Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:40 PM GMT

PDB ID	:	1GQY
Title	:	MURC - CRYSTAL STRUCTURE OF THE ENZYME FROM HAEMOPHILUS INFLUENZAE COMPLEXED WITH AMPPCP
Authors	:	Skarzynski, T.; Cleasby, A.; Domenici, E.; Gevi, M.; Shaw, J.
Deposited on	:	2001-12-06
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

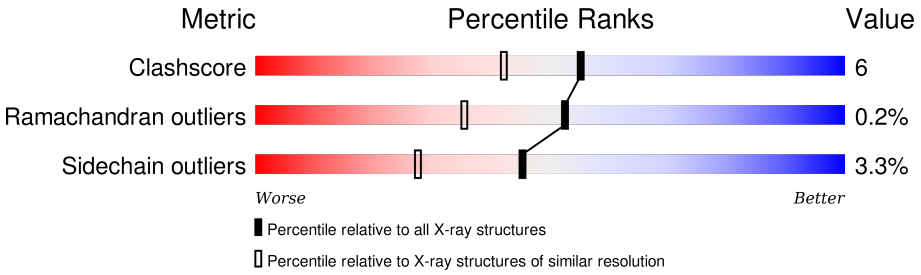
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	83% 15%
1	B	475	82% 16%

2 Entry composition

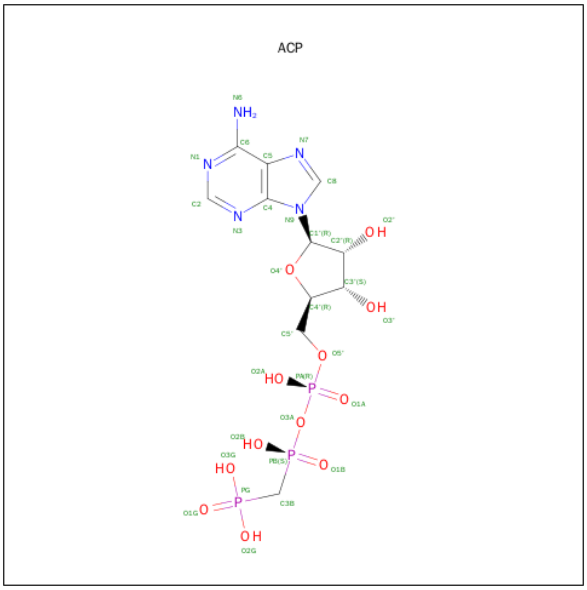
There are 4 unique types of molecules in this entry. The entry contains 8186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3595	2263	634	681	17			
1	B	469	Total	C	N	O	S	0	0	0
			3602	2268	631	686	17			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	413	Total O 413 413	0	0
4	B	512	Total O 512 512	0	0

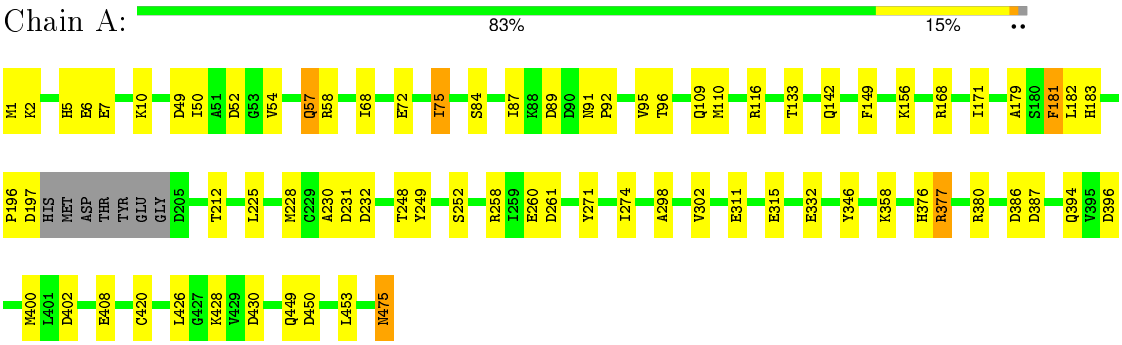
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

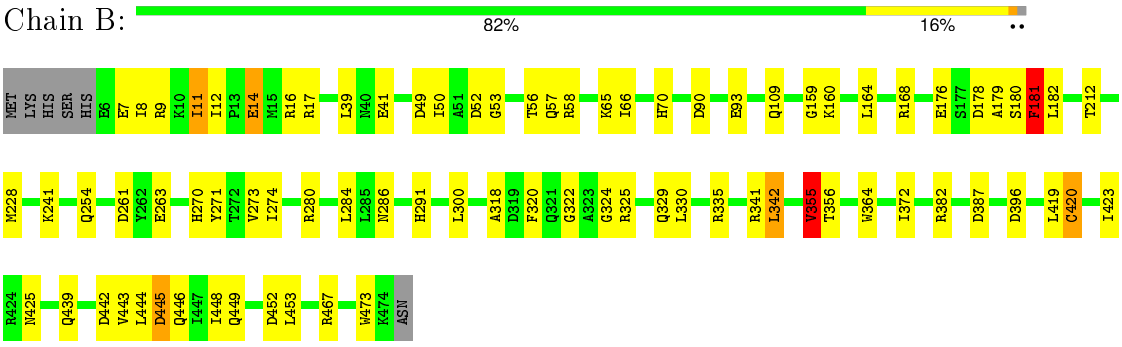
- Molecule 1: UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE

Chain A:



- Molecule 1: UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.60Å 93.20Å 86.80Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	89.5 (20.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8186	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACP

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	1.02	4/3656 (0.1%)	1.01	14/4942 (0.3%)
1	B	1.01	4/3664 (0.1%)	1.02	11/4956 (0.2%)
All	All	1.02	8/7320 (0.1%)	1.02	25/9898 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	VAL	CB-CG1	-11.46	1.28	1.52
1	A	271	TYR	CD2-CE2	6.42	1.49	1.39
1	A	346	TYR	CD1-CE1	6.25	1.48	1.39
1	B	420	CYS	CB-SG	-5.85	1.72	1.81
1	B	271	TYR	CD1-CE1	5.45	1.47	1.39
1	A	149	PHE	CE1-CZ	5.19	1.47	1.37
1	A	302	VAL	CB-CG1	5.15	1.63	1.52
1	B	273	VAL	CB-CG1	5.13	1.63	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	228	MET	CG-SD-CE	-11.49	81.81	100.20
1	A	228	MET	CG-SD-CE	-9.96	84.27	100.20
1	B	442	ASP	CB-CG-OD2	8.01	125.50	118.30
1	A	261	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	377	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	396	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	261	ASP	CB-CG-OD2	6.36	124.03	118.30
1	B	396	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	445	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	387	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	386	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	452	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	382	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	387	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	430	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	232	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	49	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	110	MET	CG-SD-CE	-5.35	91.64	100.20
1	B	90	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	89	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	450	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	453	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	B	356	THR	OG1-CB-CG2	-5.14	98.18	110.00
1	A	231	ASP	CB-CG-OD2	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3595	0	3602	45	0
1	B	3602	0	3598	46	0
2	A	31	0	14	0	0
2	B	31	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	413	0	0	11	0
4	B	512	0	0	9	0
All	All	8186	0	7228	91	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 6.

All (91) 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:B:180:SER:HA	4:B:2116:HOH:O	1.85	0.76
1:B:176:GLU:HB3	4:B:2215:HOH:O	1.88	0.72
1:B:330:LEU:HD12	1:B:342:LEU:HD13	1.74	0.70
1:A:449:GLN:NE2	4:A:2393:HOH:O	2.21	0.70
1:B:329:GLN:HB3	4:B:2393:HOH:O	1.91	0.69
1:B:8:ILE:HD13	1:B:41:GLU:HG2	1.74	0.69
1:A:400:MET:HG3	1:A:420:CYS:SG	2.33	0.68
1:B:449:GLN:NE2	4:B:2498:HOH:O	2.26	0.68
1:A:72:GLU:CG	1:A:96:THR:HG21	2.25	0.67
1:A:376:HIS:ND1	1:A:380:ARG:NH2	2.42	0.66
1:A:311:GLU:OE1	4:A:2258:HOH:O	2.12	0.66
1:A:91:ASN:O	1:A:95:VAL:HG12	1.95	0.65
1:A:168:ARG:HD3	4:A:2143:HOH:O	1.97	0.64
1:A:7:GLU:OE1	1:A:10:LYS:NZ	2.30	0.64
1:A:258:ARG:NE	1:A:260:GLU:OE2	2.28	0.63
1:A:92:PRO:O	1:A:96:THR:HG23	2.00	0.62
1:B:8:ILE:HD12	1:B:164:LEU:HD11	1.81	0.61
1:A:475:ASN:C	1:A:475:ASN:ND2	2.52	0.60
1:B:291:HIS:ND1	1:B:355:VAL:HG13	2.18	0.59
1:B:179:ALA:O	1:B:180:SER:C	2.41	0.58
1:A:1:MET:SD	1:A:6:GLU:HG2	2.43	0.58
1:A:142:GLN:NE2	1:A:315:GLU:OE1	2.36	0.56
1:A:84:SER:O	1:A:87:ILE:HG13	2.05	0.56
1:B:8:ILE:CD1	1:B:41:GLU:HG2	2.34	0.55
4:A:2254:HOH:O	1:B:16:ARG:HD3	2.06	0.55
1:B:263:GLU:HG3	4:B:2313:HOH:O	2.08	0.54
1:A:475:ASN:C	1:A:475:ASN:HD22	2.13	0.52
1:A:49:ASP:O	1:A:68:ILE:HA	2.09	0.52
1:A:156:LYS:NZ	4:A:2129:HOH:O	2.43	0.52
1:B:109:GLN:OE1	4:B:2125:HOH:O	2.19	0.52
1:A:197:ASP:HB2	4:A:2163:HOH:O	2.09	0.52
1:B:324:GLY:O	1:B:325:ARG:HB2	2.10	0.52
1:B:335:ARG:HD2	1:B:473:TRP:CE2	2.45	0.52
1:B:330:LEU:HD12	1:B:342:LEU:CD1	2.40	0.51
1:A:87:ILE:HD12	1:A:87:ILE:O	2.10	0.50
1:A:249:TYR:CZ	1:A:298:ALA:HB2	2.47	0.50
1:A:311:GLU:HG2	4:A:2259:HOH:O	2.10	0.50
1:B:159:GLY:C	1:B:160:LYS:HG2	2.32	0.50
1:A:109:GLN:OE1	1:A:183:HIS:CD2	2.65	0.50
1:B:364:TRP:CE2	1:B:453:LEU:HB2	2.46	0.50
1:A:179:ALA:HB1	1:A:182:LEU:HD12	1.93	0.50
1:A:116:ARG:HD3	4:A:2090:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HG22	1:B:12:ILE:CD1	2.43	0.49
1:A:181:PHE:HE2	1:A:212:THR:HG22	1.77	0.48
1:A:332:GLU:OE2	4:A:2283:HOH:O	2.20	0.48
1:B:439:GLN:O	1:B:443:VAL:HG23	2.12	0.48
1:B:270:HIS:CE1	1:B:284:LEU:HD13	2.48	0.48
1:B:70:HIS:HA	1:B:93:GLU:OE2	2.14	0.48
1:B:14:GLU:HG2	4:B:2009:HOH:O	2.13	0.48
1:A:258:ARG:NH2	1:A:260:GLU:OE2	2.45	0.48
1:A:72:GLU:HG3	1:A:96:THR:HG21	1.94	0.47
1:A:58:ARG:NH1	4:A:2048:HOH:O	2.37	0.47
1:A:377:ARG:NH1	1:A:408:GLU:OE2	2.39	0.47
1:A:75:ILE:HG23	1:A:75:ILE:O	2.13	0.47
1:A:1:MET:HE2	1:A:5:HIS:C	2.35	0.47
1:A:394:GLN:OE1	1:A:428:LYS:NZ	2.45	0.47
1:B:181:PHE:HE2	1:B:212:THR:HG22	1.80	0.46
1:A:72:GLU:CD	1:A:96:THR:HG21	2.35	0.46
1:B:56:THR:HG22	1:B:66:ILE:HG21	1.98	0.46
1:B:419:LEU:O	1:B:423:ILE:HG13	2.16	0.45
1:A:109:GLN:OE1	1:A:183:HIS:HD2	1.99	0.45
1:A:358:LYS:NZ	4:A:2308:HOH:O	2.47	0.44
1:B:53:GLY:O	1:B:57:GLN:HG2	2.16	0.44
1:B:448:ILE:HG23	1:B:449:GLN:N	2.32	0.44
1:B:14:GLU:H	1:B:14:GLU:HG2	1.54	0.44
1:A:230:ALA:HB2	1:A:248:THR:HB	1.99	0.44
1:A:1:MET:HE3	1:A:5:HIS:HB3	1.99	0.43
1:B:335:ARG:HD3	1:B:445:ASP:OD1	2.17	0.43
1:B:372:ILE:HD11	1:B:444:LEU:HD11	1.99	0.43
1:B:9:ARG:HA	1:B:12:ILE:O	2.19	0.43
1:B:56:THR:CG2	1:B:66:ILE:HG21	2.49	0.43
1:B:241:LYS:HD3	4:B:2093:HOH:O	2.19	0.43
1:B:291:HIS:CE1	1:B:355:VAL:HG13	2.54	0.43
1:B:274:ILE:HD12	1:B:280:ARG:HG2	2.00	0.43
1:B:448:ILE:CG2	1:B:449:GLN:N	2.81	0.42
1:A:54:VAL:O	1:A:58:ARG:HB2	2.20	0.42
1:A:274:ILE:N	1:A:274:ILE:HD12	2.35	0.42
1:B:320:PHE:CE2	1:B:322:GLY:HA2	2.55	0.42
1:B:50:ILE:HA	1:B:50:ILE:HD12	1.85	0.42
1:A:1:MET:CE	1:A:5:HIS:HB3	2.51	0.41
1:B:52:ASP:OD1	1:B:57:GLN:NE2	2.54	0.41
1:A:52:ASP:OD1	1:A:57:GLN:NE2	2.51	0.41
1:A:197:ASP:C	1:A:197:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:HB2	1:B:318:ALA:O	2.20	0.41
1:B:300:LEU:C	1:B:300:LEU:HD23	2.41	0.40
1:B:182:LEU:HB2	4:B:2217:HOH:O	2.21	0.40
1:A:2:LYS:HB3	1:A:2:LYS:HE2	1.61	0.40
1:A:133:THR:HG23	1:A:171:ILE:HG22	2.03	0.40
1:B:178:ASP:C	1:B:180:SER:N	2.75	0.40
1:B:291:HIS:CG	1:B:355:VAL:CG1	3.05	0.40
1:B:291:HIS:CG	1:B:355:VAL:HG13	2.56	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	464/475 (98%)	453 (98%)	10 (2%)	1 (0%)	52 35
1	B	467/475 (98%)	460 (98%)	6 (1%)	1 (0%)	52 35
All	All	931/950 (98%)	913 (98%)	16 (2%)	2 (0%)	52 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	PHE
1	A	196	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	381/387 (98%)	373 (98%)	8 (2%)	61 47
1	B	381/387 (98%)	364 (96%)	17 (4%)	34 16
All	All	762/774 (98%)	737 (97%)	25 (3%)	45 27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	57	GLN
1	A	75	ILE
1	A	181	PHE
1	A	225	LEU
1	A	252	SER
1	A	426	LEU
1	A	475	ASN
1	B	7	GLU
1	B	11	ILE
1	B	14	GLU
1	B	17	ARG
1	B	39	LEU
1	B	58	ARG
1	B	65	LYS
1	B	168	ARG
1	B	181	PHE
1	B	254	GLN
1	B	341	ARG
1	B	342	LEU
1	B	355	VAL
1	B	420	CYS
1	B	425	ASN
1	B	446	GLN
1	B	467	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	99	GLN
1	A	183	HIS

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Mol	Chain	Res	Type
1	A	475	ASN
1	B	57	GLN
1	B	61	GLN
1	B	99	GLN
1	B	185	GLN
1	B	254	GLN
1	B	394	GLN
1	B	449	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ACP	A	1476	3	25,33,33	2.90	8 (32%)	31,52,52	2.38	16 (51%)
2	ACP	B	1475	3	25,33,33	1.98	6 (24%)	31,52,52	1.78	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACP	A	1476	3	-	0/15/38/38	0/3/3/3
2	ACP	B	1475	3	-	0/15/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1476	ACP	PG-O1G	-5.88	1.37	1.50
2	A	1476	ACP	PB-O1B	-3.86	1.41	1.51
2	B	1475	ACP	PB-O1B	-3.70	1.42	1.51
2	A	1476	ACP	PA-O2A	-3.36	1.40	1.54
2	B	1475	ACP	PB-O2B	-2.32	1.50	1.56
2	B	1475	ACP	PA-O2A	-2.31	1.45	1.54
2	A	1476	ACP	PG-O2G	-2.09	1.49	1.54
2	B	1475	ACP	C3'-C4'	2.61	1.60	1.53
2	A	1476	ACP	C3'-C4'	2.83	1.60	1.53
2	A	1476	ACP	O2'-C2'	3.52	1.51	1.43
2	A	1476	ACP	C2-N3	3.66	1.38	1.32
2	B	1475	ACP	O2'-C2'	3.87	1.52	1.43
2	B	1475	ACP	O4'-C1'	5.58	1.48	1.41
2	A	1476	ACP	O4'-C1'	9.62	1.53	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1476	ACP	C4'-O4'-C1'	-3.94	105.39	109.72
2	B	1475	ACP	N6-C6-N1	-3.80	111.05	119.20
2	A	1476	ACP	O3G-PG-O1G	-3.38	103.76	112.40
2	A	1476	ACP	N6-C6-N1	-3.28	112.16	119.20
2	A	1476	ACP	O2'-C2'-C3'	-3.28	101.16	111.83
2	A	1476	ACP	O4'-C1'-N9	-2.82	102.20	108.10
2	B	1475	ACP	O2'-C2'-C3'	-2.77	102.82	111.83
2	A	1476	ACP	C4-C5-N7	-2.68	107.02	109.48
2	B	1475	ACP	O4'-C1'-N9	-2.50	102.86	108.10
2	A	1476	ACP	C1'-N9-C4	-2.48	123.21	126.94
2	A	1476	ACP	O5'-PA-O1A	-2.38	100.38	109.62
2	A	1476	ACP	O3G-PG-C3B	-2.00	101.55	106.40
2	A	1476	ACP	O2B-PB-C3B	2.03	115.71	106.88
2	B	1475	ACP	O2A-PA-O3A	2.07	114.51	105.09
2	A	1476	ACP	O3G-PG-O2G	2.11	114.32	108.13
2	A	1476	ACP	O4'-C4'-C3'	2.27	109.72	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1475	ACP	C2'-C1'-N9	2.60	118.27	114.29
2	A	1476	ACP	O2A-PA-O3A	2.69	117.31	105.09
2	A	1476	ACP	O2G-PG-O1G	2.85	119.70	112.40
2	B	1475	ACP	O3G-PG-O2G	3.24	117.61	108.13
2	B	1475	ACP	C4'-O4'-C1'	3.88	113.98	109.72
2	A	1476	ACP	N3-C2-N1	4.27	132.16	128.89
2	A	1476	ACP	C2'-C1'-N9	5.41	122.55	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.