Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 12:37 PM EDT

PDB ID	:	6P63
Title	:	Wild-type NIS synthetase DesD bound to AMP and substrate analog cadaverine
Authors	:	Hoffmann, K.M.
Deposited on	:	2019-05-31
Resolution	:	2.40 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:

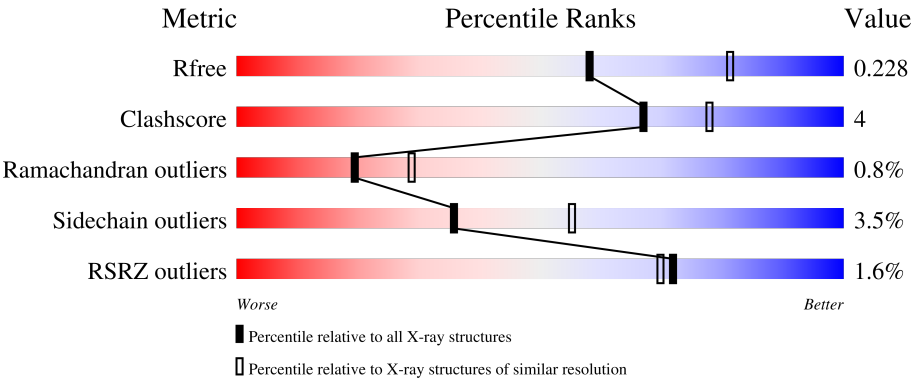
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	595	2% 85% 13%
1	B	595	% 88% 11%
1	C	595	2% 89% 10%
1	D	595	2% 87% 11%

2 Entry composition

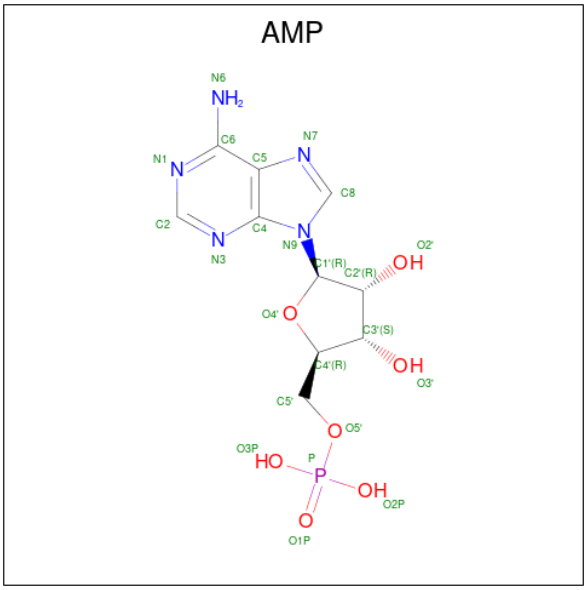
There are 5 unique types of molecules in this entry. The entry contains 38340 atoms, of which 18495 are hydrogens and 0 are deuteriums.

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 Siderophore Synthetase Type C DesD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	594	Total	C	H	N	O	S	183	0	0
			9291	2986	4598	813	879	15			
1	B	594	Total	C	H	N	O	S	183	0	0
			9291	2986	4598	813	879	15			
1	C	595	Total	C	H	N	O	S	183	0	0
			9310	2991	4609	814	880	16			
1	D	594	Total	C	H	N	O	S	183	1	0
			9311	2991	4610	816	879	15			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	4	0
			35	10	12	5	7	1		
2	B	1	Total	C	H	N	O	P	4	0
			35	10	12	5	7	1		

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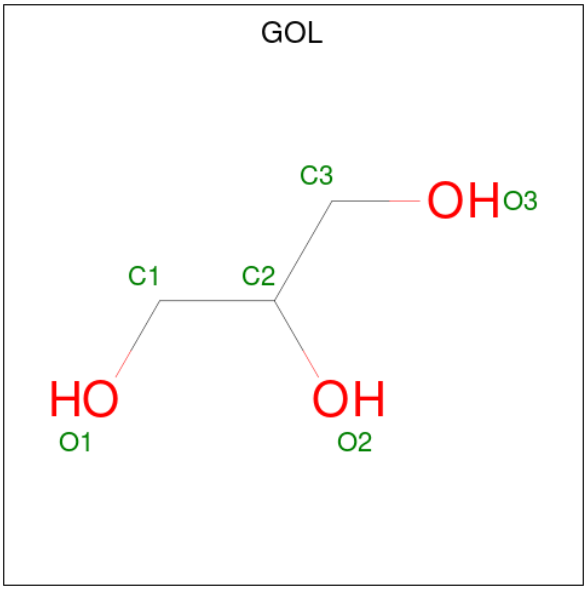
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C H N O P 35 10 12 5 7 1	4	0
2	D	1	Total C H N O P 35 10 12 5 7 1	4	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	2	0
4	B	1	Total C H O 14 3 8 3	2	0
4	C	1	Total C H O 14 3 8 3	2	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 is water.

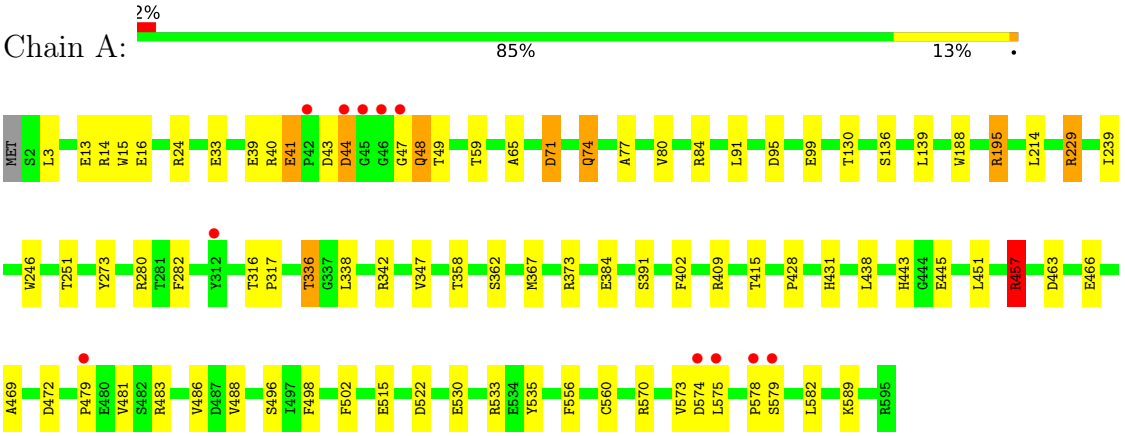
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total	O	0	0
			192	192		
5	B	283	Total	O	0	0
			283	283		
5	C	225	Total	O	0	0
			225	225		
5	D	237	Total	O	0	0
			237	237		

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.

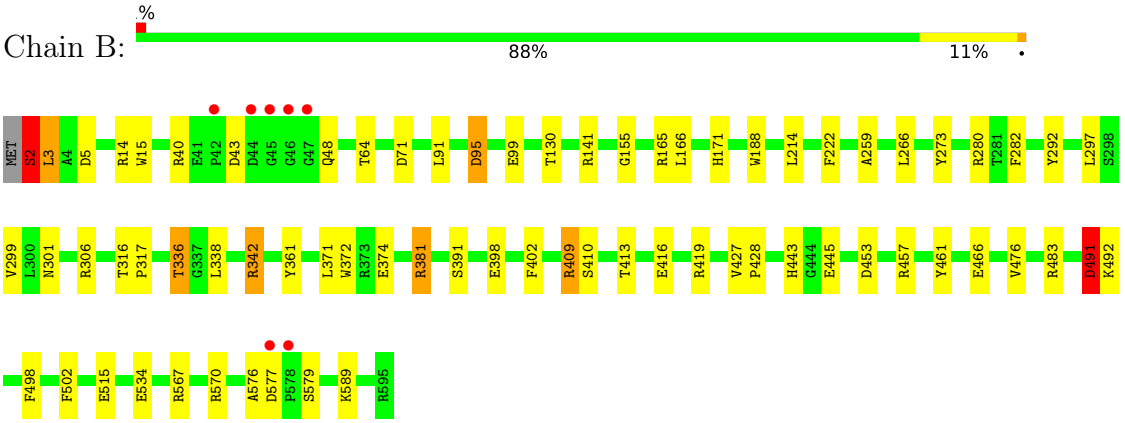
• Molecule 1: Siderophore Synthetase Type C DesD

Chain A:



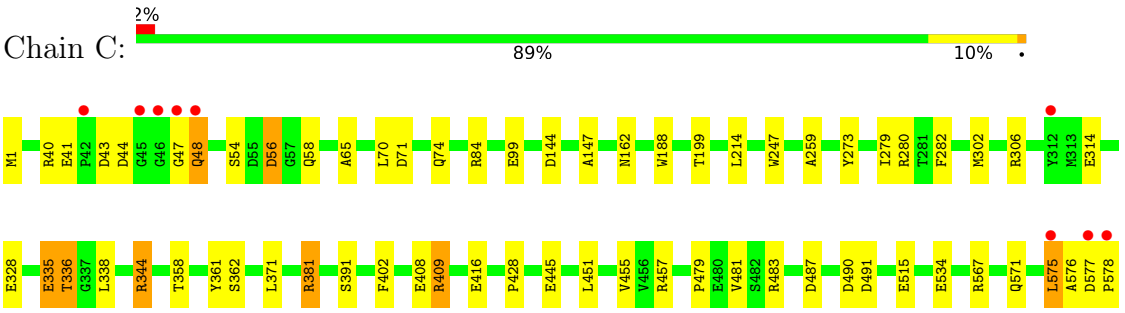
• Molecule 1: Siderophore Synthetase Type C DesD

Chain B:



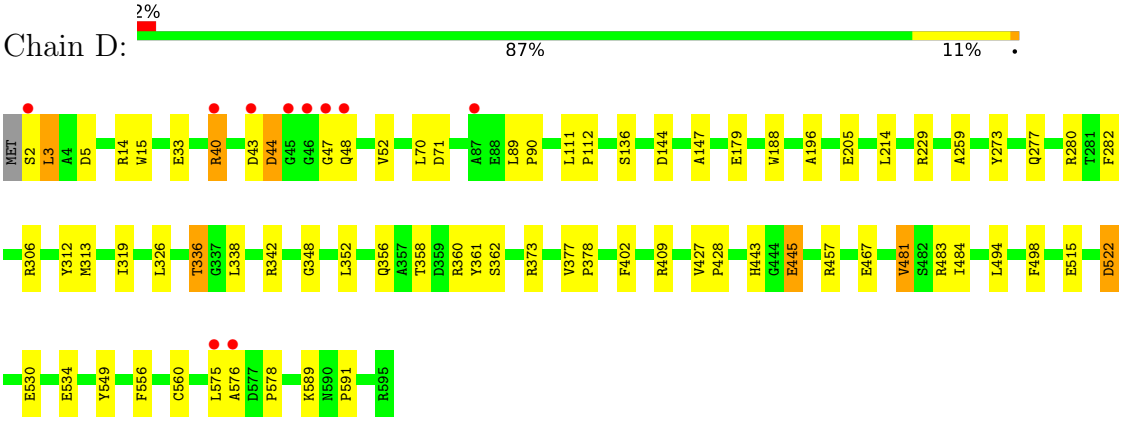
• Molecule 1: Siderophore Synthetase Type C DesD

Chain C:



• Molecule 1: Siderophore Synthetase Type C DesD

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.43Å 74.24Å 183.17Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	69.83 – 2.40 69.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (69.83-2.40) 95.9 (69.73-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.227 0.176 , 0.228	Depositor DCC
R_{free} test set	4971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	38340	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.73 % 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 4.6678e-05. 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: AMP, MG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.86	6/4808 (0.1%)	1.00	4/6544 (0.1%)
1	B	0.83	3/4808 (0.1%)	1.02	4/6544 (0.1%)
1	C	0.87	7/4816 (0.1%)	1.02	7/6554 (0.1%)
1	D	0.83	4/4819 (0.1%)	0.98	3/6558 (0.0%)
All	All	0.85	20/19251 (0.1%)	1.01	18/26200 (0.1%)

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	3
1	B	0	2
1	C	0	3
1	D	0	1
All	All	0	9

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	GLU	CD-OE1	8.02	1.34	1.25
1	A	445	GLU	CD-OE2	7.50	1.33	1.25
1	A	445	GLU	CD-OE1	7.01	1.33	1.25
1	C	416	GLU	CD-OE1	6.86	1.33	1.25
1	D	515	GLU	CD-OE1	6.32	1.32	1.25
1	C	534	GLU	CD-OE1	6.12	1.32	1.25
1	B	534	GLU	CD-OE1	6.05	1.32	1.25
1	C	71	ASP	CG-OD2	5.95	1.39	1.25
1	A	13	GLU	CD-OE2	5.76	1.31	1.25
1	B	466	GLU	CD-OE1	5.70	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	GLU	CD-OE1	5.58	1.31	1.25
1	C	335	GLU	CD-OE2	5.58	1.31	1.25
1	B	515	GLU	CD-OE1	5.52	1.31	1.25
1	A	515	GLU	CD-OE1	5.50	1.31	1.25
1	D	445	GLU	CD-OE1	5.44	1.31	1.25
1	A	16	GLU	CD-OE1	5.43	1.31	1.25
1	D	445	GLU	CD-OE2	5.42	1.31	1.25
1	C	515	GLU	CD-OE2	5.35	1.31	1.25
1	A	466	GLU	CD-OE1	5.25	1.31	1.25
1	C	416	GLU	CD-OE2	5.08	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	344	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	14	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	C	56	ASP	CB-CA-C	-7.21	95.98	110.40
1	B	306	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	595	ARG	CA-C-O	-6.61	106.23	120.10
1	C	381	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	461	TYR	CB-CG-CD1	6.10	124.66	121.00
1	A	457	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	595	ARG	CG-CD-NE	5.86	124.11	111.80
1	C	71	ASP	CB-CA-C	5.83	122.05	110.40
1	C	409	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	463	ASP	CB-CA-C	5.63	121.67	110.40
1	D	14	ARG	CG-CD-NE	-5.49	100.28	111.80
1	B	409	ARG	CB-CA-C	5.46	121.33	110.40
1	B	491	ASP	CB-CA-C	-5.45	99.50	110.40
1	A	463	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	71	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	14	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	GLU	Peptide
1	A	44	ASP	Peptide
1	A	47	GLY	Peptide
1	B	2	SER	Peptide
1	B	342	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	41	GLU	Peptide
1	C	47	GLY	Peptide
1	C	490	ASP	Peptide
1	D	3	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4693	4598	4579	42	0
1	B	4693	4598	4579	37	0
1	C	4701	4609	4591	31	0
1	D	4701	4610	4592	40	0
2	A	23	12	12	0	0
2	B	23	12	12	1	0
2	C	23	12	12	0	0
2	D	23	12	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	1	0
5	A	192	0	0	7	0
5	B	283	0	0	1	0
5	C	225	0	0	2	0
5	D	237	0	0	3	0
All	All	19845	18495	18421	146	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 4.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASP:OD1	5:A:701:HOH:O	1.85	0.93
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.39	0.88
1:B:336:THR:HG22	1:B:338:LEU:H	1.48	0.79
1:A:336:THR:HG22	1:A:338:LEU:H	1.48	0.78
1:C:344:ARG:HD3	5:C:776:HOH:O	1.83	0.77
1:C:336:THR:HG22	1:C:338:LEU:H	1.49	0.77
1:B:336:THR:HG21	1:B:428:PRO:HG3	1.66	0.77
1:C:336:THR:HG21	1:C:428:PRO:HG3	1.67	0.74
1:C:56:ASP:HB3	1:C:58:GLN:H	1.53	0.73
1:C:361:TYR:CZ	1:C:576:ALA:HB2	2.23	0.72
1:A:336:THR:HG21	1:A:428:PRO:HG3	1.75	0.68
1:B:371:LEU:C	1:B:371:LEU:HD12	2.16	0.66
1:A:74:GLN:NE2	5:A:703:HOH:O	2.31	0.63
1:B:336:THR:CG2	1:B:428:PRO:HG3	2.29	0.63
1:A:195:ARG:HD3	5:A:839:HOH:O	1.97	0.62
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.64	0.62
1:B:491:ASP:HB3	1:B:492:LYS:HG3	1.82	0.62
1:B:445:GLU:OE2	5:B:701:HOH:O	2.16	0.62
1:D:3:LEU:HD22	1:D:5:ASP:OD2	2.00	0.62
1:C:338:LEU:HD22	1:C:428:PRO:HB3	1.82	0.60
1:D:306:ARG:HD2	5:D:814:HOH:O	2.01	0.60
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.67	0.60
1:B:361:TYR:CZ	1:B:576:ALA:HB2	2.36	0.59
1:D:277:GLN:HG2	4:D:603:GOL:H31	1.83	0.59
1:D:33:GLU:OE1	1:D:560:CYS:HB3	2.01	0.59
1:D:361:TYR:CZ	1:D:576:ALA:HB2	2.38	0.59
1:A:457:ARG:HG2	1:A:457:ARG:NH1	2.11	0.59
1:C:40:ARG:CZ	1:C:48:GLN:OE1	2.51	0.58
1:A:391:SER:O	1:A:402:PHE:HB3	2.06	0.56
1:D:336:THR:CG2	1:D:428:PRO:HG3	2.35	0.56
1:A:15:TRP:HB2	1:C:259:ALA:HB1	1.86	0.56
1:D:336:THR:HG21	1:D:428:PRO:HG3	1.88	0.56
1:D:144:ASP:HB3	1:D:147:ALA:HB3	1.87	0.55
1:D:361:TYR:CE1	1:D:576:ALA:HB2	2.41	0.55
1:C:199:THR:HG21	1:C:314:GLU:O	2.06	0.55
1:A:336:THR:CG2	1:A:428:PRO:HG3	2.36	0.54
1:C:188:TRP:CE2	1:C:214:LEU:HD21	2.42	0.54
1:C:361:TYR:CZ	1:C:576:ALA:CB	2.91	0.54
1:C:273:TYR:HB3	1:C:282:PHE:HB3	1.90	0.54
1:C:361:TYR:CE1	1:C:576:ALA:HB2	2.43	0.54
1:D:481:VAL:O	1:D:484:ILE:HB	2.08	0.53
1:C:336:THR:CG2	1:C:428:PRO:HG3	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:LEU:C	1:C:371:LEU:HD12	2.29	0.53
1:A:239:ILE:HD12	1:A:347:VAL:HG13	1.89	0.53
1:D:336:THR:HG22	1:D:338:LEU:H	1.74	0.52
1:A:358:THR:HB	1:A:362:SER:HB2	1.92	0.52
1:D:427:VAL:N	1:D:428:PRO:CD	2.72	0.52
1:A:438:LEU:HA	1:A:469:ALA:O	2.11	0.51
1:B:48:GLN:HG3	1:B:64:THR:HB	1.92	0.51
1:D:273:TYR:HB3	1:D:282:PHE:HB3	1.92	0.51
1:D:358:THR:HB	1:D:362:SER:HB2	1.94	0.50
1:D:443:HIS:CE1	1:D:445:GLU:HB3	2.47	0.50
1:A:59:THR:OG1	1:A:84:ARG:NH1	2.38	0.49
1:B:95:ASP:O	1:B:99:GLU:HG3	2.13	0.49
1:A:384:GLU:HA	1:A:451:LEU:O	2.13	0.48
1:B:165:ARG:HD2	1:B:301:ASN:OD1	2.13	0.48
1:D:312:TYR:CE2	1:D:483[B]:ARG:CZ	2.96	0.48
1:D:530:GLU:O	1:D:534:GLU:HG3	2.13	0.48
1:D:326:LEU:C	1:D:326:LEU:HD23	2.34	0.48
1:B:259:ALA:HB1	1:D:15:TRP:HB2	1.95	0.48
1:A:80:VAL:HG12	1:A:91:LEU:HD21	1.95	0.47
1:B:14:ARG:CZ	1:B:130:THR:HG22	2.46	0.46
1:D:319:ILE:HD13	1:D:484:ILE:HD11	1.96	0.46
1:D:196:ALA:HA	1:D:348:GLY:O	2.15	0.46
1:B:171:HIS:N	1:B:171:HIS:ND1	2.64	0.46
1:B:292:TYR:O	1:B:372:TRP:HA	2.15	0.46
1:C:358:THR:HB	1:C:362:SER:HB2	1.98	0.46
1:D:494:LEU:HD22	1:D:549:TYR:HB3	1.98	0.46
1:A:336:THR:HG22	1:A:338:LEU:N	2.23	0.46
1:A:43:ASP:HB2	1:A:49:THR:HG21	1.97	0.46
1:B:2:SER:HB3	1:B:5:ASP:HB2	1.98	0.46
1:B:155:GLY:HA2	2:B:601:AMP:N7	2.30	0.45
1:B:413:THR:OG1	1:B:416:GLU:HG3	2.16	0.45
1:A:14:ARG:CZ	1:A:130:THR:HG22	2.47	0.45
1:A:367:MET:HB2	5:A:704:HOH:O	2.17	0.45
1:D:522:ASP:OD1	1:D:522:ASP:N	2.49	0.45
1:B:297:LEU:HG	1:B:299:VAL:HG13	1.97	0.45
1:A:316:THR:HB	1:A:317:PRO:HD3	1.98	0.45
1:A:486:VAL:HG23	1:A:488:VAL:HG23	1.98	0.45
1:D:188:TRP:CZ2	1:D:214:LEU:HD21	2.52	0.45
1:D:377:VAL:N	1:D:378:PRO:CD	2.81	0.44
1:D:2:SER:O	1:D:3:LEU:C	2.55	0.44
1:B:416:GLU:HG2	1:B:419:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:OG	1:C:56:ASP:HB2	2.17	0.44
1:A:24:ARG:HD3	1:A:77:ALA:HB2	1.99	0.44
1:C:70:LEU:HD21	1:C:591:PRO:HD3	2.00	0.44
1:A:373:ARG:HD2	5:A:809:HOH:O	2.18	0.44
1:B:2:SER:HB2	1:B:3:LEU:H	1.61	0.44
1:C:162:ASN:HA	1:C:302:MET:HG3	1.99	0.43
1:B:342:ARG:NH2	1:B:374:GLU:OE2	2.35	0.43
1:D:498:PHE:HB3	1:D:556:PHE:CE1	2.54	0.43
1:A:229:ARG:NH2	5:A:716:HOH:O	2.51	0.43
1:B:273:TYR:HB3	1:B:282:PHE:HB3	2.00	0.43
1:D:352:LEU:O	1:D:356:GLN:HG3	2.17	0.43
1:B:371:LEU:C	1:B:371:LEU:CD1	2.86	0.43
1:C:575:LEU:H	1:C:575:LEU:HD23	1.84	0.43
1:B:427:VAL:N	1:B:428:PRO:CD	2.81	0.43
1:A:3:LEU:HD23	1:C:247:TRP:CZ2	2.54	0.43
1:D:111:LEU:N	1:D:112:PRO:HD2	2.34	0.43
1:A:431:HIS:HA	1:A:535:TYR:OH	2.19	0.43
1:A:95:ASP:O	1:A:99:GLU:HG3	2.19	0.43
1:C:144:ASP:HB3	1:C:147:ALA:HB3	2.01	0.42
1:C:306:ARG:HA	1:C:306:ARG:HD3	1.77	0.42
1:C:451:LEU:HA	1:C:455:VAL:O	2.19	0.42
1:D:89:LEU:HB3	1:D:90:PRO:HD2	2.01	0.42
1:C:84:ARG:NH2	1:C:99:GLU:OE2	2.52	0.42
1:D:70:LEU:HD21	1:D:591:PRO:HD3	2.01	0.42
1:A:498:PHE:HB3	1:A:556:PHE:CE1	2.54	0.42
1:D:319:ILE:HD13	1:D:484:ILE:CD1	2.49	0.42
1:C:487:ASP:C	1:C:487:ASP:OD1	2.57	0.42
1:D:342:ARG:O	1:D:373:ARG:HA	2.19	0.42
1:C:577:ASP:CG	1:C:578:PRO:HD2	2.40	0.42
1:D:467:GLU:OE2	5:D:701:HOH:O	2.22	0.42
1:A:188:TRP:CZ2	1:A:214:LEU:HD21	2.54	0.42
1:A:530:GLU:OE2	5:A:702:HOH:O	2.22	0.42
1:B:361:TYR:CE1	1:B:576:ALA:HB2	2.55	0.42
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.73	0.42
1:D:483[B]:ARG:HG3	1:D:484:ILE:HD12	2.00	0.42
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.99	0.41
1:B:498:PHE:O	1:B:502:PHE:HB2	2.21	0.41
1:A:246:TRP:O	1:A:251:THR:HG23	2.20	0.41
1:A:136:SER:HB3	1:A:402:PHE:HA	2.02	0.41
1:A:358:THR:HB	1:A:362:SER:CB	2.51	0.41
1:C:445:GLU:OE2	5:C:701:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:PHE:O	1:A:502:PHE:HB2	2.20	0.41
1:C:65:ALA:HA	1:C:74:GLN:O	2.20	0.41
1:B:188:TRP:CE2	1:B:214:LEU:HD21	2.56	0.41
1:C:358:THR:HB	1:C:362:SER:CB	2.51	0.41
1:A:65:ALA:HA	1:A:74:GLN:O	2.21	0.41
1:B:391:SER:O	1:B:402:PHE:HB3	2.19	0.41
1:C:391:SER:O	1:C:402:PHE:HB3	2.20	0.41
1:D:136:SER:HB3	1:D:402:PHE:HA	2.02	0.41
1:D:313:MET:CE	1:D:313:MET:HA	2.51	0.41
1:A:33:GLU:OE1	1:A:560:CYS:HB3	2.21	0.40
1:A:273:TYR:HB3	1:A:282:PHE:HB3	2.02	0.40
1:A:498:PHE:HB3	1:A:556:PHE:CD1	2.56	0.40
1:A:573:VAL:HG13	1:A:578:PRO:HA	2.02	0.40
1:B:410:SER:HA	1:B:453:ASP:O	2.22	0.40
1:A:342:ARG:O	1:A:373:ARG:HA	2.20	0.40
1:B:222:PHE:CD1	1:B:266:LEU:HB3	2.56	0.40
1:B:316:THR:HB	1:B:317:PRO:HD3	2.03	0.40
1:B:15:TRP:HB2	1:D:259:ALA:HB1	2.03	0.40
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.75	0.40
1:B:381:ARG:HH11	1:B:381:ARG:CG	2.30	0.40
1:D:40:ARG:HH12	1:D:48:GLN:CB	2.34	0.40
1:D:409:ARG:NH1	5:D:726:HOH:O	2.54	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	592/595 (100%)	565 (95%)	21 (4%)	6 (1%)	15	23
1	B	592/595 (100%)	563 (95%)	25 (4%)	4 (1%)	22	32
1	C	593/595 (100%)	566 (95%)	21 (4%)	6 (1%)	15	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	593/595 (100%)	565 (95%)	25 (4%)	3 (0%)	29 41
All	All	2370/2380 (100%)	2259 (95%)	92 (4%)	19 (1%)	19 29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	LEU
1	A	579	SER
1	B	491	ASP
1	B	579	SER
1	C	44	ASP
1	C	491	ASP
1	A	44	ASP
1	A	48	GLN
1	B	3	LEU
1	B	43	ASP
1	C	43	ASP
1	D	44	ASP
1	C	48	GLN
1	C	579	SER
1	D	47	GLY
1	C	279	ILE
1	A	41	GLU
1	A	472	ASP
1	D	578	PRO

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	488/489 (100%)	466 (96%)	22 (4%)	27 44
1	B	488/489 (100%)	470 (96%)	18 (4%)	34 53
1	C	489/489 (100%)	475 (97%)	14 (3%)	42 62
1	D	489/489 (100%)	474 (97%)	15 (3%)	40 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1954/1956 (100%)	1885 (96%)	69 (4%)	36 55

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	GLU
1	A	48	GLN
1	A	71	ASP
1	A	74	GLN
1	A	139	LEU
1	A	195	ARG
1	A	229	ARG
1	A	280	ARG
1	A	336	THR
1	A	409	ARG
1	A	415	THR
1	A	443	HIS
1	A	457	ARG
1	A	479	PRO
1	A	481	VAL
1	A	483	ARG
1	A	496	SER
1	A	522	ASP
1	A	533	ARG
1	A	570	ARG
1	A	589	LYS
1	B	2	SER
1	B	40	ARG
1	B	71	ASP
1	B	95	ASP
1	B	280	ARG
1	B	336	THR
1	B	381	ARG
1	B	398	GLU
1	B	409	ARG
1	B	443	HIS
1	B	457	ARG
1	B	476	VAL
1	B	483	ARG
1	B	491	ASP
1	B	567	ARG

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Mol	Chain	Res	Type
1	B	570	ARG
1	B	577	ASP
1	B	589	LYS
1	C	1	MET
1	C	280	ARG
1	C	328	GLU
1	C	335	GLU
1	C	336	THR
1	C	381	ARG
1	C	409	ARG
1	C	457	ARG
1	C	479	PRO
1	C	481	VAL
1	C	483	ARG
1	C	567	ARG
1	C	571	GLN
1	C	575	LEU
1	D	40	ARG
1	D	43	ASP
1	D	44	ASP
1	D	52	VAL
1	D	71	ASP
1	D	205	GLU
1	D	229	ARG
1	D	280	ARG
1	D	336	THR
1	D	360	ARG
1	D	457	ARG
1	D	481	VAL
1	D	522	ASP
1	D	575	LEU
1	D	589	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	443	HIS

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)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	603	-	5,5,5	0.23	0	5,5,5	0.72	0
2	AMP	D	601	3	22,25,25	0.57	0	25,38,38	0.79	0
4	GOL	A	603	-	5,5,5	0.15	0	5,5,5	0.40	0
2	AMP	A	601	3	22,25,25	0.66	0	25,38,38	1.00	3 (12%)
4	GOL	D	603	-	5,5,5	0.07	0	5,5,5	0.30	0
2	AMP	B	601	3	22,25,25	0.63	0	25,38,38	0.87	1 (4%)
2	AMP	C	601	3	22,25,25	0.62	0	25,38,38	0.90	1 (4%)
4	GOL	C	603	-	5,5,5	0.15	0	5,5,5	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	603	-	-	2/4/4/4	-
2	AMP	D	601	3	-	2/6/26/26	0/3/3/3
4	GOL	A	603	-	-	2/4/4/4	-
2	AMP	A	601	3	-	2/6/26/26	0/3/3/3
4	GOL	D	603	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	B	601	3	-	2/6/26/26	0/3/3/3
2	AMP	C	601	3	-	2/6/26/26	0/3/3/3
4	GOL	C	603	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	AMP	C5-C6-N6	2.32	123.88	120.35
2	B	601	AMP	C5-C6-N6	2.19	123.68	120.35
2	A	601	AMP	C1'-N9-C4	2.04	130.23	126.64
2	C	601	AMP	C1'-N9-C4	2.03	130.21	126.64
2	A	601	AMP	O3'-C3'-C2'	2.02	118.36	111.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	AMP	O4'-C4'-C5'-O5'
2	D	601	AMP	O4'-C4'-C5'-O5'
2	A	601	AMP	O4'-C4'-C5'-O5'
2	A	601	AMP	C3'-C4'-C5'-O5'
2	C	601	AMP	O4'-C4'-C5'-O5'
2	C	601	AMP	C3'-C4'-C5'-O5'
2	B	601	AMP	C3'-C4'-C5'-O5'
2	D	601	AMP	C3'-C4'-C5'-O5'
4	A	603	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-O2
4	B	603	GOL	O1-C1-C2-O2

There are no ring outliers.

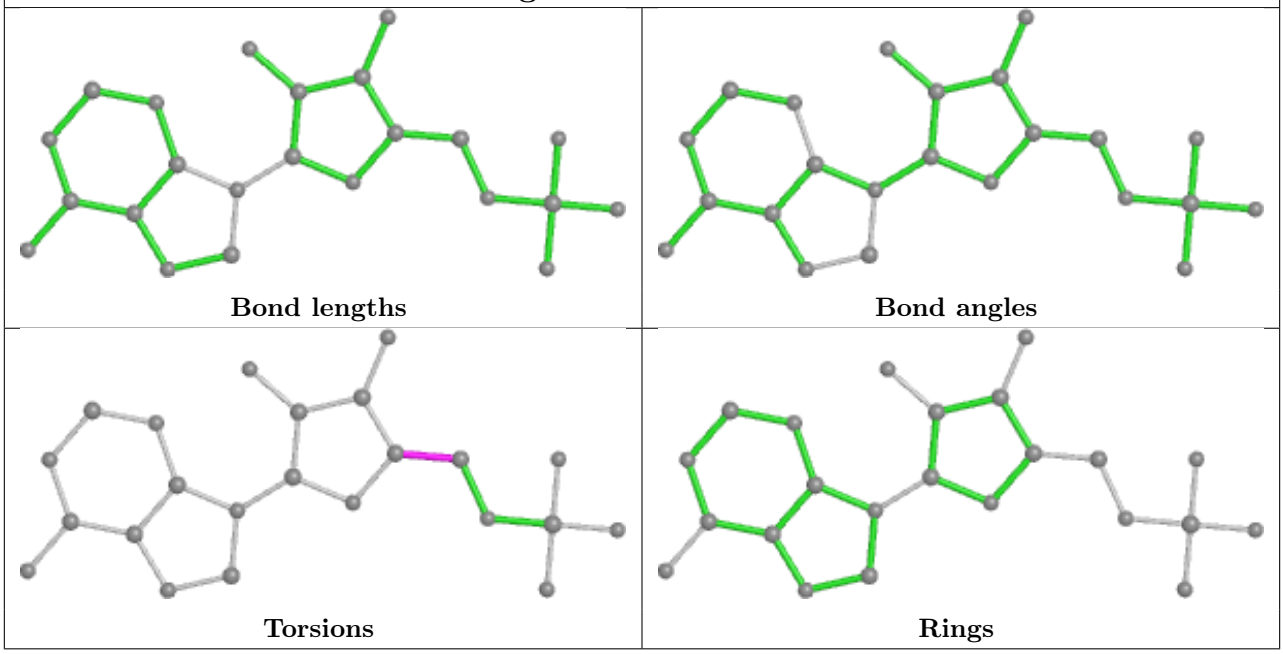
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	GOL	1	0
2	B	601	AMP	1	0

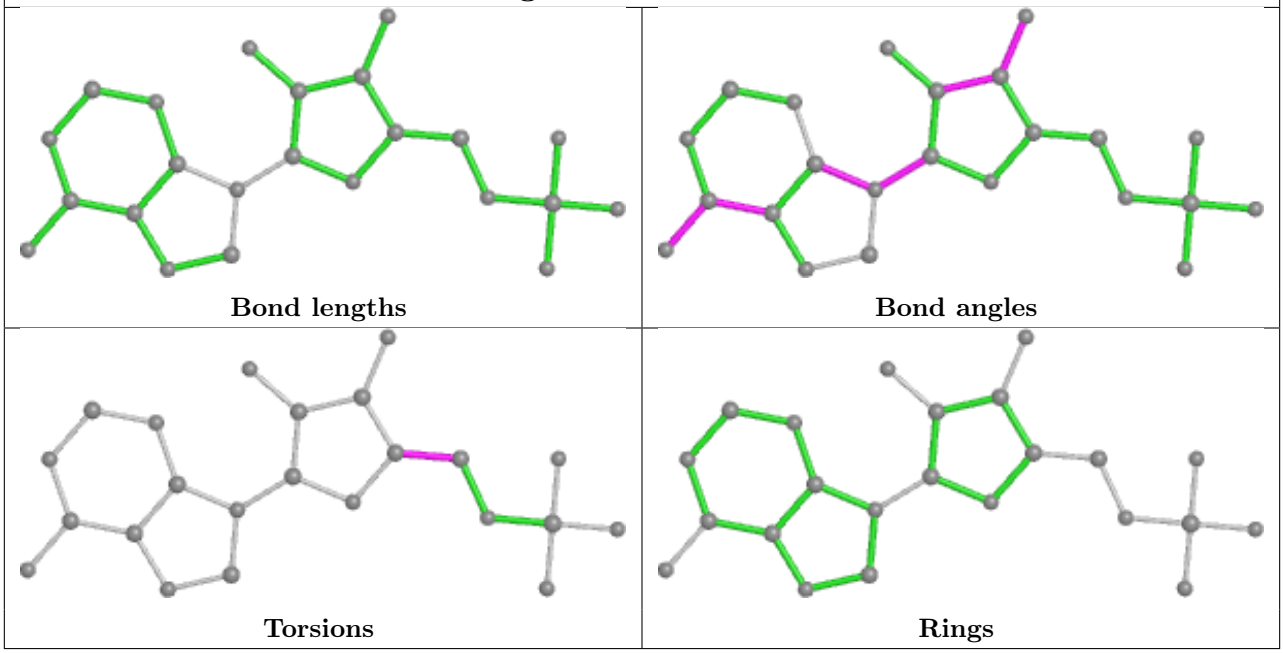
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

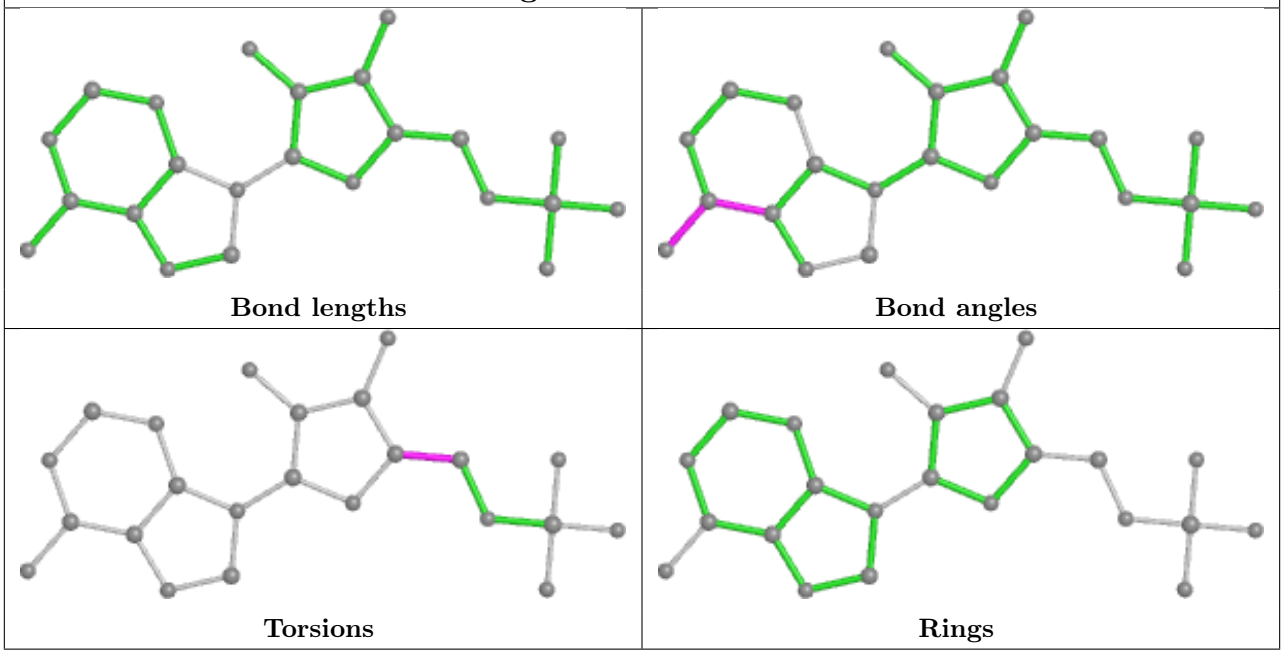
Ligand AMP D 601



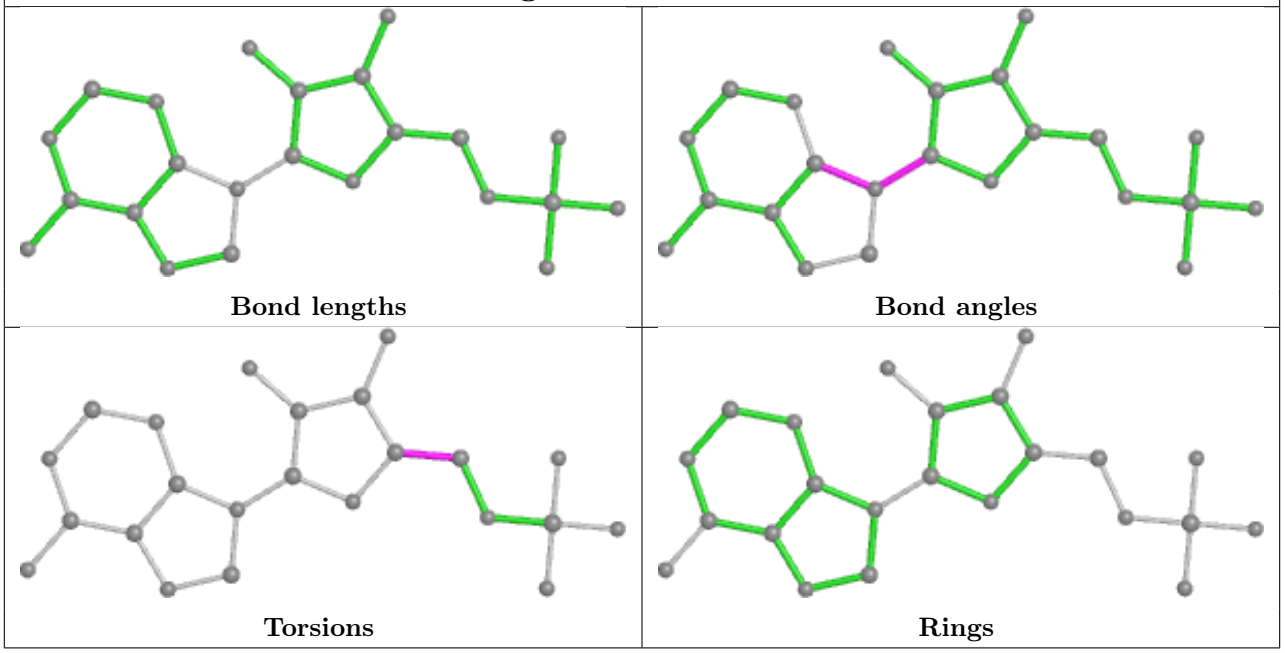
Ligand AMP A 601



Ligand AMP B 601



Ligand AMP C 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	594/595 (99%)	-0.20	11 (1%)	66 64	14, 25, 45, 93	0
1	B	594/595 (99%)	-0.27	7 (1%)	79 77	10, 19, 39, 83	0
1	C	595/595 (100%)	-0.27	10 (1%)	70 68	10, 20, 41, 83	0
1	D	594/595 (99%)	-0.23	10 (1%)	70 68	14, 23, 44, 93	0
All	All	2377/2380 (99%)	-0.24	38 (1%)	72 70	10, 22, 43, 93	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	PRO	7.6
1	A	46	GLY	6.6
1	C	46	GLY	6.3
1	B	46	GLY	6.2
1	D	45	GLY	5.7
1	B	578	PRO	5.4
1	A	579	SER	5.4
1	A	45	GLY	4.8
1	A	47	GLY	4.8
1	D	47	GLY	4.3
1	D	46	GLY	4.2
1	C	575	LEU	4.1
1	C	47	GLY	4.0
1	A	44	ASP	4.0
1	B	45	GLY	3.6
1	C	578	PRO	3.6
1	B	44	ASP	3.6
1	D	43	ASP	3.2
1	C	579	SER	3.2
1	C	42	PRO	3.2
1	B	47	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	577	ASP	2.9
1	D	48	GLN	2.9
1	A	578	PRO	2.8
1	D	575	LEU	2.8
1	A	575	LEU	2.7
1	D	576	ALA	2.7
1	D	2	SER	2.6
1	D	40	ARG	2.6
1	A	479	PRO	2.6
1	A	574	ASP	2.4
1	A	312	TYR	2.4
1	B	42	PRO	2.4
1	B	577	ASP	2.4
1	C	48	GLN	2.4
1	C	45	GLY	2.4
1	C	312	TYR	2.2
1	D	87	ALA	2.1

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)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	603	6/6	0.84	0.13	35,38,39,39	2
3	MG	A	602	1/1	0.88	0.17	36,36,36,36	0
4	GOL	B	603	6/6	0.88	0.20	23,25,30,30	2
3	MG	C	602	1/1	0.91	0.13	29,29,29,29	0
3	MG	B	602	1/1	0.93	0.10	27,27,27,27	0
2	AMP	D	601	23/23	0.95	0.14	20,23,27,28	4

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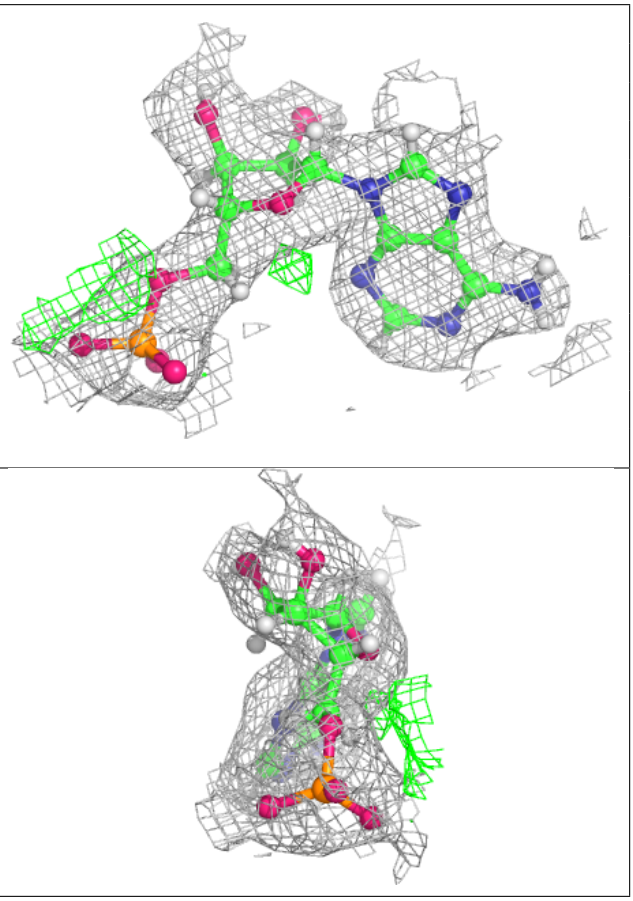
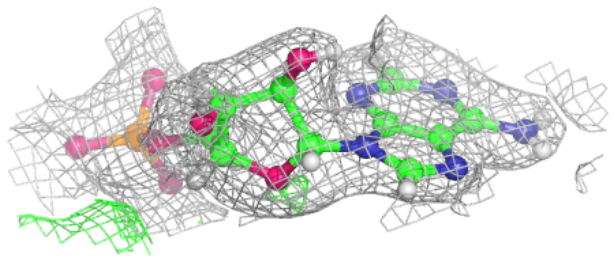
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	602	1/1	0.95	0.13	29,29,29,29	0
2	AMP	B	601	23/23	0.96	0.13	19,22,29,32	4
2	AMP	A	601	23/23	0.96	0.13	21,24,30,31	4
4	GOL	C	603	6/6	0.96	0.17	18,18,20,20	2
2	AMP	C	601	23/23	0.97	0.13	20,22,25,25	4
4	GOL	D	603	6/6	0.97	0.18	29,29,30,30	2

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 AMP D 601:

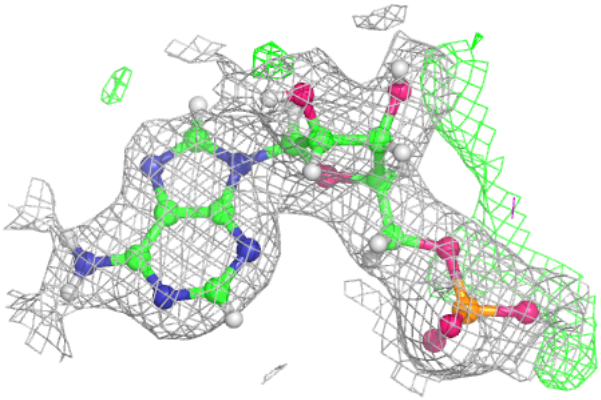
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

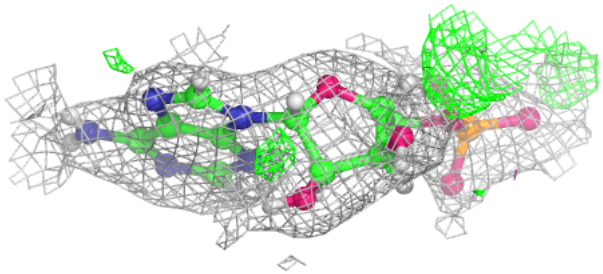


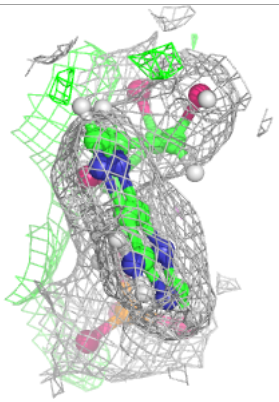


Electron density around AMP B 601:

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

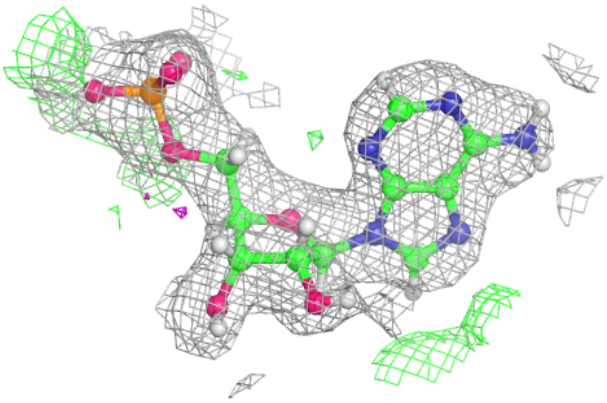


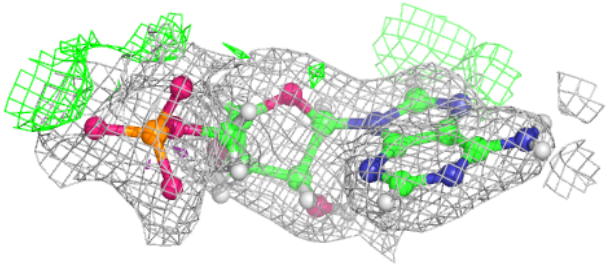


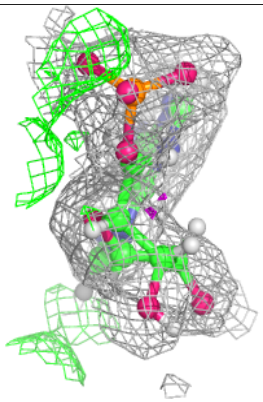


Electron density around AMP A 601:

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

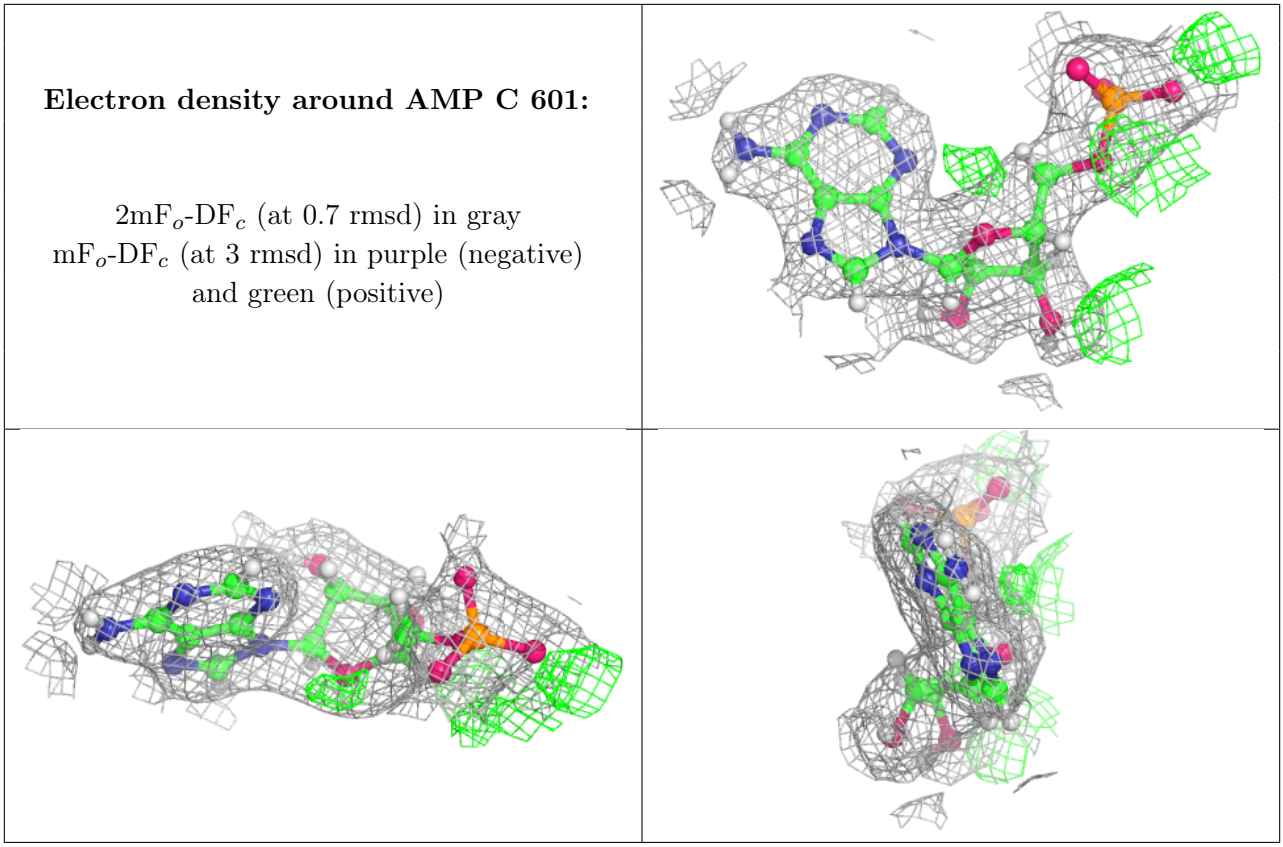






Electron density around AMP C 601:

$2mF_o$-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

There are no such residues in this entry.