



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2016 – 11:12 AM GMT

PDB ID : 5BPH
Title : Crystal structure of AMP complexed D-alanine-D-alanine ligase(DDL) from *Yersinia pestis*
Authors : Tran, H.T.; Kang, L.W.; Hong, M.K.
Deposited on : 2015-05-28
Resolution : 1.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

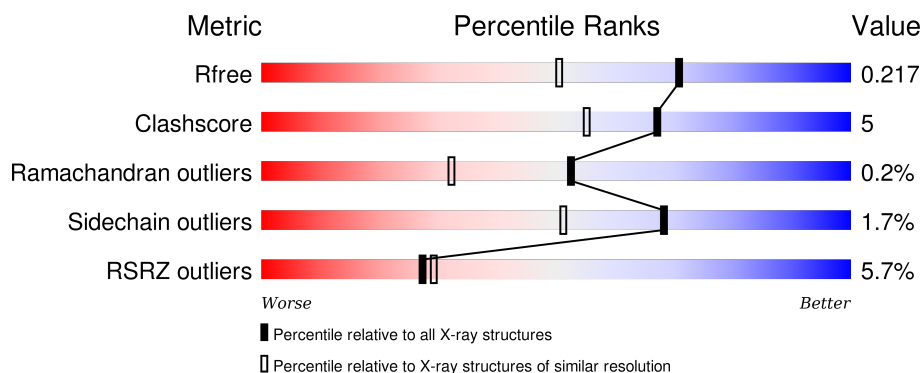
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
1	B	306	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	C	306	<div> <div>8%</div> <div>91%</div> <div>9%</div> </div>
1	D	306	<div> <div>9%</div> <div>84%</div> <div>13%</div> <div>...</div> </div>

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	ACT	D	406	-	-	X	X
5	GOL	D	405	-	-	-	X

2 Entry composition [i](#)

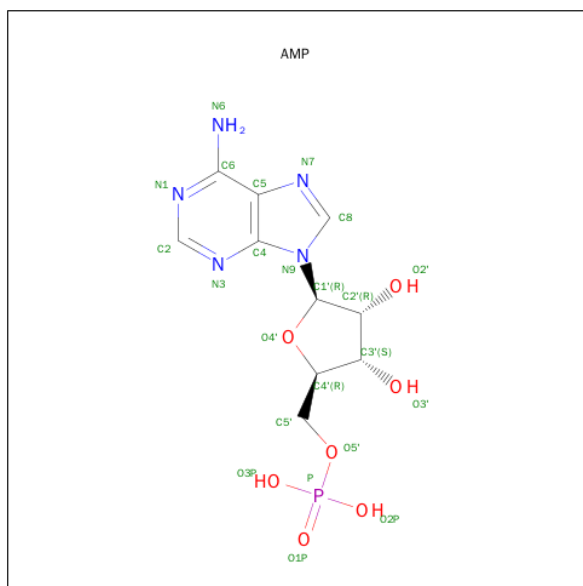
There are 6 unique types of molecules in this entry. The entry contains 10189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	B	305	Total	C	N	O	S	0	0	0
			2324	1482	383	449	10			
1	C	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	D	303	Total	C	N	O	S	0	0	0
			2308	1470	381	446	11			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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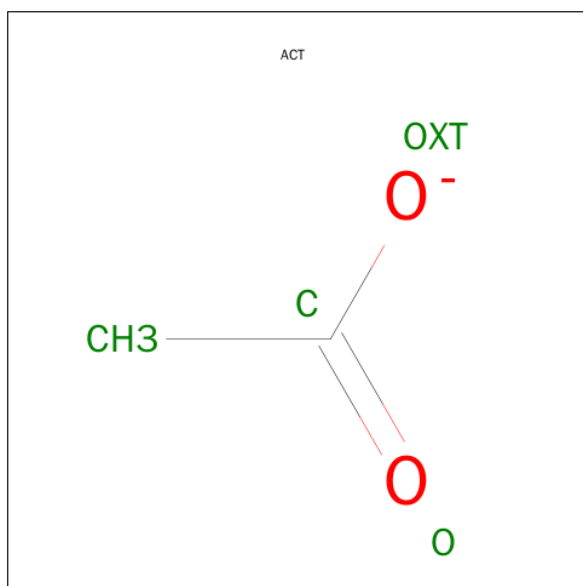
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	2	Total	Na	0	0
			2	2		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

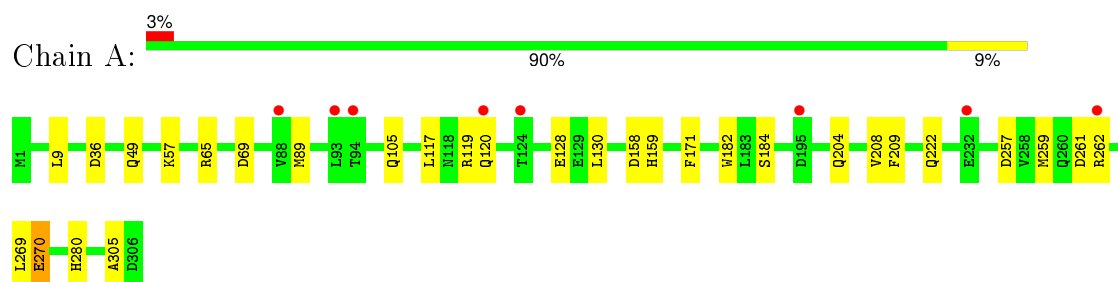
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total 221	O 221	0	0
6	B	216	Total 216	O 216	0	0
6	C	146	Total 146	O 146	0	0
6	D	147	Total 147	O 147	0	0

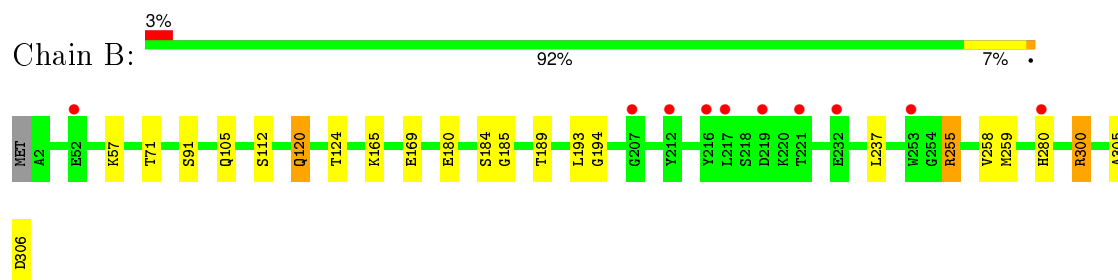
3 Residue-property plots

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.

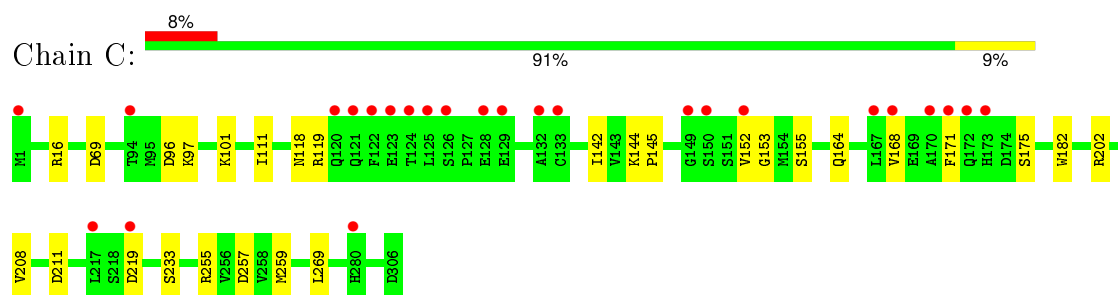
- Molecule 1: D-alanine–D-alanine ligase



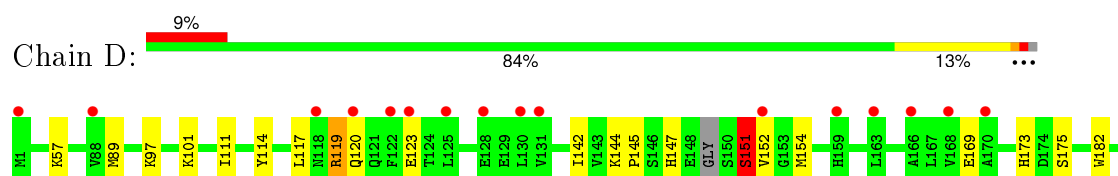
- Molecule 1: D-alanine–D-alanine ligase

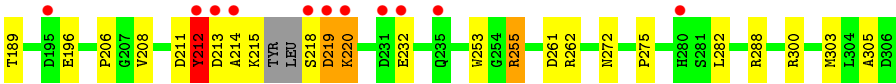


- Molecule 1: D-alanine–D-alanine ligase



- Molecule 1: D-alanine–D-alanine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 106.07Å 210.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 1.70 34.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.96-1.70) 99.6 (34.96-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.209 0.187 , 0.217	Depositor DCC
R_{free} test set	7688 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 153242 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10189	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ACT, NA, 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	1.10	1/2379 (0.0%)	1.13	7/3226 (0.2%)
1	B	1.15	6/2371 (0.3%)	1.10	6/3216 (0.2%)
1	C	1.05	0/2379	1.02	5/3226 (0.2%)
1	D	0.96	2/2352 (0.1%)	1.15	8/3186 (0.3%)
All	All	1.07	9/9481 (0.1%)	1.10	26/12854 (0.2%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	GLY	N-CA	8.99	1.59	1.46
1	A	105	GLN	CD-NE2	6.30	1.48	1.32
1	B	91	SER	CA-CB	5.79	1.61	1.52
1	B	105	GLN	CD-NE2	5.60	1.46	1.32
1	B	112	SER	CB-OG	5.43	1.49	1.42
1	B	194	GLY	C-O	-5.35	1.15	1.23
1	B	180	GLU	CD-OE2	5.34	1.31	1.25
1	D	196	GLU	CG-CD	5.31	1.59	1.51
1	D	288	ARG	C-O	5.18	1.33	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	MET	CG-SD-CE	-19.47	69.05	100.20
1	A	89	MET	CG-SD-CE	-18.89	69.98	100.20
1	D	303	MET	CG-SD-CE	-17.48	72.23	100.20
1	B	259	MET	CA-CB-CG	10.79	131.64	113.30
1	D	300	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	D	300	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	D	255	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	261	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	255	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	185	GLY	N-CA-C	-7.11	95.33	113.10
1	C	16	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	105	GLN	CA-CB-CG	6.44	127.58	113.40
1	C	96	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	69	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	261	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	306	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	158	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	257	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	300	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	105	GLN	CA-CB-CG	5.63	125.79	113.40
1	C	202	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	196	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	C	211	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	C	69	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	36	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	196	GLU	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2332	0	2323	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2324	0	2311	9	0
1	C	2332	0	2323	26	0
1	D	2308	0	2298	38	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	2	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	4	0	3	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	8	0	6	2	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	D	12	0	16	0	0
6	A	221	0	0	5	0
6	B	216	0	0	3	0
6	C	146	0	0	0	0
6	D	147	0	0	3	0
All	All	10189	0	9377	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 5.

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:C:142:ILE:HD11	1:C:182:TRP:CZ3	1.75	1.21
1:C:142:ILE:HD11	1:C:182:TRP:CE3	1.81	1.15
1:A:280:HIS:HE1	6:A:615:HOH:O	1.56	0.87
1:C:142:ILE:CD1	1:C:182:TRP:CE3	2.58	0.86
1:A:280:HIS:CE1	6:A:615:HOH:O	2.30	0.84
1:C:182:TRP:CH2	1:C:208:VAL:HG13	2.11	0.84
1:C:142:ILE:HD11	1:C:182:TRP:HZ3	1.42	0.84
1:C:142:ILE:CD1	1:C:182:TRP:HE3	2.03	0.71
1:B:280:HIS:CD2	6:B:509:HOH:O	2.43	0.71
1:A:49:GLN:HG2	6:A:650:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:O	1:D:212:TYR:CD2	2.44	0.70
1:D:262:ARG:NH2	6:D:501:HOH:O	2.23	0.69
1:C:142:ILE:CD1	1:C:182:TRP:CZ3	2.66	0.69
1:A:117:LEU:HD11	1:A:130:LEU:HD22	1.75	0.69
1:D:182:TRP:CH2	1:D:208:VAL:HG13	2.29	0.68
1:A:159:HIS:HD2	6:A:695:HOH:O	1.75	0.68
1:B:120:GLN:O	1:B:124:THR:HG22	1.94	0.67
1:D:152:VAL:HG21	1:D:173:HIS:CD2	2.30	0.66
1:D:212:TYR:HA	1:D:215:LYS:HB2	1.78	0.65
1:C:142:ILE:CG1	1:C:182:TRP:HE3	2.11	0.62
1:D:151:SER:HA	1:D:212:TYR:HE2	1.64	0.62
1:D:101:LYS:HE3	1:D:111:ILE:HD12	1.82	0.61
1:D:211:ASP:O	1:D:212:TYR:CG	2.53	0.61
1:B:300:ARG:NH2	6:B:501:HOH:O	2.33	0.61
1:C:182:TRP:HH2	1:C:208:VAL:HG13	1.61	0.61
1:D:218:SER:OG	1:D:220:LYS:N	2.23	0.61
1:B:189:THR:OG1	1:B:255:ARG:HG2	2.01	0.60
1:D:152:VAL:HG21	1:D:173:HIS:NE2	2.18	0.59
1:C:142:ILE:CG1	1:C:182:TRP:CE3	2.85	0.58
1:D:212:TYR:HD1	1:D:213:ASP:H	1.52	0.57
1:D:119:ARG:O	1:D:123:GLU:HG2	2.04	0.57
1:C:164:GLN:O	1:C:168:VAL:HG13	2.04	0.57
1:C:259:MET:HG3	1:C:269:LEU:HD11	1.87	0.56
1:D:182:TRP:HH2	1:D:208:VAL:HG13	1.70	0.56
1:C:182:TRP:CH2	1:C:208:VAL:CG1	2.88	0.55
1:D:144:LYS:HB3	1:D:154:MET:CE	2.36	0.55
1:D:212:TYR:HD1	1:D:213:ASP:N	2.05	0.55
1:B:71:THR:HG21	6:B:612:HOH:O	2.06	0.54
1:D:144:LYS:HB3	1:D:154:MET:HE2	1.90	0.54
1:A:204:GLN:NE2	1:A:222:GLN:OE1	2.41	0.53
1:B:237:LEU:HD11	1:B:258:VAL:HG21	1.91	0.53
1:C:255:ARG:NH1	1:C:257:ASP:OD1	2.41	0.53
1:D:97:LYS:O	1:D:101:LYS:HG3	2.08	0.52
1:C:119:ARG:NH2	1:C:171:PHE:O	2.43	0.52
1:A:208:VAL:HG23	1:A:209:PHE:CD2	2.44	0.52
1:C:142:ILE:HG12	1:C:182:TRP:HE3	1.73	0.52
1:C:142:ILE:CD1	1:C:182:TRP:HZ3	2.17	0.52
1:D:151:SER:HA	1:D:212:TYR:CE2	2.45	0.51
1:A:119:ARG:NH1	1:A:171:PHE:O	2.42	0.51
1:D:189:THR:OG1	1:D:255:ARG:HG2	2.12	0.50
1:C:97:LYS:O	1:C:101:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:SER:OG	1:D:219:ASP:N	2.45	0.50
1:A:262:ARG:NH1	6:A:505:HOH:O	2.44	0.49
1:C:118:ASN:HA	1:C:175:SER:O	2.12	0.49
1:D:101:LYS:HG3	6:D:610:HOH:O	2.12	0.49
1:D:57:LYS:HE3	1:D:305:ALA:O	2.13	0.49
1:A:159:HIS:HE1	1:C:233:SER:OG	1.96	0.48
1:A:259:MET:HG3	1:A:269:LEU:HD11	1.95	0.48
1:D:144:LYS:HE2	1:D:154:MET:CE	2.44	0.48
1:C:152:VAL:HG22	1:C:153:GLY:N	2.29	0.47
1:B:165:LYS:O	1:B:169:GLU:HG3	2.14	0.47
1:D:211:ASP:H	1:D:214:ALA:HB3	1.79	0.47
1:D:142:ILE:HD11	1:D:154:MET:CE	2.45	0.47
1:D:255:ARG:HH22	4:D:406:ACT:H3	1.80	0.47
1:D:169:GLU:HA	1:D:169:GLU:OE1	2.16	0.46
1:A:57:LYS:HE2	1:A:305:ALA:O	2.15	0.46
1:D:213:ASP:O	1:D:218:SER:N	2.49	0.46
1:D:142:ILE:HD11	1:D:154:MET:HE1	1.97	0.46
1:A:182:TRP:CH2	1:A:184:SER:HA	2.51	0.46
1:D:101:LYS:HG2	6:D:586:HOH:O	2.17	0.45
1:D:253:TRP:CH2	1:D:275:PRO:HD2	2.52	0.44
1:D:255:ARG:HH22	4:D:406:ACT:CH3	2.30	0.44
1:A:57:LYS:NZ	1:A:305:ALA:O	2.50	0.44
1:D:189:THR:HG21	1:D:282:LEU:HD13	1.99	0.44
1:D:101:LYS:HE2	1:D:114:TYR:CG	2.52	0.44
1:C:182:TRP:HH2	1:C:208:VAL:CG1	2.27	0.44
1:A:117:LEU:HD11	1:A:130:LEU:CD2	2.46	0.44
1:A:128:GLU:H	1:A:128:GLU:CD	2.21	0.44
1:D:212:TYR:CD1	1:D:213:ASP:N	2.83	0.43
1:A:269:LEU:C	1:A:270:GLU:HG3	2.39	0.43
1:C:142:ILE:HA	1:C:142:ILE:HD13	1.69	0.43
1:D:206:PRO:HB3	1:D:220:LYS:HB3	2.01	0.42
1:C:142:ILE:HD12	1:C:142:ILE:HG23	1.76	0.41
1:B:189:THR:OG1	1:B:255:ARG:CG	2.69	0.41
1:D:152:VAL:CG2	1:D:173:HIS:CD2	3.03	0.41
1:B:57:LYS:HE2	1:B:305:ALA:HB3	2.02	0.41
1:D:145:PRO:HB2	1:D:147:HIS:O	2.21	0.40
1:A:57:LYS:CE	1:A:305:ALA:O	2.69	0.40
1:A:9:LEU:HD12	1:A:9:LEU:C	2.42	0.40
1:C:101:LYS:HE3	1:C:111:ILE:HD12	2.02	0.40
1:C:144:LYS:HA	1:C:145:PRO:HD3	1.89	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	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	B	303/306 (99%)	295 (97%)	8 (3%)	0	100	100
1	C	304/306 (99%)	298 (98%)	6 (2%)	0	100	100
1	D	297/306 (97%)	288 (97%)	7 (2%)	2 (1%)	26	9
All	All	1208/1224 (99%)	1180 (98%)	26 (2%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	SER
1	D	212	TYR

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	251/251 (100%)	248 (99%)	3 (1%)	78	65
1	B	250/251 (100%)	248 (99%)	2 (1%)	86	79
1	C	251/251 (100%)	249 (99%)	2 (1%)	86	79
1	D	249/251 (99%)	239 (96%)	10 (4%)	38	16
All	All	1001/1004 (100%)	984 (98%)	17 (2%)	68	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	120	GLN
1	A	270	GLU
1	B	120	GLN
1	B	193	LEU
1	C	155	SER
1	C	219	ASP
1	D	117	LEU
1	D	119	ARG
1	D	120	GLN
1	D	151	SER
1	D	175	SER
1	D	212	TYR
1	D	219	ASP
1	D	220	LYS
1	D	232	GLU
1	D	272	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	173	HIS
1	A	204	GLN
1	B	120	GLN
1	B	265	HIS
1	B	280	HIS
1	C	105	GLN
1	C	265	HIS
1	D	105	GLN
1	D	272	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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	AMP	A	401	-	22,25,25	1.37	3 (13%)	22,38,38	1.51	3 (13%)
4	ACT	A	403	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	A	404	-	5,5,5	0.44	0	5,5,5	0.69	0
5	GOL	A	405	-	5,5,5	0.32	0	5,5,5	0.66	0
2	AMP	B	401	-	22,25,25	1.42	3 (13%)	22,38,38	1.25	2 (9%)
4	ACT	B	403	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	B	404	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	B	405	-	5,5,5	0.87	0	5,5,5	0.67	0
2	AMP	C	401	-	22,25,25	1.15	1 (4%)	22,38,38	2.27	4 (18%)
4	ACT	C	403	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	C	404	-	5,5,5	0.12	0	5,5,5	0.48	0
5	GOL	C	405	-	5,5,5	0.84	0	5,5,5	1.34	1 (20%)
2	AMP	D	401	-	22,25,25	1.05	2 (9%)	22,38,38	1.82	5 (22%)
4	ACT	D	403	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	D	404	-	5,5,5	0.21	0	5,5,5	1.07	0
5	GOL	D	405	-	5,5,5	0.17	0	5,5,5	1.08	0
4	ACT	D	406	-	0,3,3	0.00	-	0,3,3	0.00	-

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	AMP	A	401	-	-	0/6/26/26	0/3/3/3
4	ACT	A	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	404	-	-	0/4/4/4	0/0/0/0
5	GOL	A	405	-	-	0/4/4/4	0/0/0/0
2	AMP	B	401	-	-	0/6/26/26	0/3/3/3
4	ACT	B	403	-	-	0/0/0/0	0/0/0/0
4	ACT	B	404	-	-	0/0/0/0	0/0/0/0
5	GOL	B	405	-	-	0/4/4/4	0/0/0/0
2	AMP	C	401	-	-	0/6/26/26	0/3/3/3
4	ACT	C	403	-	-	0/0/0/0	0/0/0/0
5	GOL	C	404	-	-	0/4/4/4	0/0/0/0
5	GOL	C	405	-	-	0/4/4/4	0/0/0/0
2	AMP	D	401	-	-	0/6/26/26	0/3/3/3
4	ACT	D	403	-	-	0/0/0/0	0/0/0/0
5	GOL	D	404	-	-	0/4/4/4	0/0/0/0
5	GOL	D	405	-	-	0/4/4/4	0/0/0/0
4	ACT	D	406	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	AMP	C2'-C1'	-2.70	1.49	1.53
2	A	401	AMP	C2'-C1'	-2.53	1.49	1.53
2	D	401	AMP	P-O2P	-2.41	1.46	1.54
2	A	401	AMP	C2'-C3'	-2.06	1.47	1.53
2	D	401	AMP	O4'-C1'	2.56	1.44	1.41
2	B	401	AMP	C5-C4	2.68	1.46	1.40
2	B	401	AMP	P-O5'	3.18	1.69	1.59
2	B	401	AMP	C2-N3	3.22	1.37	1.32
2	A	401	AMP	C5-C4	3.54	1.48	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	AMP	O5'-P-O1P	-7.11	89.21	107.08
2	A	401	AMP	N3-C2-N1	-5.34	124.68	128.87
2	B	401	AMP	N3-C2-N1	-3.49	126.13	128.87
2	D	401	AMP	O3P-P-O5'	-2.74	98.74	106.72
2	C	401	AMP	O3P-P-O5'	-2.38	99.77	106.72
2	D	401	AMP	O2P-P-O1P	-2.30	103.13	110.63
2	A	401	AMP	O2'-C2'-C1'	-2.23	104.65	111.61
2	A	401	AMP	O2P-P-O1P	2.05	117.31	110.63
5	C	405	GOL	O3-C3-C2	2.28	121.51	109.97
2	B	401	AMP	C4'-O4'-C1'	2.50	112.30	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	AMP	O2P-P-O5'	2.90	115.18	106.72
2	D	401	AMP	O3P-P-O2P	3.06	118.66	107.44
2	C	401	AMP	O2P-P-O5'	3.74	117.63	106.72
2	D	401	AMP	N3-C2-N1	5.60	133.27	128.87
2	C	401	AMP	O3P-P-O2P	5.69	128.33	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	406	ACT	2	0

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, 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	306/306 (100%)	0.02	8 (2%) 59 64	16, 24, 41, 62	0
1	B	305/306 (99%)	0.16	10 (3%) 50 54	16, 25, 45, 70	0
1	C	306/306 (100%)	0.31	25 (8%) 14 16	16, 26, 58, 79	0
1	D	303/306 (99%)	0.53	27 (8%) 12 13	17, 32, 61, 93	0
All	All	1220/1224 (99%)	0.25	70 (5%) 27 29	16, 27, 54, 93	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	TYR	10.3
1	D	1	MET	6.0
1	C	125	LEU	5.1
1	D	213	ASP	5.0
1	C	124	THR	4.7
1	B	216	TYR	4.5
1	C	149	GLY	4.3
1	D	220	LYS	4.1
1	C	120	GLN	4.0
1	D	219	ASP	4.0
1	C	132	ALA	4.0
1	B	217	LEU	3.8
1	D	120	GLN	3.7
1	C	150	SER	3.7
1	D	130	LEU	3.6
1	B	219	ASP	3.4
1	A	120	GLN	3.4
1	D	218	SER	3.3
1	D	280	HIS	3.3
1	C	171	PHE	3.2
1	C	217	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	VAL	3.1
1	D	128	GLU	3.0
1	B	280	HIS	3.0
1	D	131	VAL	2.9
1	C	170	ALA	2.9
1	B	212	TYR	2.9
1	C	123	GLU	2.9
1	A	232	GLU	2.9
1	C	172	GLN	2.8
1	D	170	ALA	2.8
1	D	214	ALA	2.7
1	C	133	CYS	2.7
1	C	126	SER	2.7
1	C	1	MET	2.7
1	B	253	TRP	2.7
1	D	123	GLU	2.6
1	D	122	PHE	2.6
1	C	121	GLN	2.6
1	D	231	ASP	2.6
1	A	262	ARG	2.6
1	C	168	VAL	2.6
1	C	122	PHE	2.5
1	C	280	HIS	2.5
1	D	163	LEU	2.5
1	C	167	LEU	2.5
1	A	195	ASP	2.4
1	C	173	HIS	2.4
1	C	128	GLU	2.4
1	B	52	GLU	2.3
1	D	125	LEU	2.3
1	D	235	GLN	2.3
1	D	118	ASN	2.3
1	A	93	LEU	2.3
1	B	207	GLY	2.2
1	D	166	ALA	2.2
1	D	152	VAL	2.2
1	C	129	GLU	2.2
1	D	195	ASP	2.1
1	B	232	GLU	2.1
1	D	88	VAL	2.1
1	C	152	VAL	2.1
1	C	219	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	221	THR	2.0
1	D	159	HIS	2.0
1	D	232	GLU	2.0
1	A	94	THR	2.0
1	A	88	VAL	2.0
1	A	124	THR	2.0
1	C	94	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	D	405	6/6	0.92	0.16	3.78	33,47,50,51	0
4	ACT	D	406	4/4	0.73	0.24	2.23	36,40,43,49	0
5	GOL	C	404	6/6	0.87	0.13	1.17	30,45,46,55	0
5	GOL	A	404	6/6	0.86	0.14	1.01	32,53,56,62	0
5	GOL	B	405	6/6	0.85	0.14	0.80	36,46,47,49	0
5	GOL	C	405	6/6	0.87	0.11	0.55	28,42,45,46	0
4	ACT	D	403	4/4	0.86	0.14	0.50	38,41,41,42	0
5	GOL	A	405	6/6	0.91	0.15	0.50	36,45,53,55	0
4	ACT	C	403	4/4	0.91	0.12	0.43	33,41,42,42	0
5	GOL	D	404	6/6	0.92	0.11	0.26	32,43,48,49	0
4	ACT	B	403	4/4	0.89	0.13	-0.16	32,37,38,42	0
2	AMP	C	401	23/23	0.96	0.10	-0.29	23,26,35,42	0
2	AMP	A	401	23/23	0.98	0.09	-0.36	20,23,27,29	0
2	AMP	B	401	23/23	0.95	0.08	-0.72	21,25,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	C	402	1/1	0.99	0.12	-0.73	18,18,18,18	0
4	ACT	B	404	4/4	0.96	0.08	-0.83	27,29,31,31	0
2	AMP	D	401	23/23	0.97	0.07	-1.24	22,30,40,45	0
3	NA	B	402	1/1	0.99	0.11	-1.54	18,18,18,18	0
4	ACT	A	403	4/4	0.97	0.07	-1.93	25,26,27,30	0
3	NA	A	402	1/1	1.00	0.06	-3.02	17,17,17,17	0
3	NA	D	402	1/1	0.99	0.07	-4.35	20,20,20,20	0
3	NA	A	406	1/1	0.91	0.08	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.