:H:100:MET:CE	2:H:147:ALA:HB2	2.48	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
1:A:356:PHE:CD1	1:A:356:PHE:C	2.91	0.44
1:G:487:SER:O	1:G:490:THR:N	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:127:VAL:HG12	3:O:128:PHE:H	1.82	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: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:518:TYR:CB	1:G:565:ALA:HB2	2.48	0.43
1:A:828:TYR:HD1	1:A:828:TYR:O	2.01	0.43
1:A:463:ARG:HD2	1:A:489:PHE:CB	2.48	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:A:391:PRO:C	1:A:393:PRO:N	2.72	0.43
1:M:56:ALA:O	1:M:59:LYS:N	2.51	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
2:B:195:LYS:O	2:B:196:LEU:C	2.57	0.43
1:A:401:LEU:C	1:A:403:GLN:H	2.21	0.43
1:M:189:ALA:O	1:M:192:THR:HG22	2.18	0.43
1:A:405:PHE:O	1:A:414:ALA:HB2	2.19	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:G:115:THR:O	1:G:117:GLU:N	2.52	0.43
1:G:172:ASN:C	1:G:174:THR:H	2.22	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: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: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: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
1:M:233:LYS:HA	1:M:236:ASN:ND2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:TYR:C	1:A:524:ASP:H	2.23	0.42
1:G:514:GLN:OE1	1:G:568:ARG:NH1	2.53	0.42
1:A:321:PRO:O	1:A:322:PRO:C	2.57	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:391:PRO:C	1:G:393:PRO:N	2.73	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
1:M:125:PHE:O	1:M:126:THR:C	2.57	0.42
3:O:109:SER:HA	7:O:201:ACO:O2A	2.19	0.42
1:A:532:LEU:CD2	1:A:551:ILE:HG12	2.49	0.42
1:M:430:GLU:CD	1:M:430:GLU:O	2.58	0.42
1:M:463:ARG:HG3	1:M:489:PHE:CZ	2.53	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:101:SER:O	1:M:102:PRO:C	2.57	0.42
1:M:185:GLU:CG	1:M:185:GLU:OE1	2.57	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: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: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
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
3:C:93:ILE:O	3:C:94:GLU:C	2.58	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:M:800:GLU:O	1:M:802:SER:N	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:ARG:C	1:G:172:ASN:N	2.74	0.41
1:G:464:PHE:HD2	2:H:122:ARG:CB	2.34	0.41
2:N:179:SER:C	2:N:181:TYR:H	2.23	0.41
1:A:233:LYS:O	1:A:235:GLN:N	2.53	0.41
1:A:811:PHE:CD2	1:A:811:PHE:C	2.93	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:A:430:GLU:CD	1:A:430:GLU:O	2.58	0.41
1:G:282:ASN:O	1:G:282:ASN:ND2	2.54	0.41
1:A:561:TYR:O	1:A:564:LEU:N	2.54	0.41
2:B:40:TRP:CZ2	2:B:99:LYS:HB2	2.55	0.41
1:G:224:TYR:C	1:G:226:ALA:H	2.24	0.41
3:C:61:THR:HA	3:C:75:VAL:HA	2.03	0.41
1:G:811:PHE:CD2	1:G:811:PHE:C	2.93	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:76:TYR:C	1:A:78:VAL:H	2.23	0.41
1:A:521:LEU:O	1:A:561:TYR:HD2	2.03	0.41
2:B:159:ARG:O	2:B:160:ALA:C	2.59	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:269:LYS:C	1:A:271:ALA:H	2.23	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:M:316:TYR:HA	1:M:317:PRO:HD3	1.95	0.41
1:M:321:PRO:O	1:M:322:PRO:C	2.59	0.41
2:N:168:THR:OG1	2:N:169:LEU:N	2.54	0.41
1:A:101:SER:O	1:A:102:PRO:C	2.60	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:G:386:ASP:C	1:G:388:THR:H	2.24	0.40
1:G:561:TYR:O	1:G:564:LEU:N	2.53	0.40
1:G:711:TYR:C	1:G:713:ASN:H	2.24	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
2:B:179:SER:C	2:B:181:TYR:H	2.24	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:GLU:O	1:G:198:LYS:CB	2.68	0.40
1:G:826:PHE:O	1:G:828:TYR:O	2.38	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
3:I:117:ASP:O	3:I:119:CYS:N	2.54	0.40
1:M:391:PRO:C	1:M:393:PRO:N	2.75	0.40
2:B:31:LYS:O	2:B:33:TYR:N	2.55	0.40
2:H:12:ASP:O	2:H:16:MET:N	2.51	0.40
1:M:628:GLN:O	1:M:631:ASP:CB	2.69	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

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 8
1	G	754/854 (88%)	494 (66%)	179 (24%)	81 (11%)	0 8
1	M	753/854 (88%)	504 (67%)	173 (23%)	76 (10%)	0 9
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 6
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 4
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 8

Continued on next page...

Continued from previous page...

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 7

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	186/759 (24%)	142 (76%)	44 (24%)	1 5
1	G	189/759 (25%)	137 (72%)	52 (28%)	0 3
1	M	188/759 (25%)	155 (82%)	33 (18%)	2 12
2	B	51/216 (24%)	43 (84%)	8 (16%)	2 16
2	H	51/216 (24%)	38 (74%)	13 (26%)	0 4
2	N	51/216 (24%)	40 (78%)	11 (22%)	1 6
3	C	29/153 (19%)	22 (76%)	7 (24%)	0 4
3	I	28/153 (18%)	25 (89%)	3 (11%)	6 27
3	O	25/153 (16%)	24 (96%)	1 (4%)	31 57
All	All	798/3384 (24%)	626 (78%)	172 (22%)	1 6

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	77	SER
1	A	93	ARG
1	A	159	ARG
1	A	170	ARG
1	A	194	SER
1	A	196	PHE
1	A	224	TYR
1	A	236	ASN
1	A	252	PHE
1	A	254	LEU
1	A	262	TYR
1	A	270	ASP
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	464	PHE
1	A	506	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	ARG
1	A	522	TYR
1	A	532	LEU
1	A	559	ARG
1	A	578	GLN
1	A	581	ASP
1	A	585	ASP
1	A	615	TYR
1	A	626	TYR
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	811	PHE
1	A	815	LYS
1	A	826	PHE
1	A	828	TYR
2	B	22	HIS
2	B	35	TYR
2	B	40	TRP
2	B	100	MET
2	B	148	GLU
2	B	152	LEU
2	B	163	HIS
2	B	165	TYR
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	31	TYR
1	G	48	LYS
1	G	76	TYR
1	G	106	HIS
1	G	117	GLU
1	G	135	ASN
1	G	159	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	394	PHE
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	519	TYR
1	G	522	TYR
1	G	532	LEU
1	G	580	GLU
1	G	584	LEU
1	G	585	ASP
1	G	599	TYR
1	G	615	TYR
1	G	626	TYR
1	G	633	ARG
1	G	705	ASP
1	G	708	THR
1	G	728	ASP
1	G	733	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	826	PHE
1	G	828	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	95	TYR
2	H	117	SER
2	H	152	LEU
2	H	163	HIS
2	H	165	TYR
2	H	200	GLN
3	I	95	PHE
3	I	113	LYS
3	I	157	PHE
1	M	48	LYS
1	M	55	ASP
1	M	74	ASP
1	M	76	TYR
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	252	PHE
1	M	254	LEU
1	M	273	ILE
1	M	330	LEU
1	M	338	LYS
1	M	407	PHE
1	M	430	GLU
1	M	447	THR
1	M	464	PHE
1	M	489	PHE
1	M	522	TYR
1	M	532	LEU
1	M	599	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	615	TYR
1	M	626	TYR
1	M	628	GLN
1	M	633	ARG
1	M	710	PHE
1	M	726	ILE
1	M	808	TRP
1	M	826	PHE
1	M	828	TYR
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	95	TYR
2	N	153	HIS
2	N	165	TYR
2	N	192	LYS
3	O	95	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	404	HIS
1	G	188	GLN
1	G	503	HIS
1	M	135	ASN
1	M	220	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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	G	901	-	30,38,38	1.78	7 (23%)	42,61,61	2.29	14 (33%)
5	G4P	A	901	-	30,38,38	1.18	2 (6%)	42,61,61	1.40	7 (16%)
7	ACO	C	201	-	45,53,53	1.12	3 (6%)	56,79,79	1.74	10 (17%)
6	CMC	H	301	-	45,53,54	0.99	2 (4%)	55,78,80	1.50	7 (12%)
6	CMC	B	301	-	45,53,54	1.00	2 (4%)	55,78,80	1.50	8 (14%)
7	ACO	I	201	-	45,53,53	1.40	9 (20%)	56,79,79	2.04	19 (33%)
7	ACO	O	201	-	45,53,53	1.09	3 (6%)	56,79,79	1.43	6 (10%)
5	G4P	M	901	-	30,38,38	1.10	3 (10%)	42,61,61	1.50	7 (16%)
6	CMC	N	301	-	45,53,54	1.01	2 (4%)	55,78,80	1.53	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G4P	G	901	-	-	2/23/43/43	0/3/3/3
5	G4P	A	901	-	-	5/23/43/43	0/3/3/3
7	ACO	C	201	-	-	18/47/67/67	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CMC	H	301	-	-	4/46/67/68	0/3/3/3
6	CMC	B	301	-	-	3/46/67/68	0/3/3/3
7	ACO	I	201	-	-	22/47/67/67	0/3/3/3
7	ACO	O	201	-	-	15/47/67/67	0/3/3/3
5	G4P	M	901	-	-	5/23/43/43	0/3/3/3
6	CMC	N	301	-	-	3/46/67/68	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	901	G4P	PD-O1D	4.96	1.66	1.50
5	G	901	G4P	O3'-C3'	3.82	1.58	1.44
7	C	201	ACO	O4B-C1B	3.71	1.46	1.41
7	I	201	ACO	C5P-N4P	3.65	1.41	1.33
7	I	201	ACO	C5A-C4A	3.43	1.50	1.40
5	A	901	G4P	O4'-C1'	3.38	1.45	1.41
6	N	301	CMC	C9P-N8P	-3.29	1.26	1.33
6	B	301	CMC	C9P-N8P	-3.24	1.26	1.33
6	H	301	CMC	C9P-N8P	-3.23	1.26	1.33
5	G	901	G4P	O4'-C1'	3.13	1.45	1.41
6	N	301	CMC	C5P-N4P	-3.13	1.26	1.33
6	H	301	CMC	C5P-N4P	-3.11	1.26	1.33
6	B	301	CMC	C5P-N4P	-3.08	1.26	1.33
7	I	201	ACO	C4A-N3A	2.80	1.39	1.35
7	O	201	ACO	O4B-C1B	2.79	1.45	1.41
7	I	201	ACO	C2A-N3A	2.74	1.36	1.32
7	C	201	ACO	C2A-N3A	2.70	1.36	1.32
7	O	201	ACO	C2A-N3A	2.65	1.36	1.32
7	O	201	ACO	C5A-C4A	2.64	1.47	1.40
7	C	201	ACO	C5A-C4A	2.62	1.47	1.40
5	A	901	G4P	PC-O3'	2.61	1.67	1.60
5	M	901	G4P	O4'-C1'	2.55	1.44	1.41
5	M	901	G4P	PC-O3'	2.49	1.67	1.60
7	I	201	ACO	O5P-C5P	2.45	1.28	1.23
5	G	901	G4P	PB-O1B	2.43	1.58	1.50
7	I	201	ACO	P3B-O3B	2.37	1.63	1.59
5	G	901	G4P	PD-O3D	2.35	1.63	1.54
7	I	201	ACO	P3B-O7A	2.33	1.58	1.50
7	I	201	ACO	C6A-C5A	2.33	1.51	1.43
7	I	201	ACO	O4B-C1B	2.29	1.44	1.41
5	G	901	G4P	O6-C6	2.17	1.27	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	901	G4P	C5-C4	2.08	1.48	1.43
5	M	901	G4P	C5-C4	2.07	1.48	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	901	G4P	PC-O3C-PD	-7.13	108.38	132.83
7	I	201	ACO	CAP-C9P-N8P	5.43	127.39	116.58
7	C	201	ACO	P2A-O3A-P1A	-5.26	114.77	132.83
7	O	201	ACO	P2A-O3A-P1A	-4.78	116.42	132.83
6	B	301	CMC	C2P-S1P-C1	4.77	109.68	101.71
7	I	201	ACO	C6P-C7P-N8P	4.74	121.46	111.90
5	M	901	G4P	PA-O3A-PB	-4.73	116.58	132.83
5	G	901	G4P	O3D-PD-O2D	4.65	125.40	107.64
6	H	301	CMC	C2P-S1P-C1	4.62	109.43	101.71
5	G	901	G4P	O3C-PC-O3'	4.61	111.79	102.48
6	N	301	CMC	C2P-S1P-C1	4.47	109.19	101.71
7	I	201	ACO	N3A-C2A-N1A	-4.19	122.13	128.68
7	I	201	ACO	P2A-O3A-P1A	-4.01	119.07	132.83
6	H	301	CMC	N3A-C2A-N1A	-3.95	122.51	128.68
6	B	301	CMC	N3A-C2A-N1A	-3.94	122.52	128.68
6	N	301	CMC	N3A-C2A-N1A	-3.92	122.56	128.68
7	C	201	ACO	CAP-C9P-N8P	3.78	124.10	116.58
7	O	201	ACO	N3A-C2A-N1A	-3.74	122.84	128.68
5	G	901	G4P	PC-O3'-C3'	3.73	132.99	119.41
5	G	901	G4P	C5'-C4'-C3'	-3.70	102.14	114.40
7	I	201	ACO	O9P-C9P-N8P	-3.69	115.07	122.99
6	H	301	CMC	C2P-C3P-N4P	-3.66	104.72	112.42
6	B	301	CMC	P2A-O3A-P1A	-3.65	120.31	132.83
6	N	301	CMC	C2P-C3P-N4P	-3.64	104.77	112.42
5	G	901	G4P	O3D-PD-O1D	-3.62	96.51	110.68
7	C	201	ACO	N3A-C2A-N1A	-3.56	123.12	128.68
6	N	301	CMC	C6P-C7P-N8P	-3.55	104.72	111.90
6	H	301	CMC	C6P-C7P-N8P	-3.51	104.82	111.90
7	C	201	ACO	O9P-C9P-N8P	-3.49	115.50	122.99
7	I	201	ACO	O5P-C5P-C6P	-3.48	115.65	122.02
6	B	301	CMC	C2P-C3P-N4P	-3.44	105.19	112.42
6	N	301	CMC	P2A-O3A-P1A	-3.44	121.03	132.83
5	A	901	G4P	PA-O3A-PB	-3.41	121.11	132.83
5	G	901	G4P	O4'-C4'-C5'	3.39	120.54	109.37
6	B	301	CMC	C6P-C7P-N8P	-3.35	105.13	111.90
7	I	201	ACO	CEP-CBP-CAP	3.31	114.57	108.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	901	G4P	O3'-PC-O1C	-3.28	97.14	109.47
6	H	301	CMC	P2A-O3A-P1A	-3.26	121.64	132.83
7	C	201	ACO	C4A-C5A-N7A	-3.21	106.06	109.40
7	O	201	ACO	C4A-C5A-N7A	-3.13	106.14	109.40
5	M	901	G4P	PC-O3'-C3'	3.07	130.56	119.41
7	C	201	ACO	C6P-C7P-N8P	3.00	117.96	111.90
7	C	201	ACO	CDP-CBP-CAP	2.97	113.97	108.82
5	M	901	G4P	O3B-PB-O2B	2.91	118.76	107.64
5	G	901	G4P	PA-O3A-PB	-2.88	122.94	132.83
7	I	201	ACO	O6A-P2A-O4A	-2.88	97.82	109.07
7	I	201	ACO	OAP-CAP-CBP	-2.87	103.49	110.25
5	A	901	G4P	C5-C6-N1	2.86	119.01	113.95
5	A	901	G4P	O3D-PD-O2D	2.76	118.19	107.64
7	I	201	ACO	O5A-P2A-O4A	2.74	125.77	112.24
7	I	201	ACO	C2P-C3P-N4P	-2.72	106.71	112.42
6	H	301	CMC	C7P-N8P-C9P	2.71	127.42	122.59
7	C	201	ACO	C2P-C3P-N4P	-2.70	106.75	112.42
5	A	901	G4P	O3C-PC-O3'	2.62	107.77	102.48
6	B	301	CMC	C7P-N8P-C9P	2.61	127.24	122.59
7	C	201	ACO	O5A-P2A-O4A	2.61	125.13	112.24
5	G	901	G4P	O5'-C5'-C4'	2.59	117.92	108.99
6	B	301	CMC	C3P-N4P-C5P	2.57	127.61	122.84
5	G	901	G4P	O2C-PC-O3'	2.57	116.91	106.78
6	N	301	CMC	C7P-N8P-C9P	2.54	127.12	122.59
6	N	301	CMC	C3P-N4P-C5P	2.53	127.53	122.84
5	M	901	G4P	C8-N7-C5	2.51	107.78	102.99
7	O	201	ACO	C7P-C6P-C5P	2.48	116.49	112.36
7	O	201	ACO	C7P-N8P-C9P	2.44	126.94	122.59
5	G	901	G4P	O3'-C3'-C2'	-2.44	102.84	111.68
6	H	301	CMC	C3P-N4P-C5P	2.40	127.29	122.84
7	I	201	ACO	CEP-CBP-CCP	2.38	112.11	108.23
7	I	201	ACO	C3B-C2B-C1B	2.34	105.08	99.89
5	M	901	G4P	PC-O3C-PD	-2.29	124.98	132.83
7	I	201	ACO	C2P-S1P-C	2.25	113.53	101.68
5	G	901	G4P	C8-N7-C5	2.25	107.27	102.99
5	A	901	G4P	O4'-C1'-C2'	-2.22	103.69	106.93
5	A	901	G4P	O3B-PB-O2B	2.20	116.03	107.64
5	M	901	G4P	C5-C6-N1	2.20	117.83	113.95
6	N	301	CMC	C3B-C2B-C1B	2.17	104.70	99.89
6	N	301	CMC	O6A-CCP-CBP	-2.16	107.07	110.55
7	O	201	ACO	N6A-C6A-N1A	2.15	123.05	118.57
6	B	301	CMC	C3B-C2B-C1B	2.14	104.62	99.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	201	ACO	O4B-C4B-C3B	2.11	109.40	104.87
7	I	201	ACO	O5P-C5P-N4P	2.11	127.00	123.01
5	A	901	G4P	PC-O3C-PD	-2.10	125.61	132.83
7	I	201	ACO	C2A-N1A-C6A	2.08	122.31	118.75
7	I	201	ACO	O2B-C2B-C3B	2.06	117.00	111.17
5	M	901	G4P	O4'-C1'-C2'	-2.04	103.94	106.93
7	I	201	ACO	CEP-CBP-CDP	-2.03	105.03	109.17
7	C	201	ACO	O2A-P1A-O1A	2.03	122.25	112.24
5	G	901	G4P	O2A-PA-O1A	2.02	122.22	112.24

There are no chirality outliers.

All (77) 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	M	901	G4P	C2'-C3'-O3'-PC
6	B	301	CMC	C5B-O5B-P1A-O1A
6	B	301	CMC	C5B-O5B-P1A-O2A
6	N	301	CMC	C5B-O5B-P1A-O1A
6	N	301	CMC	C5B-O5B-P1A-O2A
7	C	201	ACO	C5B-O5B-P1A-O2A
7	C	201	ACO	C5B-O5B-P1A-O3A
7	C	201	ACO	N8P-C9P-CAP-OAP
7	C	201	ACO	CAP-C9P-N8P-C7P
7	C	201	ACO	C3P-C2P-S1P-C
7	C	201	ACO	O-C-S1P-C2P
7	C	201	ACO	CH3-C-S1P-C2P
7	I	201	ACO	C3B-O3B-P3B-O9A
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

Continued on next page...

Continued from previous page...

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	CCP-O6A-P2A-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	C4'-C3'-O3'-PC
7	I	201	ACO	C2B-C3B-O3B-P3B
5	A	901	G4P	C4'-C5'-O5'-PA
7	C	201	ACO	O9P-C9P-CAP-OAP
7	I	201	ACO	OAP-CAP-CBP-CEP
5	G	901	G4P	C4'-C5'-O5'-PA
5	M	901	G4P	C4'-C5'-O5'-PA
6	H	301	CMC	P1A-O3A-P2A-O4A
7	C	201	ACO	C5B-O5B-P1A-O1A
7	O	201	ACO	C5B-O5B-P1A-O2A
7	O	201	ACO	CCP-O6A-P2A-O4A
7	O	201	ACO	CCP-O6A-P2A-O5A
7	I	201	ACO	O5P-C5P-C6P-C7P
7	C	201	ACO	C9P-CAP-CBP-CCP
7	I	201	ACO	N4P-C5P-C6P-C7P
7	I	201	ACO	OAP-CAP-CBP-CDP
5	M	901	G4P	C3'-C4'-C5'-O5'
7	C	201	ACO	S1P-C2P-C3P-N4P
7	C	201	ACO	N8P-C9P-CAP-CBP
6	H	301	CMC	O9P-C9P-CAP-OAP
5	M	901	G4P	O4'-C4'-C5'-O5'
7	C	201	ACO	C9P-CAP-CBP-CDP
7	C	201	ACO	C9P-CAP-CBP-CEP
6	B	301	CMC	C5B-O5B-P1A-O3A
6	N	301	CMC	C5B-O5B-P1A-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
6	H	301	CMC	C6P-C7P-N8P-C9P

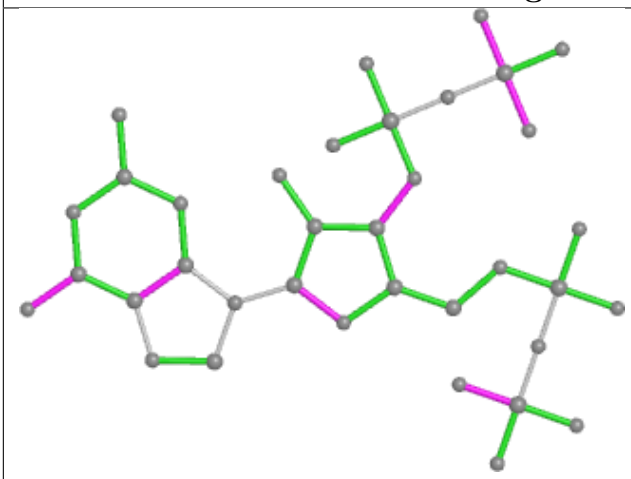
There are no ring outliers.

5 monomers are involved in 28 short contacts:

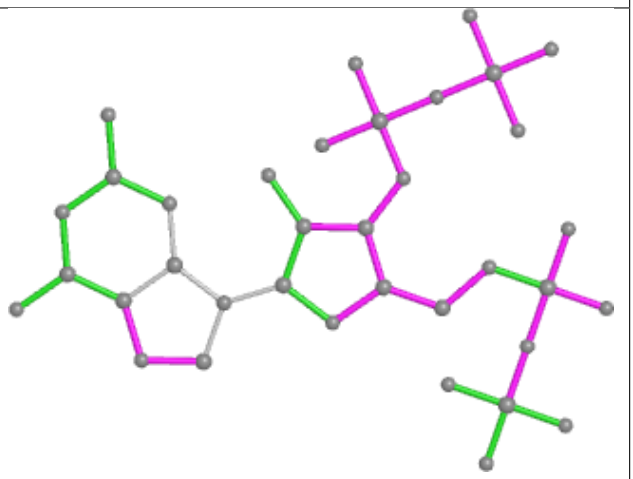
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	901	G4P	3	0
5	A	901	G4P	1	0
7	C	201	ACO	10	0
7	I	201	ACO	9	0
7	O	201	ACO	5	0

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

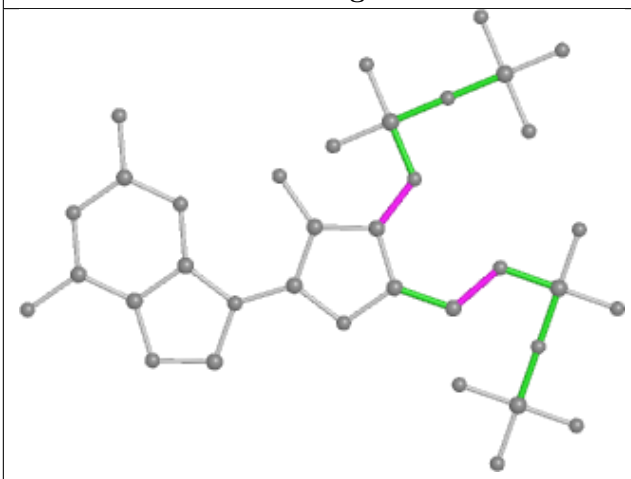
Ligand G4P G 901



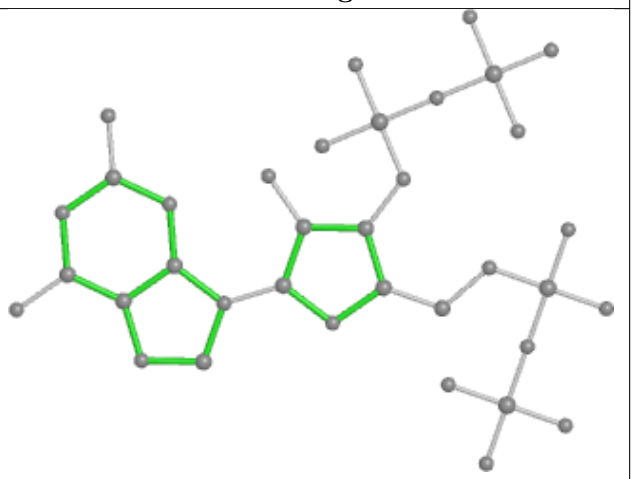
Bond lengths



Bond angles

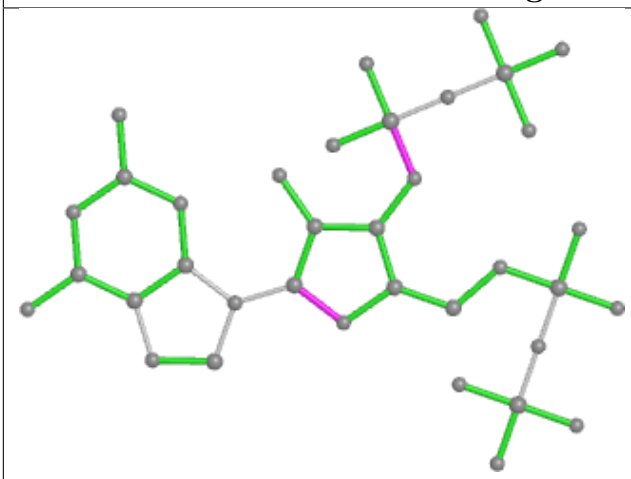


Torsions

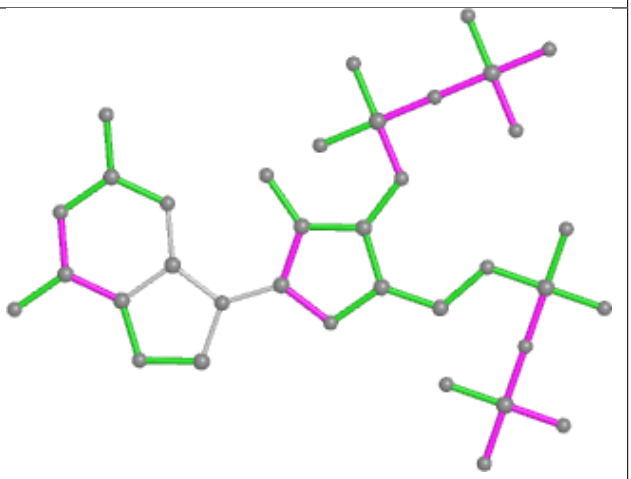


Rings

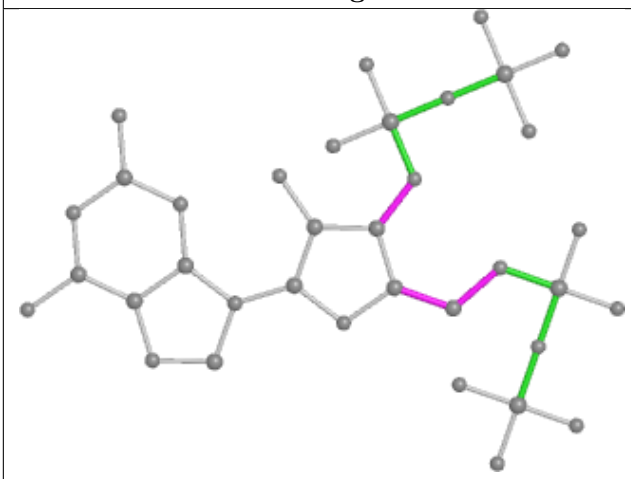
Ligand G4P A 901



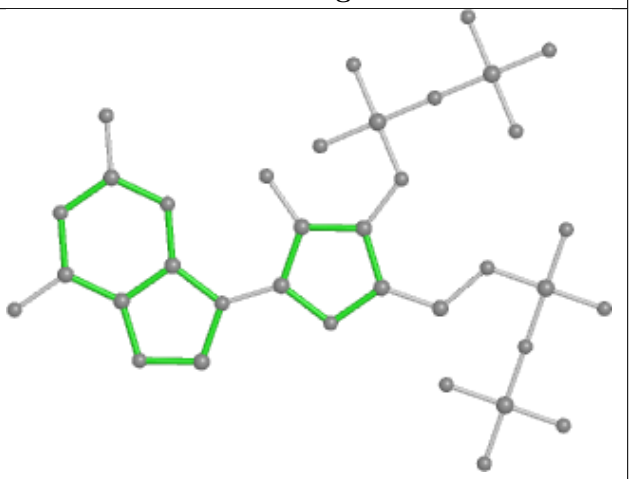
Bond lengths



Bond angles

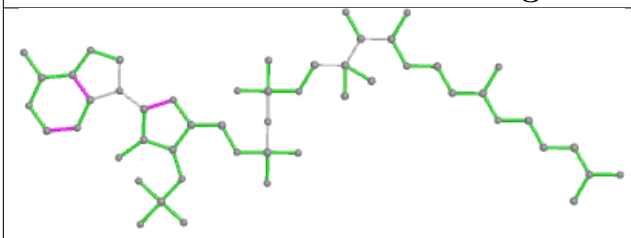


Torsions

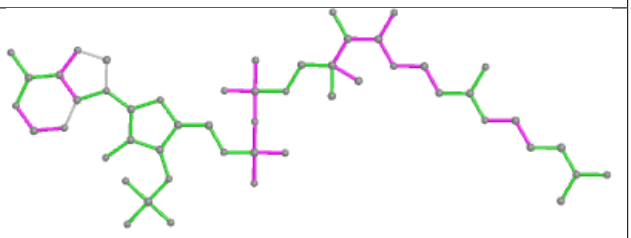


Rings

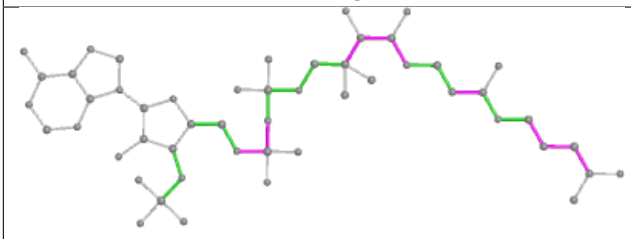
Ligand ACO C 201



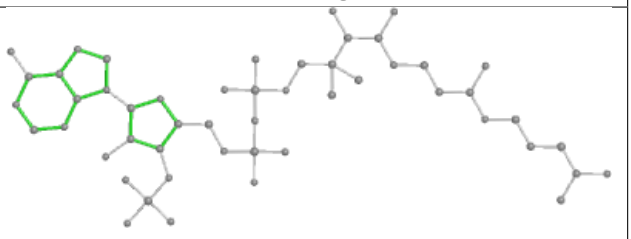
Bond lengths



Bond angles

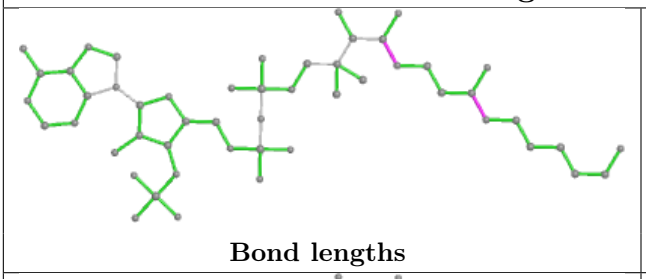


Torsions

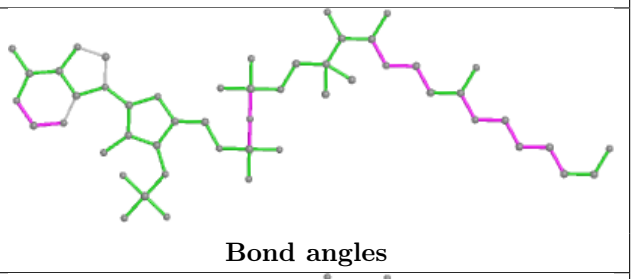


Rings

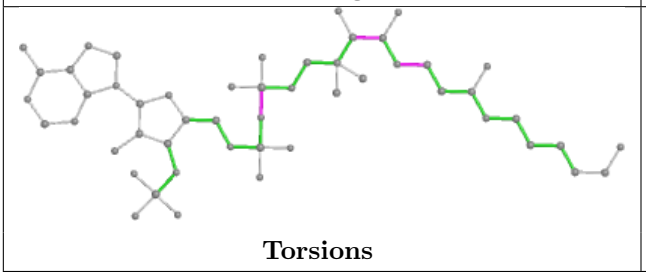
Ligand CMC H 301



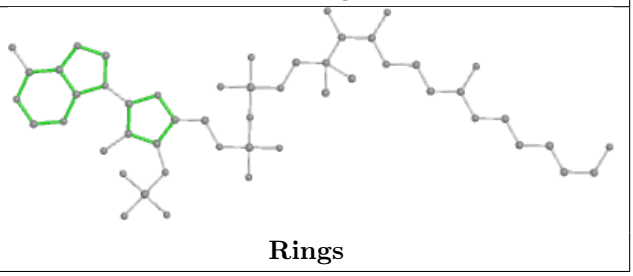
Bond lengths



Bond angles

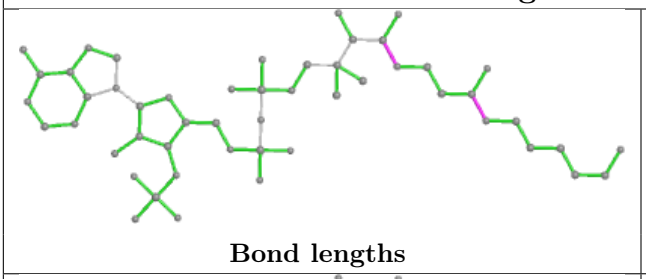


Torsions

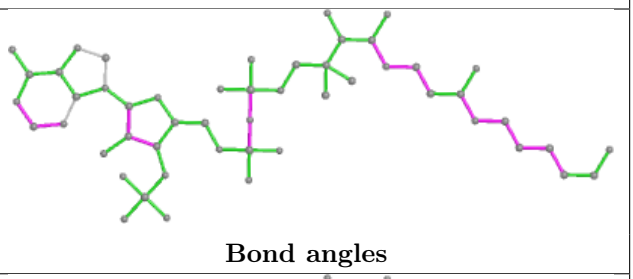


Rings

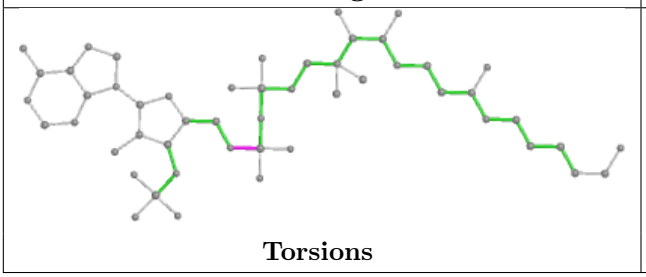
Ligand CMC B 301



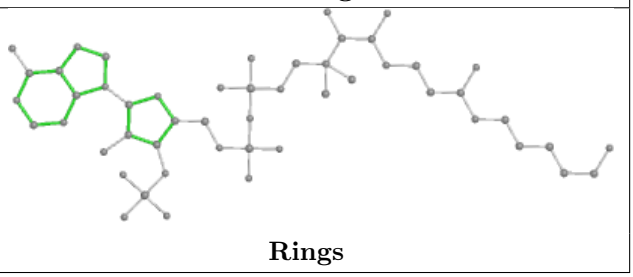
Bond lengths



Bond angles

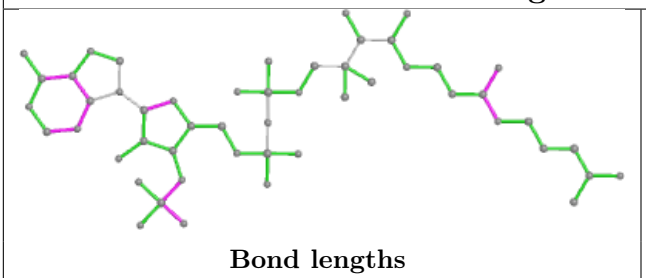


Torsions

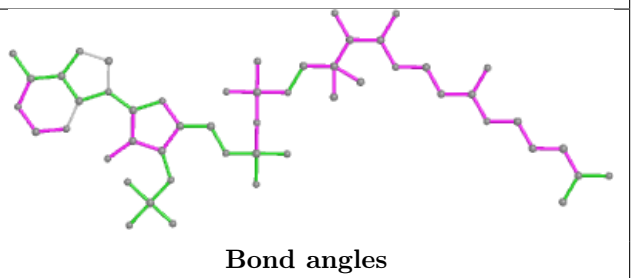


Rings

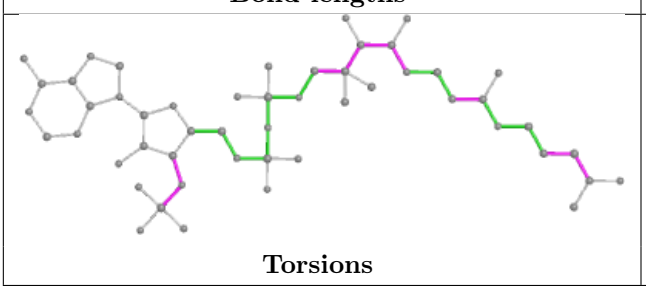
Ligand ACO I 201



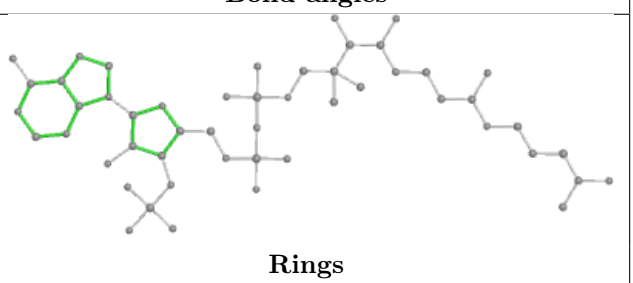
Bond lengths



Bond angles

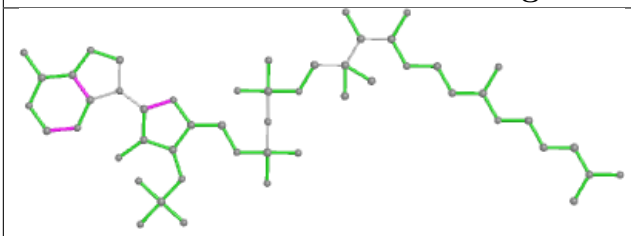


Torsions

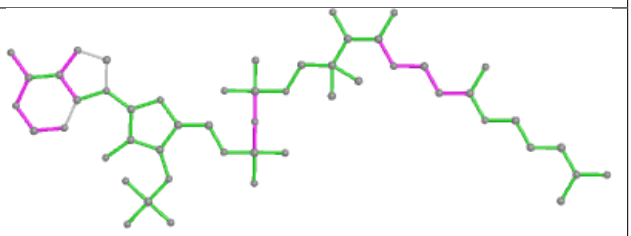


Rings

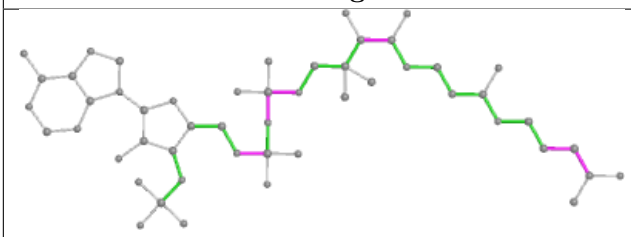
Ligand ACO O 201



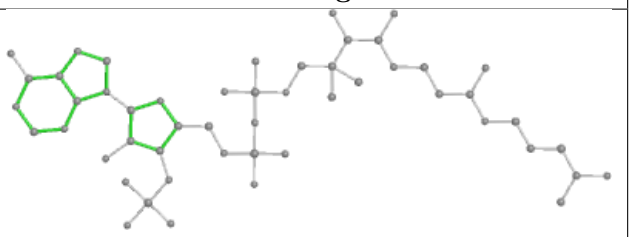
Bond lengths



Bond angles

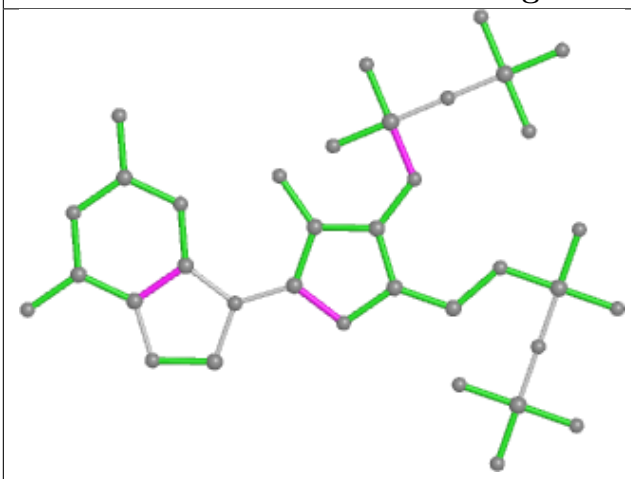


Torsions

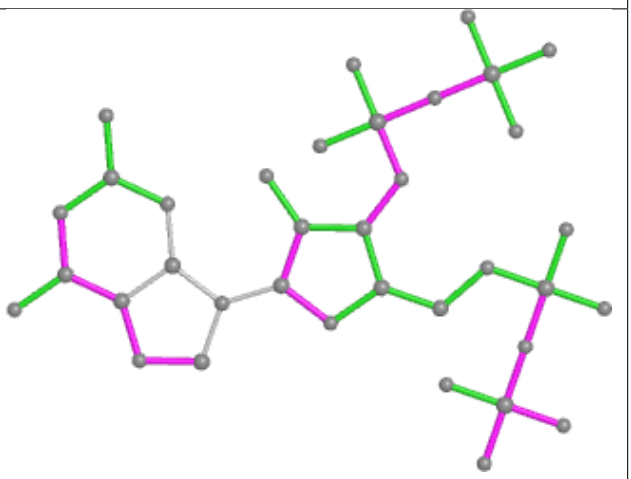


Rings

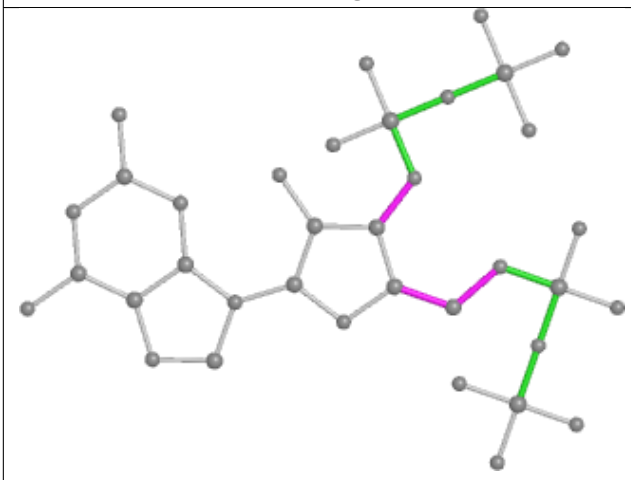
Ligand G4P M 901



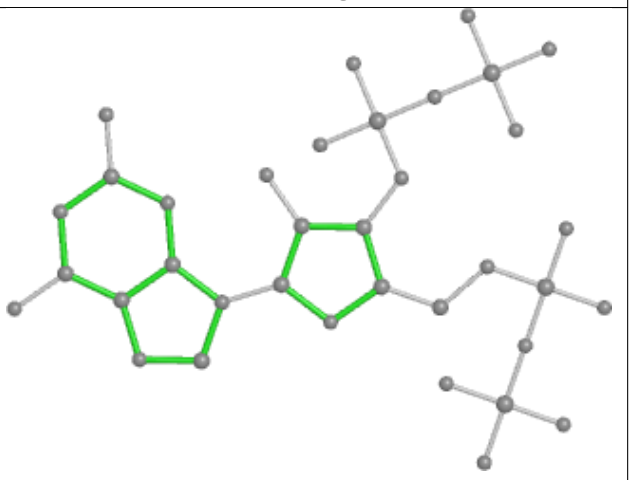
Bond lengths



Bond angles

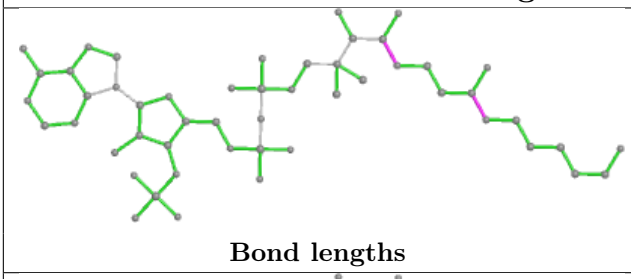


Torsions

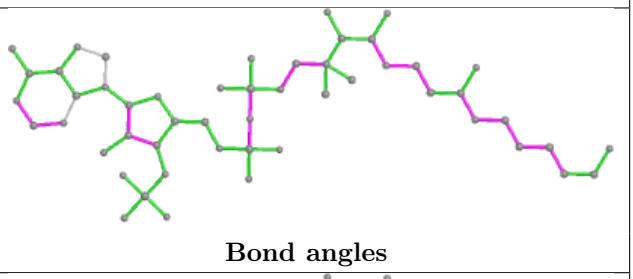


Rings

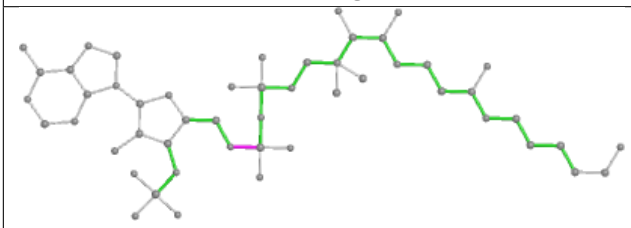
Ligand CMC N 301



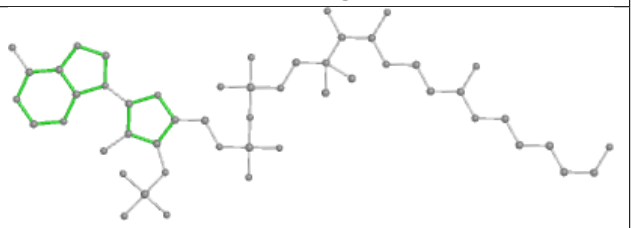
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.12	7 (0%) 84 77	83, 86, 91, 94	0
1	G	770/854 (90%)	-0.08	5 (0%) 89 84	73, 85, 88, 88	0
1	M	769/854 (90%)	-0.14	4 (0%) 91 85	84, 86, 90, 92	0
2	B	164/238 (68%)	-0.13	4 (2%) 59 49	48, 84, 86, 88	0
2	H	164/238 (68%)	-0.18	1 (0%) 89 84	84, 85, 86, 87	0
2	N	164/238 (68%)	-0.18	0 100 100	54, 86, 87, 88	0
3	C	156/176 (88%)	-0.01	1 (0%) 89 84	84, 86, 88, 88	2 (1%)
3	I	155/176 (88%)	0.01	0 100 100	85, 87, 89, 90	2 (1%)
3	O	154/176 (87%)	-0.06	0 100 100	86, 90, 93, 93	1 (0%)
4	E	6/8 (75%)	0.48	0 100 100	83, 83, 84, 84	0
4	K	6/8 (75%)	0.33	1 (16%) 1 2	84, 84, 85, 85	0
4	Q	6/8 (75%)	0.32	0 100 100	85, 85, 85, 85	0
All	All	3283/3828 (85%)	-0.11	23 (0%) 87 82	48, 86, 90, 94	5 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	GLU	4.0
1	G	775	PRO	3.5
1	A	64	HIS	3.1
1	G	384	GLY	2.9
1	M	732	ASN	2.9
4	K	6	HIS	2.9
2	H	183	ASP	2.8
3	C	174	HIS	2.8
1	G	64	HIS	2.7
1	M	96	GLU	2.5
1	A	674	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	183	ASP	2.4
1	A	63	SER	2.3
2	B	200	GLN	2.3
1	M	63	SER	2.3
2	B	166	ARG	2.2
1	M	384	GLY	2.2
1	A	673	LYS	2.2
1	G	96	GLU	2.2
1	A	319	CYS	2.2
2	B	148	GLU	2.1
1	A	384	GLY	2.1
1	G	319	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.