Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 09:16 PM EDT

PDB ID	:	4NNJ
Title	:	Crystal structure of Uba1 in complex with ubiquitin-AMP and thioesterified ubiquitin
Authors	:	Schaefer, A.; Schindelin, H.
Deposited on	:	2013-11-18
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 (i) 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 (i)) were used in the production of this report:

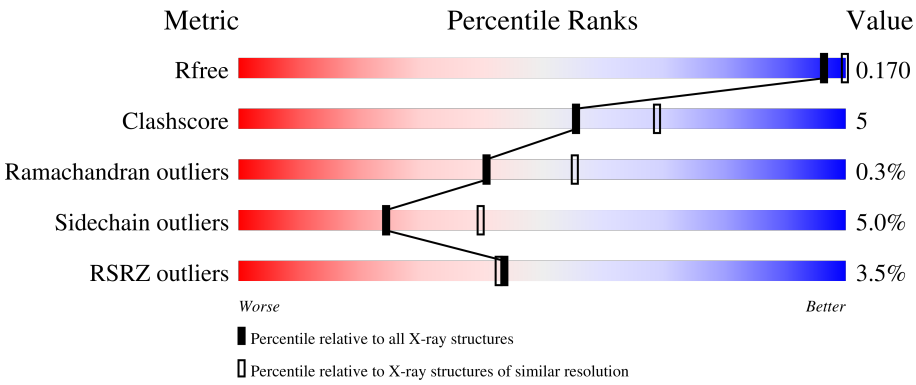
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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	1040	3%, 86%, 9%
1	C	1040	3%, 85%, 10%
2	B	79	4%, 87%, 9%
2	D	79	80%, 14%
2	E	79	22%, 65%, 28%, 5%

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
4	GOL	C	1104[A]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36909 atoms, of which 17908 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1006	15830	5070	7873	1315	1548	24	1	2	0
1	C	1006	15807	5062	7863	1312	1547	23	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP P22515
A	-14	GLY	-	expression tag	UNP P22515
A	-13	SER	-	expression tag	UNP P22515
A	-12	SER	-	expression tag	UNP P22515
A	-11	HIS	-	expression tag	UNP P22515
A	-10	HIS	-	expression tag	UNP P22515
A	-9	HIS	-	expression tag	UNP P22515
A	-8	HIS	-	expression tag	UNP P22515
A	-7	HIS	-	expression tag	UNP P22515
A	-6	HIS	-	expression tag	UNP P22515
A	-5	SER	-	expression tag	UNP P22515
A	-4	SER	-	expression tag	UNP P22515
A	-3	GLY	-	expression tag	UNP P22515
A	-2	GLU	-	expression tag	UNP P22515
A	-1	ASN	-	expression tag	UNP P22515
A	0	LEU	-	expression tag	UNP P22515
A	1	TYR	-	expression tag	UNP P22515
A	2	PHE	-	expression tag	UNP P22515
A	3	GLN	-	expression tag	UNP P22515
A	4	GLY	-	expression tag	UNP P22515
A	5	SER	-	expression tag	UNP P22515
A	6	HIS	-	expression tag	UNP P22515
A	7	MET	-	expression tag	UNP P22515
A	8	ALA	-	expression tag	UNP P22515
C	-15	MET	-	expression tag	UNP P22515

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLY	-	expression tag	UNP P22515
C	-13	SER	-	expression tag	UNP P22515
C	-12	SER	-	expression tag	UNP P22515
C	-11	HIS	-	expression tag	UNP P22515
C	-10	HIS	-	expression tag	UNP P22515
C	-9	HIS	-	expression tag	UNP P22515
C	-8	HIS	-	expression tag	UNP P22515
C	-7	HIS	-	expression tag	UNP P22515
C	-6	HIS	-	expression tag	UNP P22515
C	-5	SER	-	expression tag	UNP P22515
C	-4	SER	-	expression tag	UNP P22515
C	-3	GLY	-	expression tag	UNP P22515
C	-2	GLU	-	expression tag	UNP P22515
C	-1	ASN	-	expression tag	UNP P22515
C	0	LEU	-	expression tag	UNP P22515
C	1	TYR	-	expression tag	UNP P22515
C	2	PHE	-	expression tag	UNP P22515
C	3	GLN	-	expression tag	UNP P22515
C	4	GLY	-	expression tag	UNP P22515
C	5	SER	-	expression tag	UNP P22515
C	6	HIS	-	expression tag	UNP P22515
C	7	MET	-	expression tag	UNP P22515
C	8	ALA	-	expression tag	UNP P22515

- Molecule 2 is a protein called Uba1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	78	1243	381	633	107	121	1	0	0	0
			Total	C	H	N	O	S			
2	D	77	1252	383	639	109	120	1	0	1	0
			Total	C	H	N	O	S			
2	E	77	1234	378	629	106	120	1	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P0CG63
B	-1	ALA	-	expression tag	UNP P0CG63
B	0	ALA	-	expression tag	UNP P0CG63
D	-2	SER	-	expression tag	UNP P0CG63
D	-1	ALA	-	expression tag	UNP P0CG63

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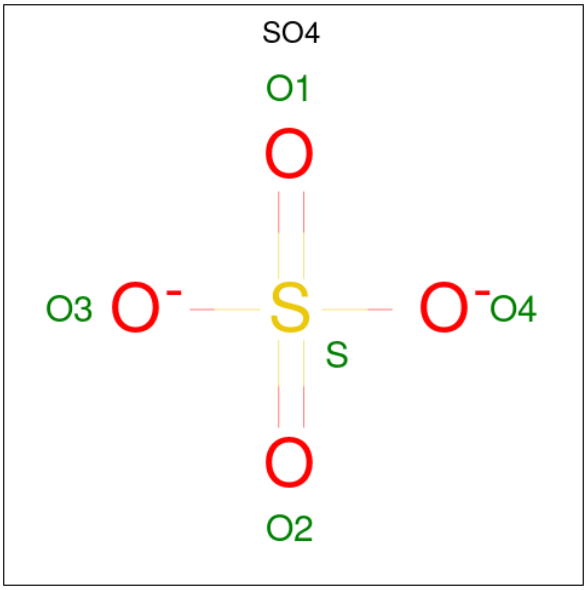
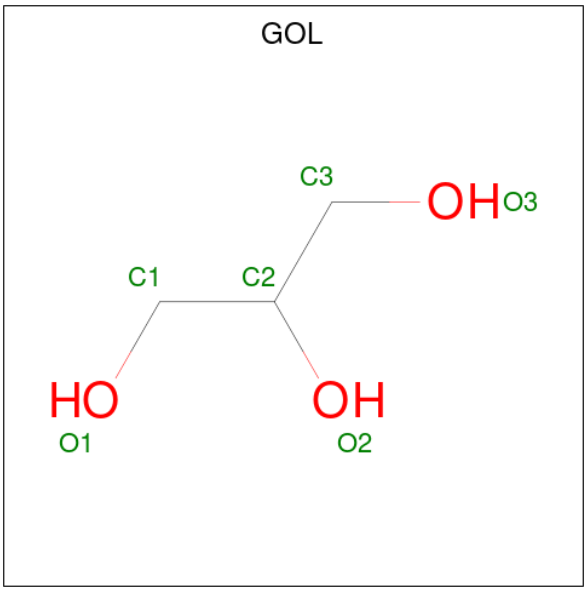
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ALA	-	expression tag	UNP P0CG63
E	-2	SER	-	expression tag	UNP P0CG63
E	-1	ALA	-	expression tag	UNP P0CG63
E	0	ALA	-	expression tag	UNP P0CG63

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0

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



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

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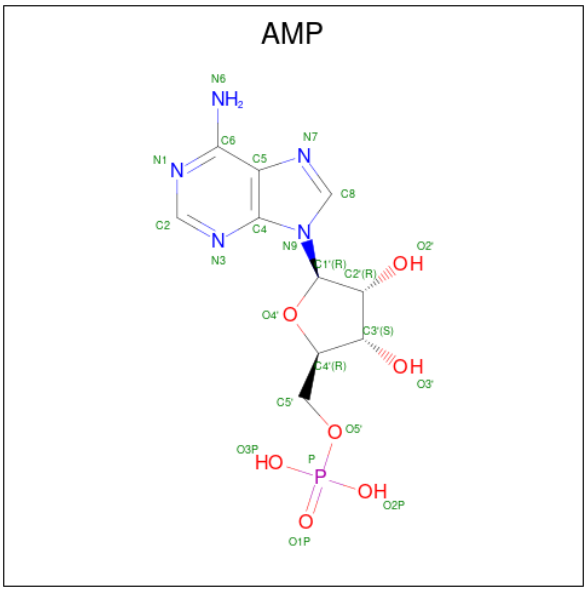
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	27	6	15	6	0	1
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	28	6	16	6	0	1
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0
			Total	C	H	O		
4	C	1	14	3	8	3	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 6 is water.

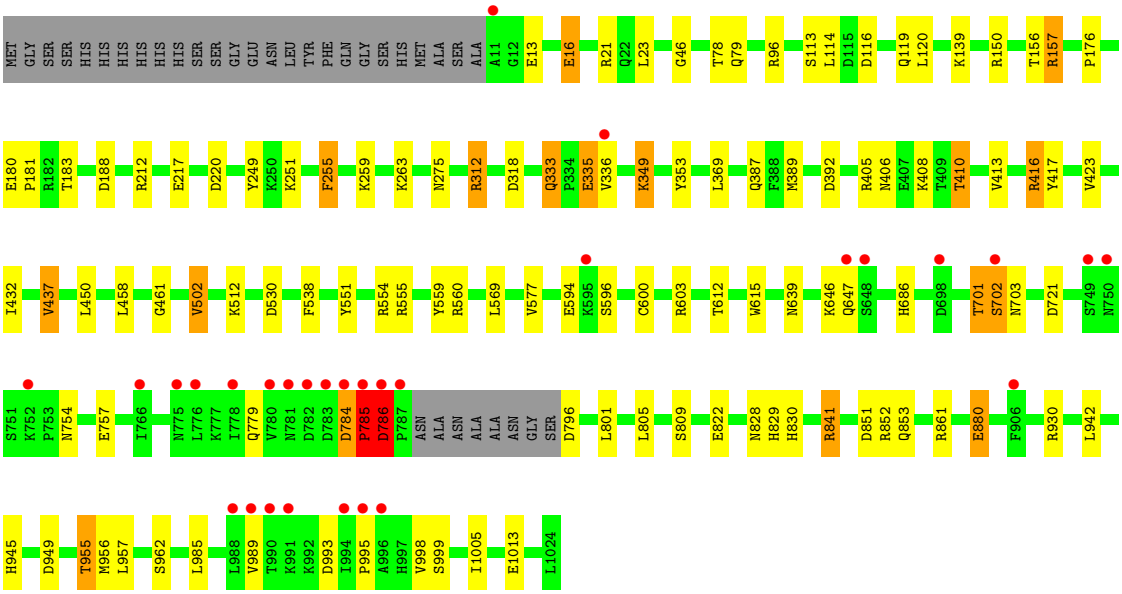
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	500	500	500	0	0
			Total	O		
6	B	35	35	35	0	0
			Total	O		
6	C	451	451	451	0	0
			Total	O		
6	D	25	25	25	0	0
			Total	O		
6	E	9	9	9	0	0

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.

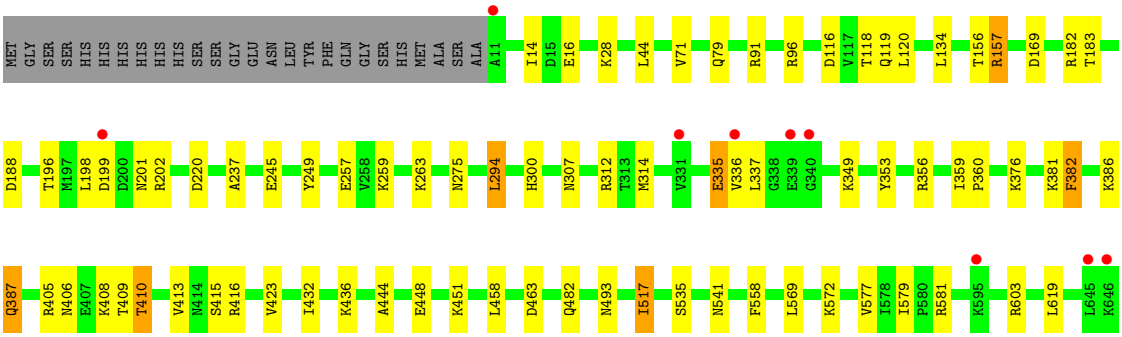
• Molecule 1: Ubiquitin-activating enzyme E1 1

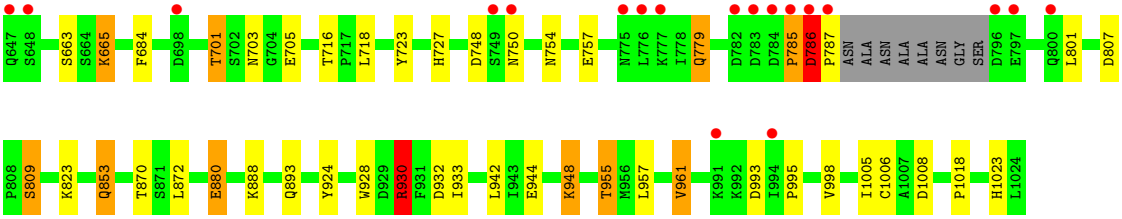
Chain A:



• Molecule 1: Ubiquitin-activating enzyme E1 1

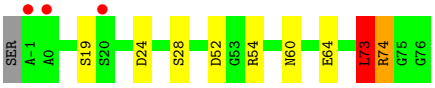
Chain C:





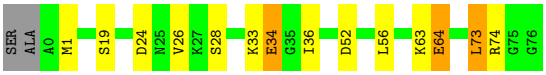
- Molecule 2: Uba1

Chain B:



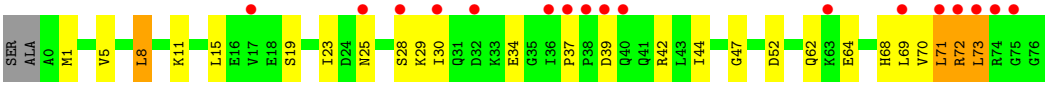
- Molecule 2: Uba1

Chain D:



- Molecule 2: Uba1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.04Å 195.65Å 230.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.40 48.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.65-2.40) 99.2 (48.65-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.164 , 0.201 0.171 , 0.170	Depositor DCC
R_{free} test set	3198 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	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	0.96	EDS
Total number of atoms	36909	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, AMP

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	0.55	0/8126	0.65	1/10997 (0.0%)
1	C	0.54	0/8109	0.63	1/10974 (0.0%)
2	B	0.55	0/615	0.90	3/826 (0.4%)
2	D	0.54	0/621	0.89	1/833 (0.1%)
2	E	0.50	0/610	1.07	5/819 (0.6%)
All	All	0.54	0/18081	0.68	11/24449 (0.0%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	73	LEU	CA-CB-CG	10.35	139.10	115.30
2	B	73	LEU	CA-CB-CG	-9.64	93.12	115.30
2	E	71	LEU	N-CA-C	-8.98	86.76	111.00
2	B	73	LEU	CB-CG-CD2	8.22	124.97	111.00
2	D	73	LEU	CA-CB-CG	-7.28	98.55	115.30
2	E	72	ARG	CA-CB-CG	-5.87	100.48	113.40
2	B	73	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	C	930	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	E	8	LEU	CA-CB-CG	5.34	127.58	115.30
2	E	72	ARG	CB-CG-CD	5.31	125.41	111.60
1	A	841	ARG	NE-CZ-NH2	-5.25	117.68	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	785	PRO	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	7957	7873	7857	66	0
1	C	7944	7863	7845	91	0
2	B	610	633	635	3	0
2	D	613	639	643	11	0
2	E	605	629	630	25	0
3	A	10	0	0	0	0
3	C	10	0	0	1	0
4	A	102	136	136	6	0
4	C	84	111	112	8	0
5	B	23	12	12	0	0
5	D	23	12	12	0	0
6	A	500	0	0	11	0
6	B	35	0	0	0	0
6	C	451	0	0	11	0
6	D	25	0	0	1	0
6	E	9	0	0	0	0
All	All	19001	17908	17882	184	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 5.

All (184) 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:554:ARG:NH2	6:A:1600:HOH:O	1.95	0.99
1:C:198:LEU:O	1:C:201:ASN:ND2	2.09	0.86
1:C:581:ARG:NH2	6:C:1633:HOH:O	2.20	0.73
2:D:1:MET:HE2	2:D:63:LYS:CA	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1107:GOL:O3	4:C:1108:GOL:H12	1.90	0.72
1:A:577:VAL:HG11	1:A:880:GLU:HG3	1.71	0.72
2:E:39:ASP:O	2:E:72:ARG:NH2	2.23	0.72
2:D:1:MET:CE	2:D:63:LYS:N	2.52	0.71
1:C:198:LEU:HG	2:E:8:LEU:HD11	1.71	0.71
2:E:42:ARG:HB3	2:E:70:VAL:CG2	2.20	0.71
1:A:437:VAL:HG21	1:A:458:LEU:HD21	1.73	0.71
1:C:16:GLU:OE1	1:C:853:GLN:NE2	2.22	0.71
2:D:1:MET:HE2	2:D:63:LYS:N	2.06	0.71
1:A:116:ASP:O	1:A:119:GLN:HG3	1.92	0.70
4:C:1104[A]:GOL:O1	6:C:1640:HOH:O	2.09	0.69
1:C:1008:ASP:OD2	4:C:1104[A]:GOL:H2	1.93	0.69
1:C:893:GLN:NE2	6:C:1575:HOH:O	2.24	0.68
1:C:199:ASP:HB2	2:E:8:LEU:HD13	1.74	0.68
1:A:405:ARG:HD2	1:A:423:VAL:O	1.95	0.67
1:A:413:VAL:HG12	1:A:413:VAL:O	1.94	0.66
1:C:1008:ASP:OD2	4:C:1104[A]:GOL:C2	2.43	0.66
1:C:237:ALA:HB3	2:E:47:GLY:HA2	1.79	0.64
1:C:572:LYS:NZ	6:C:1517:HOH:O	2.28	0.64
1:C:201:ASN:OD1	6:C:1462:HOH:O	2.15	0.64
1:A:985:LEU:O	1:A:989:VAL:HG23	1.99	0.63
1:A:945[A]:HIS:ND1	1:A:949:ASP:OD2	2.33	0.62
1:C:558:PHE:O	1:C:930:ARG:NH1	2.32	0.62
1:C:603:ARG:NH2	1:C:779:GLN:HG3	2.15	0.62
1:C:413:VAL:O	1:C:413:VAL:HG12	1.98	0.61
1:C:955:THR:HG21	6:C:1366:HOH:O	2.00	0.61
1:C:199:ASP:HB2	2:E:8:LEU:CD1	2.31	0.60
1:A:852:ARG:HB2	4:A:1112:GOL:H32	1.85	0.59
1:A:530:ASP:OD2	1:A:999:SER:OG	2.20	0.58
1:A:413:VAL:O	1:A:413:VAL:CG1	2.51	0.58
1:C:198:LEU:HD12	2:E:8:LEU:HD12	1.84	0.58
1:A:721:ASP:OD2	4:A:1118:GOL:H2	2.04	0.58
1:C:196:THR:CG2	2:E:44:ILE:HD11	2.34	0.58
1:A:333:GLN:O	1:A:336:VAL:HG22	2.04	0.57
1:C:1008:ASP:OD2	4:C:1104[A]:GOL:O2	2.22	0.57
2:D:1:MET:HE2	2:D:63:LYS:HA	1.85	0.57
1:A:779:GLN:NE2	1:A:784:ASP:O	2.38	0.57
1:A:176:PRO:HD2	1:A:259:LYS:HG3	1.87	0.57
1:A:336:VAL:CG1	6:A:1596:HOH:O	2.52	0.56
1:C:569:LEU:HB3	2:D:73:LEU:HD22	1.86	0.56
1:C:807:ASP:OD2	1:C:809:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:HD2	1:A:353:TYR:CE2	2.41	0.56
1:A:995:PRO:HG2	1:A:998:VAL:HG23	1.87	0.56
1:A:639:ASN:HB2	6:A:1657:HOH:O	2.05	0.56
1:A:600[B]:CYS:SG	1:A:603:ARG:NH2	2.79	0.56
2:E:25:ASN:O	2:E:29:LYS:HG3	2.05	0.56
2:D:74[B]:ARG:NH1	6:D:206:HOH:O	2.39	0.55
1:A:349:LYS:HD3	1:A:353:TYR:CZ	2.42	0.55
1:C:237:ALA:HB3	2:E:47:GLY:CA	2.36	0.55
2:E:42:ARG:HB3	2:E:70:VAL:HG22	1.89	0.54
1:A:785:PRO:O	1:A:786:ASP:HB3	2.07	0.53
2:E:11:LYS:NZ	2:E:34:GLU:OE1	2.28	0.53
1:A:569:LEU:HB3	2:B:73:LEU:HD22	1.90	0.53
1:C:14:ILE:HD12	1:C:28:LYS:HG3	1.91	0.53
1:C:405:ARG:HD2	1:C:423:VAL:O	2.09	0.53
2:E:23:ILE:HB	2:E:52:ASP:HA	1.90	0.53
2:E:44:ILE:CG1	2:E:68:HIS:HB2	2.39	0.53
1:A:369:LEU:HD22	1:A:389:MET:HE1	1.90	0.52
1:C:957:LEU:HD12	1:C:1005:ILE:CG2	2.39	0.52
1:C:1008:ASP:OD2	4:C:1104[B]:GOL:H31	2.09	0.52
1:C:336:VAL:HG23	1:C:337:LEU:N	2.23	0.52
1:A:612:THR:HG22	1:A:841:ARG:HG2	1.91	0.52
2:D:34:GLU:HB3	2:D:36:ILE:HD12	1.92	0.52
1:A:703:ASN:C	1:A:703:ASN:OD1	2.48	0.52
1:C:335:GLU:HA	1:C:335:GLU:OE1	2.10	0.52
1:A:349:LYS:CD	1:A:353:TYR:CE2	2.93	0.51
1:C:444:ALA:HA	1:C:482:GLN:HG2	1.92	0.51
1:C:71:VAL:HG22	1:C:91:ARG:HG2	1.92	0.51
1:C:517:ILE:HG23	1:C:517:ILE:O	2.10	0.51
1:C:294:LEU:HD21	1:C:336:VAL:HG21	1.93	0.51
1:C:665:LYS:HE3	6:C:1585:HOH:O	2.10	0.51
1:A:180:GLU:OE2	1:A:181:PRO:HD2	2.10	0.51
1:A:551:TYR:CZ	1:A:555:ARG:HD2	2.46	0.51
1:C:116:ASP:OD1	1:C:118:THR:HB	2.11	0.51
1:A:406:ASN:O	1:A:410:THR:HB	2.11	0.50
1:A:46:GLY:HA3	1:A:78:THR:OG1	2.11	0.50
1:A:255:PHE:C	1:A:255:PHE:CD1	2.84	0.50
2:E:5:VAL:CG1	2:E:69:LEU:HB2	2.41	0.50
1:A:335:GLU:HB2	6:A:1380:HOH:O	2.10	0.50
1:C:944:GLU:HG2	1:C:948:LYS:HD3	1.92	0.50
1:A:851:ASP:HB2	4:A:1112:GOL:H2	1.94	0.50
1:C:823:LYS:HE3	6:C:1588:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASP:OD1	2:E:71:LEU:O	2.29	0.50
1:C:349:LYS:HD3	1:C:353:TYR:CE2	2.47	0.50
1:C:381:LYS:O	1:C:382:PHE:HB2	2.12	0.50
1:A:461:GLY:O	1:A:512:LYS:NZ	2.45	0.50
1:C:198:LEU:CG	2:E:8:LEU:HD11	2.39	0.50
1:A:861:ARG:NH1	6:A:1511:HOH:O	2.44	0.49
1:C:754:ASN:HB3	1:C:757:GLU:OE1	2.12	0.49
1:C:785:PRO:CB	1:C:786:ASP:HA	2.41	0.49
1:C:955:THR:HG22	1:C:1006:CYS:HB2	1.94	0.49
1:A:530:ASP:OD1	1:A:559:TYR:OH	2.22	0.49
2:B:74:ARG:HG3	2:B:74:ARG:O	2.13	0.49
1:C:493:ASN:HB3	1:C:517:ILE:HD11	1.94	0.49
1:A:957:LEU:HD12	1:A:1005:ILE:CG2	2.43	0.49
1:A:188:ASP:HA	1:A:249:TYR:CE1	2.48	0.49
1:C:577:VAL:HG21	1:C:880:GLU:HG3	1.94	0.48
1:C:933:ILE:CD1	1:C:942:LEU:CD1	2.91	0.48
1:A:150:ARG:NH1	4:A:1104:GOL:H32	2.28	0.48
1:C:202:ARG:NH2	3:C:1114:SO4:O3	2.47	0.48
1:C:888:LYS:HE3	6:C:1575:HOH:O	2.14	0.48
1:A:336:VAL:HG12	6:A:1596:HOH:O	2.14	0.48
1:A:114:LEU:HG	1:A:114:LEU:O	2.13	0.47
2:D:24:ASP:OD2	2:D:52:ASP:O	2.32	0.47
1:C:701:THR:OG1	1:C:705:GLU:O	2.32	0.47
2:E:42:ARG:HB3	2:E:70:VAL:HG23	1.95	0.47
1:A:156:THR:C	1:A:157:ARG:HG2	2.35	0.47
1:C:182:ARG:HD2	1:C:257:GLU:OE1	2.14	0.47
1:A:646:LYS:HG2	1:A:647:GLN:N	2.30	0.47
1:C:198:LEU:HD12	2:E:8:LEU:CD1	2.44	0.47
1:C:995:PRO:HG2	1:C:998:VAL:HG23	1.96	0.47
1:C:957:LEU:HD12	1:C:1005:ILE:HG22	1.97	0.46
1:A:822:GLU:H	1:A:830:HIS:HD1	1.63	0.46
1:C:134:LEU:HB2	1:C:300:HIS:CG	2.49	0.46
1:C:406:ASN:H	1:C:409:THR:CG2	2.28	0.46
1:C:684:PHE:HB3	1:C:718:LEU:HD22	1.96	0.46
1:C:493:ASN:CB	1:C:517:ILE:HD11	2.46	0.46
2:D:26:VAL:HG21	2:D:56:LEU:HD21	1.97	0.46
1:A:942:LEU:C	1:A:942:LEU:HD23	2.36	0.46
1:C:376:LYS:HG2	1:C:382:PHE:HB2	1.97	0.46
2:E:42:ARG:HB2	2:E:72:ARG:HD3	1.98	0.45
2:B:24:ASP:OD2	2:B:52:ASP:O	2.35	0.45
1:A:217:GLU:OE2	1:A:251:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:MET:CG	1:C:410:THR:HG21	2.46	0.45
1:C:957:LEU:CD1	1:C:1005:ILE:CG2	2.95	0.45
1:C:1008:ASP:OD1	4:C:1104[A]:GOL:O2	2.33	0.45
1:C:577:VAL:CG1	1:C:579:ILE:HD11	2.46	0.45
1:C:872:LEU:C	1:C:872:LEU:HD23	2.37	0.45
2:E:44:ILE:HG12	2:E:68:HIS:HB2	1.97	0.45
1:A:615:TRP:CE3	1:A:841:ARG:HD2	2.53	0.44
1:C:932:ASP:OD1	1:C:1023:HIS:HE1	2.00	0.44
1:C:196:THR:HG21	2:E:44:ILE:HD11	2.00	0.44
2:D:63:LYS:O	2:D:64:GLU:HB2	2.17	0.44
1:C:381:LYS:O	1:C:382:PHE:CB	2.65	0.44
1:A:416:ARG:HD3	6:A:1210:HOH:O	2.18	0.43
1:A:828:ASN:O	1:A:829:HIS:HB2	2.19	0.43
1:C:924:TYR:CD2	1:C:1018:PRO:HG3	2.54	0.43
1:C:1008:ASP:CG	4:C:1104[A]:GOL:O2	2.57	0.43
1:A:560:ARG:NH1	1:A:930:ARG:NE	2.66	0.43
1:A:957:LEU:HD12	1:A:1005:ILE:HG22	2.00	0.43
1:C:336:VAL:CG2	1:C:337:LEU:N	2.81	0.43
1:A:16:GLU:OE1	1:A:853:GLN:HG2	2.19	0.43
1:A:841:ARG:NH2	6:A:1294:HOH:O	2.51	0.43
2:D:1:MET:HE3	2:D:63:LYS:HB3	2.01	0.43
1:A:432:ILE:HG23	1:A:458:LEU:HD12	2.00	0.42
1:A:701:THR:O	1:A:702:SER:C	2.57	0.42
1:C:944:GLU:CG	1:C:948:LYS:HD3	2.50	0.42
2:E:37:PRO:HB2	2:E:39:ASP:OD2	2.19	0.42
1:C:928:TRP:O	1:C:930:ARG:NH2	2.50	0.42
1:A:754:ASN:OD1	1:A:757:GLU:HG3	2.19	0.42
1:C:336:VAL:HG23	1:C:337:LEU:HG	2.01	0.42
1:C:432:ILE:O	1:C:458:LEU:HD12	2.20	0.42
1:A:437:VAL:CG1	1:A:538:PHE:CE2	3.03	0.42
1:C:156:THR:C	1:C:157:ARG:HG2	2.40	0.42
1:C:237:ALA:CB	2:E:47:GLY:HA2	2.48	0.42
1:C:349:LYS:HD3	1:C:353:TYR:CZ	2.54	0.42
1:C:183:THR:HG22	6:C:1512:HOH:O	2.20	0.42
1:C:448:GLU:HG3	1:C:870:THR:HG22	2.02	0.42
1:A:955:THR:HG21	6:A:1280:HOH:O	2.18	0.42
1:C:786:ASP:O	1:C:787:PRO:O	2.38	0.42
1:A:312:ARG:HG2	1:A:318:ASP:OD2	2.20	0.41
1:C:188:ASP:HA	1:C:249:TYR:CE1	2.56	0.41
1:A:416:ARG:HD2	1:A:417:TYR:CE1	2.56	0.41
1:C:727:HIS:CD2	1:C:727:HIS:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LYS:HA	1:C:387:GLN:HA	1.83	0.41
1:C:961:VAL:O	1:C:961:VAL:HG13	2.21	0.41
1:A:450:LEU:HB3	1:A:502:VAL:HG21	2.02	0.41
1:A:139:LYS:HD3	1:C:723:TYR:CZ	2.55	0.41
1:C:359:ILE:HA	1:C:360:PRO:HD3	1.97	0.41
1:C:541:ASN:HB3	6:C:1361:HOH:O	2.21	0.41
1:C:314:MET:HG2	1:C:410:THR:HG21	2.03	0.41
1:A:945[A]:HIS:NE2	6:A:1444:HOH:O	2.37	0.41
1:C:786:ASP:HB3	1:C:787:PRO:CD	2.50	0.41
1:C:436:LYS:HD2	1:C:535:SER:O	2.21	0.40
1:A:852:ARG:HG3	4:A:1112:GOL:H12	2.02	0.40
1:C:116:ASP:O	1:C:119:GLN:HG3	2.21	0.40
2:E:15:LEU:HD11	2:E:30:ILE:HG13	2.02	0.40
1:C:716:THR:O	1:C:716:THR:HG23	2.22	0.40
1:A:801:LEU:O	1:A:805:LEU:HD13	2.22	0.40
4:A:1116:GOL:H31	6:A:1467:HOH:O	2.21	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	1004/1040 (96%)	971 (97%)	31 (3%)	2 (0%)	47 62
1	C	1002/1040 (96%)	965 (96%)	32 (3%)	5 (0%)	29 41
2	B	76/79 (96%)	76 (100%)	0	0	100 100
2	D	76/79 (96%)	76 (100%)	0	0	100 100
2	E	75/79 (95%)	74 (99%)	1 (1%)	0	100 100
All	All	2233/2317 (96%)	2162 (97%)	64 (3%)	7 (0%)	41 55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	786	ASP
1	C	703	ASN
1	A	785	PRO
1	C	382	PHE
1	C	665	LYS
1	C	786	ASP
1	C	785	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	890/913 (98%)	849 (95%)	41 (5%)	27	43
1	C	888/913 (97%)	848 (96%)	40 (4%)	27	44
2	B	69/70 (99%)	62 (90%)	7 (10%)	7	11
2	D	70/70 (100%)	65 (93%)	5 (7%)	14	23
2	E	69/70 (99%)	63 (91%)	6 (9%)	10	15
All	All	1986/2036 (98%)	1887 (95%)	99 (5%)	24	40

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	16	GLU
1	A	21	ARG
1	A	23	LEU
1	A	79	GLN
1	A	96	ARG
1	A	113	SER
1	A	120	LEU
1	A	157	ARG
1	A	183	THR
1	A	212	ARG
1	A	220	ASP
1	A	255	PHE

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	275	ASN
1	A	312	ARG
1	A	333	GLN
1	A	335	GLU
1	A	349	LYS
1	A	387	GLN
1	A	392	ASP
1	A	408	LYS
1	A	410	THR
1	A	416	ARG
1	A	437	VAL
1	A	502	VAL
1	A	594	GLU
1	A	596	SER
1	A	686	HIS
1	A	701	THR
1	A	702	SER
1	A	784	ASP
1	A	786	ASP
1	A	796	ASP
1	A	809	SER
1	A	880	GLU
1	A	955	THR
1	A	956	MET
1	A	962	SER
1	A	993	ASP
1	A	1013	GLU
2	B	19	SER
2	B	28	SER
2	B	54	ARG
2	B	60	ASN
2	B	64	GLU
2	B	73	LEU
2	B	74	ARG
1	C	44	LEU
1	C	79	GLN
1	C	96	ARG
1	C	120	LEU
1	C	157	ARG
1	C	169	ASP
1	C	220	ASP

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Mol	Chain	Res	Type
1	C	245	GLU
1	C	259	LYS
1	C	263	LYS
1	C	275	ASN
1	C	294	LEU
1	C	307	ASN
1	C	312	ARG
1	C	335	GLU
1	C	356	ARG
1	C	387	GLN
1	C	408	LYS
1	C	410	THR
1	C	415	SER
1	C	416	ARG
1	C	451	LYS
1	C	463	ASP
1	C	517	ILE
1	C	619	LEU
1	C	663	SER
1	C	701	THR
1	C	748	ASP
1	C	750	ASN
1	C	779	GLN
1	C	786	ASP
1	C	801	LEU
1	C	809	SER
1	C	853	GLN
1	C	880	GLU
1	C	930	ARG
1	C	948	LYS
1	C	955	THR
1	C	961	VAL
1	C	993	ASP
2	D	19	SER
2	D	28	SER
2	D	33	LYS
2	D	34	GLU
2	D	64	GLU
2	E	1	MET
2	E	19	SER
2	E	28	SER
2	E	62	GLN

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Mol	Chain	Res	Type
2	E	64	GLU
2	E	73	LEU

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	853	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

37 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	$\#\|Z\| > 2$
4	GOL	A	1114	-	5,5,5	0.32	0	5,5,5	0.43	0
4	GOL	A	1113	-	5,5,5	0.32	0	5,5,5	0.39	0
4	GOL	C	1111	-	5,5,5	0.52	0	5,5,5	0.25	0
4	GOL	A	1117	-	5,5,5	0.57	0	5,5,5	0.42	0
4	GOL	C	1113	-	5,5,5	0.42	0	5,5,5	0.31	0
4	GOL	C	1108	-	5,5,5	0.64	0	5,5,5	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	1108	-	5,5,5	0.27	0	5,5,5	0.43	0
4	GOL	C	1107	-	5,5,5	0.34	0	5,5,5	0.82	0
4	GOL	A	1112	-	5,5,5	0.36	0	5,5,5	0.26	0
3	SO4	A	1119	-	4,4,4	0.09	0	6,6,6	0.23	0
4	GOL	C	1104[B]	-	5,5,5	0.37	0	5,5,5	0.43	0
4	GOL	A	1116	-	5,5,5	0.45	0	5,5,5	0.39	0
4	GOL	A	1105	-	5,5,5	0.43	0	5,5,5	0.54	0
4	GOL	C	1106[A]	-	5,5,5	0.39	0	5,5,5	0.39	0
4	GOL	A	1103	-	5,5,5	0.41	0	5,5,5	0.54	0
4	GOL	A	1115	-	5,5,5	0.40	0	5,5,5	0.08	0
4	GOL	A	1111	-	5,5,5	0.47	0	5,5,5	0.79	0
4	GOL	C	1105	-	5,5,5	0.41	0	5,5,5	0.42	0
4	GOL	A	1118	-	5,5,5	0.48	0	5,5,5	0.82	0
4	GOL	C	1110	-	5,5,5	0.49	0	5,5,5	0.23	0
4	GOL	A	1110	-	5,5,5	0.46	0	5,5,5	0.34	0
3	SO4	C	1101	-	4,4,4	0.44	0	6,6,6	0.62	0
4	GOL	C	1109	-	5,5,5	0.42	0	5,5,5	0.27	0
4	GOL	A	1106	-	5,5,5	0.38	0	5,5,5	0.16	0
5	AMP	D	101	2	22,25,25	0.96	1 (4%)	25,38,38	1.29	1 (4%)
4	GOL	C	1106[B]	-	5,5,5	0.39	0	5,5,5	0.34	0
5	AMP	B	101	2	22,25,25	0.96	2 (9%)	25,38,38	1.27	3 (12%)
4	GOL	A	1102	-	5,5,5	0.55	0	5,5,5	0.25	0
4	GOL	A	1109	-	5,5,5	0.32	0	5,5,5	0.54	0
4	GOL	A	1107	-	5,5,5	0.21	0	5,5,5	0.79	0
3	SO4	C	1114	-	4,4,4	0.13	0	6,6,6	0.25	0
4	GOL	C	1103	-	5,5,5	0.52	0	5,5,5	0.64	0
4	GOL	C	1102	-	5,5,5	0.30	0	5,5,5	0.35	0
3	SO4	A	1101	-	4,4,4	0.13	0	6,6,6	0.37	0
4	GOL	C	1112	-	5,5,5	0.30	0	5,5,5	0.29	0
4	GOL	A	1104	-	5,5,5	0.35	0	5,5,5	0.53	0
4	GOL	C	1104[A]	-	5,5,5	0.35	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	A	1114	-	-	2/4/4/4	-
4	GOL	A	1113	-	-	4/4/4/4	-
4	GOL	C	1111	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1117	-	-	4/4/4/4	-
4	GOL	C	1113	-	-	3/4/4/4	-
4	GOL	C	1108	-	-	3/4/4/4	-
4	GOL	A	1108	-	-	3/4/4/4	-
4	GOL	C	1107	-	-	2/4/4/4	-
4	GOL	A	1112	-	-	4/4/4/4	-
4	GOL	C	1104[B]	-	-	2/4/4/4	-
4	GOL	A	1116	-	-	4/4/4/4	-
4	GOL	A	1105	-	-	0/4/4/4	-
4	GOL	C	1106[A]	-	-	2/4/4/4	-
4	GOL	A	1103	-	-	2/4/4/4	-
4	GOL	A	1115	-	-	4/4/4/4	-
4	GOL	A	1111	-	-	2/4/4/4	-
4	GOL	C	1105	-	-	0/4/4/4	-
4	GOL	A	1118	-	-	4/4/4/4	-
4	GOL	C	1110	-	-	4/4/4/4	-
4	GOL	A	1110	-	-	4/4/4/4	-
4	GOL	C	1109	-	-	2/4/4/4	-
4	GOL	A	1106	-	-	2/4/4/4	-
5	AMP	D	101	2	-	2/6/26/26	0/3/3/3
4	GOL	C	1106[B]	-	-	2/4/4/4	-
5	AMP	B	101	2	-	1/6/26/26	0/3/3/3
4	GOL	A	1102	-	-	2/4/4/4	-
4	GOL	A	1109	-	-	4/4/4/4	-
4	GOL	A	1107	-	-	0/4/4/4	-
4	GOL	C	1103	-	-	4/4/4/4	-
4	GOL	C	1102	-	-	4/4/4/4	-
4	GOL	C	1112	-	-	2/4/4/4	-
4	GOL	A	1104	-	-	2/4/4/4	-
4	GOL	C	1104[A]	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	AMP	C5-C4	2.26	1.46	1.40
5	D	101	AMP	C5-C4	2.16	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	AMP	C2-N3	2.05	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	101	AMP	N3-C2-N1	-3.89	122.59	128.68
5	B	101	AMP	N3-C2-N1	-3.88	122.61	128.68
5	B	101	AMP	O3P-P-O2P	2.32	116.51	107.64
5	B	101	AMP	C4-C5-N7	-2.10	107.21	109.40

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	GOL	C1-C2-C3-O3
4	A	1102	GOL	O2-C2-C3-O3
4	A	1103	GOL	O1-C1-C2-C3
4	A	1106	GOL	O1-C1-C2-C3
4	A	1108	GOL	O1-C1-C2-C3
4	A	1109	GOL	O1-C1-C2-C3
4	A	1109	GOL	C1-C2-C3-O3
4	A	1110	GOL	O1-C1-C2-C3
4	A	1112	GOL	O1-C1-C2-C3
4	A	1112	GOL	C1-C2-C3-O3
4	A	1113	GOL	O1-C1-C2-C3
4	A	1113	GOL	C1-C2-C3-O3
4	A	1113	GOL	O2-C2-C3-O3
4	A	1114	GOL	C1-C2-C3-O3
4	A	1115	GOL	C1-C2-C3-O3
4	A	1115	GOL	O2-C2-C3-O3
4	A	1116	GOL	O1-C1-C2-C3
4	A	1116	GOL	C1-C2-C3-O3
4	A	1117	GOL	O1-C1-C2-O2
4	A	1117	GOL	O1-C1-C2-C3
4	A	1118	GOL	C1-C2-C3-O3
4	C	1104[A]	GOL	O1-C1-C2-C3
4	C	1104[B]	GOL	O1-C1-C2-C3
4	C	1107	GOL	O1-C1-C2-C3
4	C	1109	GOL	C1-C2-C3-O3
4	C	1111	GOL	O1-C1-C2-C3
4	C	1113	GOL	O1-C1-C2-C3
4	A	1103	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1115	GOL	O1-C1-C2-O2
4	C	1107	GOL	O1-C1-C2-O2
4	C	1113	GOL	O1-C1-C2-O2
4	A	1104	GOL	C1-C2-C3-O3
4	A	1111	GOL	C1-C2-C3-O3
4	A	1115	GOL	O1-C1-C2-C3
4	A	1118	GOL	O1-C1-C2-C3
4	C	1102	GOL	O1-C1-C2-C3
4	C	1103	GOL	O1-C1-C2-C3
4	C	1106[B]	GOL	C1-C2-C3-O3
4	C	1110	GOL	O1-C1-C2-C3
4	C	1110	GOL	C1-C2-C3-O3
4	C	1112	GOL	C1-C2-C3-O3
4	C	1113	GOL	C1-C2-C3-O3
4	A	1106	GOL	O1-C1-C2-O2
4	A	1109	GOL	O1-C1-C2-O2
4	A	1109	GOL	O2-C2-C3-O3
4	A	1110	GOL	O1-C1-C2-O2
4	A	1112	GOL	O1-C1-C2-O2
4	A	1113	GOL	O1-C1-C2-O2
4	A	1114	GOL	O2-C2-C3-O3
4	A	1116	GOL	O2-C2-C3-O3
4	C	1104[A]	GOL	O1-C1-C2-O2
4	C	1104[B]	GOL	O1-C1-C2-O2
4	C	1106[B]	GOL	O2-C2-C3-O3
4	C	1112	GOL	O2-C2-C3-O3
4	A	1108	GOL	O1-C1-C2-O2
4	A	1111	GOL	O2-C2-C3-O3
4	A	1118	GOL	O2-C2-C3-O3
4	C	1109	GOL	O2-C2-C3-O3
4	C	1111	GOL	O1-C1-C2-O2
4	A	1110	GOL	O2-C2-C3-O3
4	C	1108	GOL	O2-C2-C3-O3
5	D	101	AMP	O4'-C4'-C5'-O5'
4	A	1108	GOL	O2-C2-C3-O3
4	A	1116	GOL	O1-C1-C2-O2
4	C	1102	GOL	O1-C1-C2-O2
4	C	1103	GOL	O1-C1-C2-O2
4	C	1103	GOL	O2-C2-C3-O3
4	C	1106[A]	GOL	O1-C1-C2-O2
4	C	1110	GOL	O2-C2-C3-O3
4	A	1104	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1112	GOL	O2-C2-C3-O3
4	C	1110	GOL	O1-C1-C2-O2
5	B	101	AMP	O4'-C4'-C5'-O5'
4	A	1117	GOL	C1-C2-C3-O3
4	C	1102	GOL	C1-C2-C3-O3
4	C	1106[A]	GOL	O1-C1-C2-C3
4	C	1108	GOL	C1-C2-C3-O3
4	A	1117	GOL	O2-C2-C3-O3
4	C	1102	GOL	O2-C2-C3-O3
4	A	1118	GOL	O1-C1-C2-O2
4	C	1108	GOL	O1-C1-C2-O2
4	A	1110	GOL	C1-C2-C3-O3
4	C	1103	GOL	C1-C2-C3-O3
5	D	101	AMP	C3'-C4'-C5'-O5'

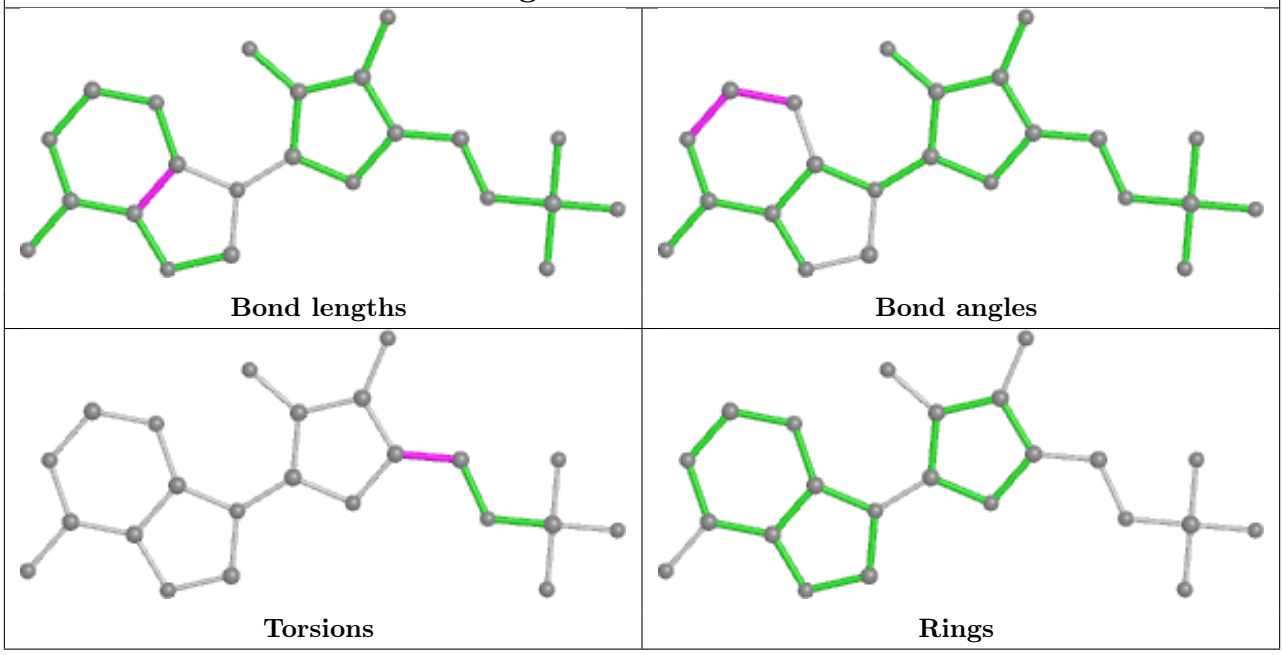
There are no ring outliers.

9 monomers are involved in 15 short contacts:

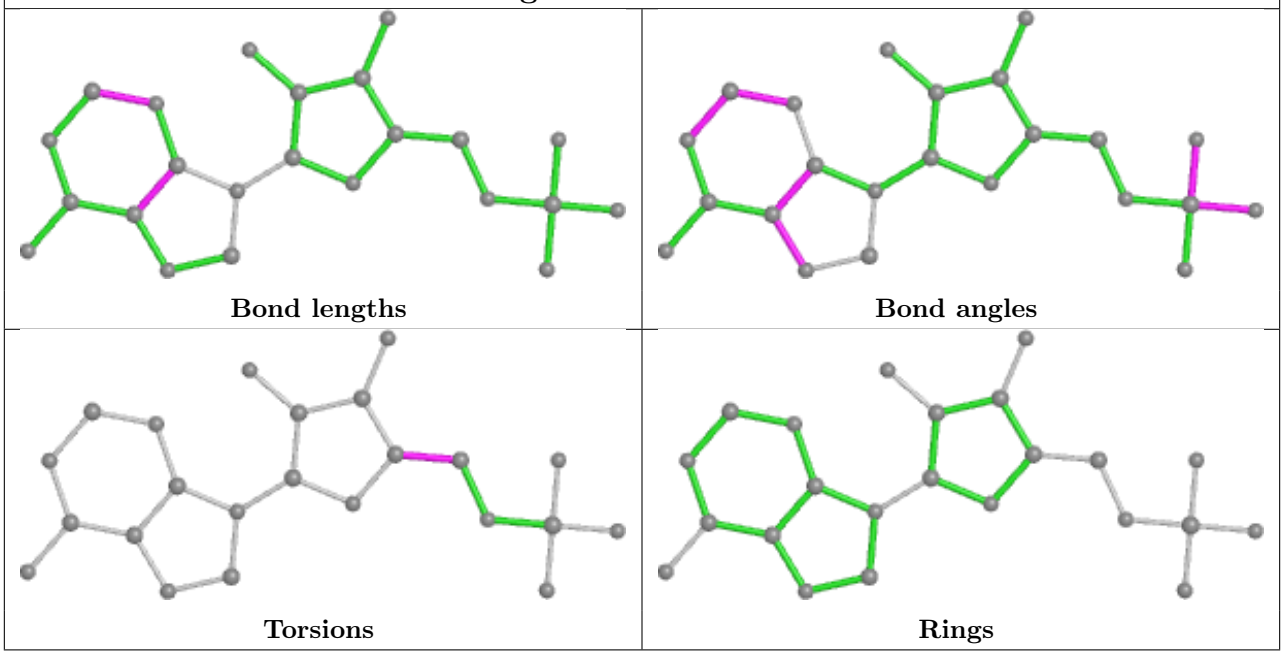
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1108	GOL	1	0
4	C	1107	GOL	1	0
4	A	1112	GOL	3	0
4	C	1104[B]	GOL	1	0
4	A	1116	GOL	1	0
4	A	1118	GOL	1	0
3	C	1114	SO4	1	0
4	A	1104	GOL	1	0
4	C	1104[A]	GOL	6	0

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 101



Ligand AMP B 101



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1006/1040 (96%)	-0.02	30 (2%) 50 49	22, 41, 86, 174	0
1	C	1006/1040 (96%)	-0.02	28 (2%) 53 51	24, 41, 87, 164	0
2	B	78/79 (98%)	0.31	3 (3%) 40 39	29, 47, 81, 96	0
2	D	77/79 (97%)	-0.07	0 100 100	29, 51, 88, 98	0
2	E	77/79 (97%)	1.24	17 (22%) 0 0	40, 80, 136, 162	0
All	All	2244/2317 (96%)	0.03	78 (3%) 44 43	22, 42, 92, 174	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	787	PRO	9.0
2	E	73	LEU	8.5
1	C	786	ASP	7.5
1	A	785	PRO	6.5
2	E	74	ARG	6.3
2	E	40	GLN	5.6
2	E	72	ARG	5.5
1	C	750	ASN	5.3
1	A	750	ASN	5.3
1	C	787	PRO	4.5
2	E	71	LEU	4.5
1	A	749	SER	4.4
1	A	780	VAL	4.4
2	E	75	GLY	4.4
1	C	645	LEU	4.4
2	E	30	ILE	4.2
1	C	785	PRO	4.2
1	A	783	ASP	3.9
2	B	0	ALA	3.7
1	C	749	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	37	PRO	3.6
1	A	996	ALA	3.6
1	C	11	ALA	3.6
1	C	340	GLY	3.5
1	A	784	ASP	3.5
1	A	995	PRO	3.5
1	A	776	LEU	3.4
1	A	647	GLN	3.4
1	C	646	LYS	3.3
1	A	989	VAL	3.2
1	A	11	ALA	3.2
1	C	595	LYS	3.2
2	E	36	ILE	3.2
1	C	199	ASP	3.1
1	C	776	LEU	3.1
2	E	38	PRO	3.1
2	B	-1	ALA	3.1
1	A	786	ASP	3.0
1	A	648	SER	2.9
2	E	25	ASN	2.9
1	A	778	ILE	2.9
1	C	782	ASP	2.8
1	A	766	ILE	2.8
1	C	336	VAL	2.8
1	C	783	ASP	2.8
2	E	28	SER	2.7
1	C	339	GLU	2.7
1	A	702	SER	2.6
1	A	994	ILE	2.6
1	C	800	GLN	2.6
1	C	991	LYS	2.5
1	A	752	LYS	2.5
1	C	994	ILE	2.5
1	A	775	ASN	2.5
1	C	775	ASN	2.5
1	A	988	LEU	2.4
1	C	648	SER	2.4
1	A	698	ASP	2.4
1	C	796	ASP	2.4
1	A	336	VAL	2.4
2	B	20	SER	2.3
1	A	991	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	647	GLN	2.3
2	E	39	ASP	2.3
1	C	331	VAL	2.2
1	A	782	ASP	2.2
1	A	990	THR	2.2
1	C	784	ASP	2.2
1	C	797	GLU	2.2
1	A	906	PHE	2.2
2	E	32	ASP	2.2
1	C	777	LYS	2.2
2	E	69	LEU	2.2
1	A	781	ASN	2.1
2	E	17	VAL	2.1
1	A	595	LYS	2.1
1	C	698	ASP	2.0
2	E	63	LYS	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	1111	6/6	0.71	0.34	85,106,121,127	0
4	GOL	A	1111	6/6	0.75	0.26	71,85,100,100	0
4	GOL	A	1116	6/6	0.77	0.25	85,102,104,106	0
4	GOL	C	1107	6/6	0.80	0.23	61,78,91,95	0
4	GOL	A	1118	6/6	0.80	0.32	67,81,82,83	0
4	GOL	A	1112	6/6	0.82	0.24	71,85,96,101	0
4	GOL	A	1105	6/6	0.83	0.18	64,77,80,82	0

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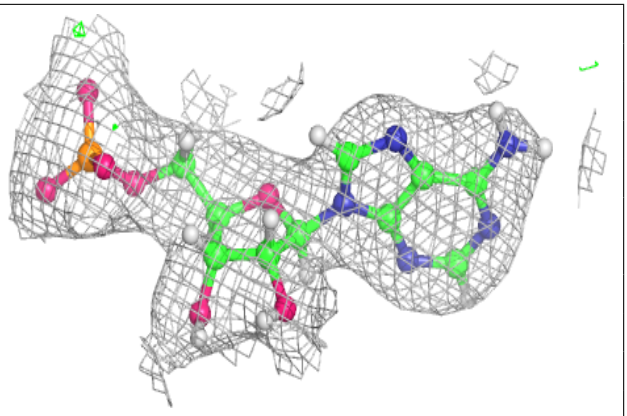
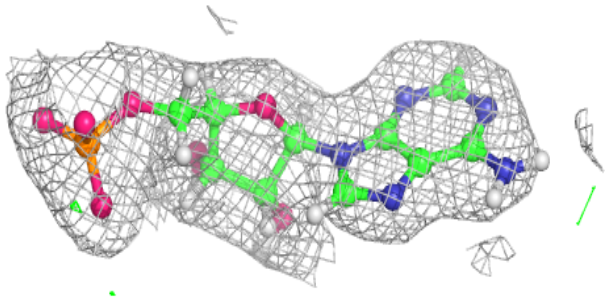
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1115	6/6	0.84	0.13	92,110,112,112	0
4	GOL	C	1112	6/6	0.84	0.21	94,113,119,121	0
4	GOL	A	1109	6/6	0.85	0.27	65,78,82,84	0
4	GOL	C	1106[B]	6/6	0.86	0.19	45,54,60,60	14
4	GOL	C	1106[A]	6/6	0.86	0.19	44,52,60,60	14
4	GOL	C	1103	6/6	0.88	0.21	53,63,65,65	0
4	GOL	C	1104[A]	6/6	0.88	0.20	67,69,82,83	13
4	GOL	C	1108	6/6	0.88	0.27	56,67,68,69	0
4	GOL	C	1104[B]	6/6	0.88	0.20	65,78,83,84	14
4	GOL	A	1107	6/6	0.88	0.19	54,64,70,73	0
4	GOL	A	1106	6/6	0.89	0.21	71,85,97,101	0
4	GOL	A	1104	6/6	0.89	0.26	56,68,72,76	0
4	GOL	A	1108	6/6	0.89	0.31	67,80,87,88	0
4	GOL	A	1102	6/6	0.89	0.23	50,60,66,70	0
4	GOL	A	1117	6/6	0.89	0.26	89,107,110,112	0
4	GOL	C	1110	6/6	0.90	0.23	65,78,88,89	0
4	GOL	A	1113	6/6	0.92	0.22	73,88,92,94	0
4	GOL	C	1109	6/6	0.92	0.24	62,75,82,86	0
4	GOL	A	1114	6/6	0.92	0.17	77,93,97,98	0
3	SO4	C	1114	5/5	0.92	0.17	108,109,109,109	0
3	SO4	A	1119	5/5	0.92	0.28	96,97,98,100	0
4	GOL	C	1105	6/6	0.93	0.18	58,69,72,73	0
4	GOL	C	1113	6/6	0.93	0.23	59,70,77,79	0
4	GOL	A	1110	6/6	0.94	0.26	68,82,88,91	0
3	SO4	C	1101	5/5	0.97	0.21	45,46,48,50	0
4	GOL	A	1103	6/6	0.97	0.22	43,52,57,57	0
4	GOL	C	1102	6/6	0.98	0.17	41,49,50,51	0
5	AMP	B	101	23/23	0.98	0.14	22,33,41,42	0
5	AMP	D	101	23/23	0.98	0.16	20,34,44,49	0
3	SO4	A	1101	5/5	1.00	0.18	39,39,40,43	0

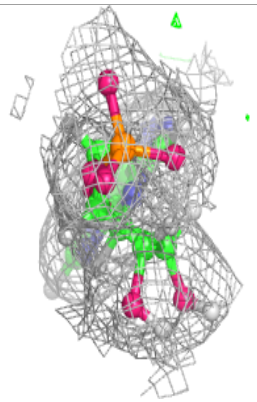
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 101:

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

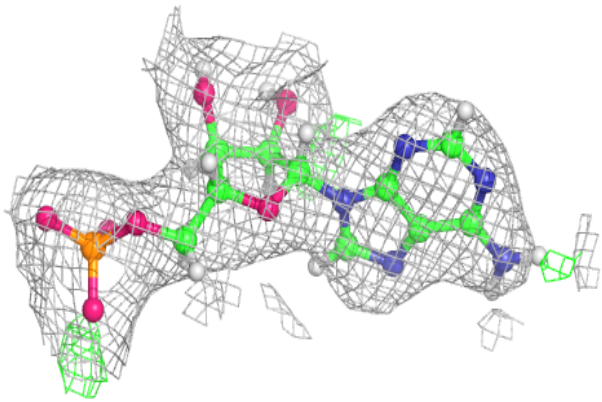


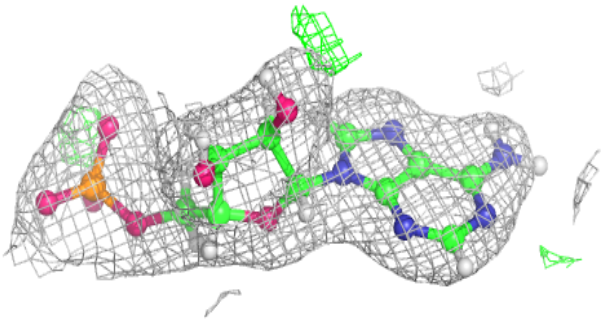


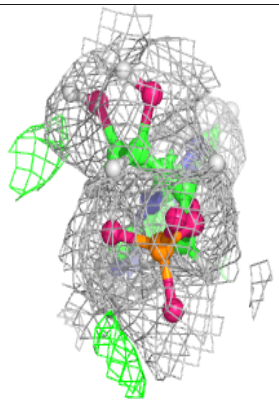


Electron density around AMP D 101:

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







6.5 Other polymers (i)

There are no such residues in this entry.