Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:57 AM GMT

PDB ID	:	2VD6
Title	:	Human adenylosuccinate lyase in complex with its substrate N6-(1,2-Dicarboxyethyl)-AMP, and its products AMP and fumarate.
Authors	:	Stenmark, P.; Moche, M.; Arrowsmith, C.; Berglund, H.; Busam, R.; Collins, R.; Dahlgren, L.G.; Edwards, A.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg-schiavone, L.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Nilsson, M.; Nyman, T.; Ogg, D.; Persson, C.; Sagemark, J.; Sundstrom, M.; Thorsell, A.G.; Tresaugues, L.; van den Berg, S.; Weigelt, J.; Welin, M.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on	:	2007-09-30
Resolution	:	2.00 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 (1)) were used in the production of this report:

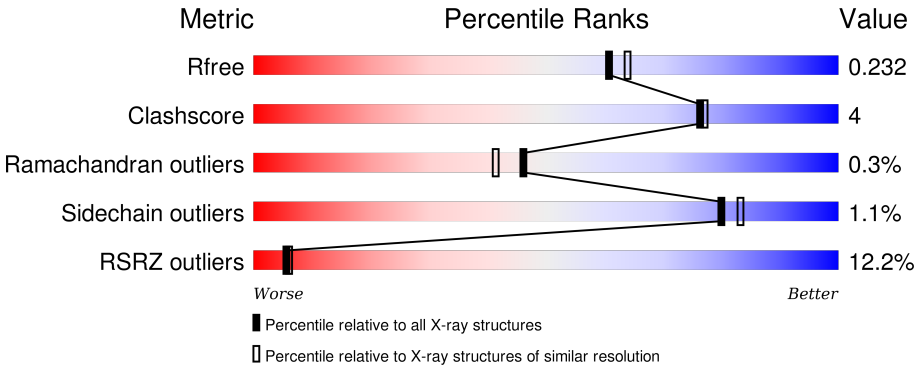
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	503	11% 84% 7% 8%
1	B	503	12% 84% 7% 8%
1	C	503	10% 82% 8% 9%
1	D	503	12% 84% 8% • 8%

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	B	1004	-	-	-	X
4	GOL	C	1003	-	-	-	X
5	CL	C	2002	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15817 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	4	0
			3706	2333	657	690	26			
1	B	461	Total	C	N	O	S	0	1	0
			3685	2322	654	683	26			
1	C	457	Total	C	N	O	S	0	4	0
			3681	2318	656	682	25			
1	D	462	Total	C	N	O	S	0	3	0
			3704	2334	657	687	26			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P30566
A	-20	HIS	-	EXPRESSION TAG	UNP P30566
A	-19	HIS	-	EXPRESSION TAG	UNP P30566
A	-18	HIS	-	EXPRESSION TAG	UNP P30566
A	-17	HIS	-	EXPRESSION TAG	UNP P30566
A	-16	HIS	-	EXPRESSION TAG	UNP P30566
A	-15	HIS	-	EXPRESSION TAG	UNP P30566
A	-14	SER	-	EXPRESSION TAG	UNP P30566
A	-13	SER	-	EXPRESSION TAG	UNP P30566
A	-12	GLY	-	EXPRESSION TAG	UNP P30566
A	-11	VAL	-	EXPRESSION TAG	UNP P30566
A	-10	ASP	-	EXPRESSION TAG	UNP P30566
A	-9	LEU	-	EXPRESSION TAG	UNP P30566
A	-8	GLY	-	EXPRESSION TAG	UNP P30566
A	-7	THR	-	EXPRESSION TAG	UNP P30566
A	-6	GLU	-	EXPRESSION TAG	UNP P30566
A	-5	ASN	-	EXPRESSION TAG	UNP P30566
A	-4	LEU	-	EXPRESSION TAG	UNP P30566
A	-3	TYR	-	EXPRESSION TAG	UNP P30566
A	-2	PHE	-	EXPRESSION TAG	UNP P30566
A	-1	GLN	-	EXPRESSION TAG	UNP P30566

Continued on next page...

Continued from previous page...

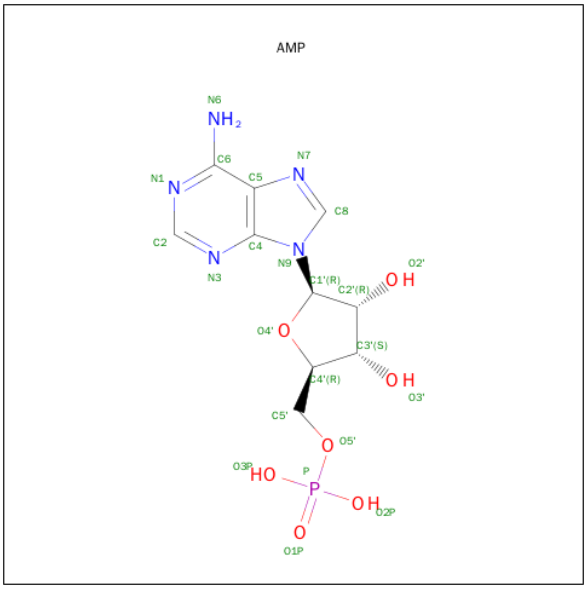
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P30566
B	-21	MET	-	EXPRESSION TAG	UNP P30566
B	-20	HIS	-	EXPRESSION TAG	UNP P30566
B	-19	HIS	-	EXPRESSION TAG	UNP P30566
B	-18	HIS	-	EXPRESSION TAG	UNP P30566
B	-17	HIS	-	EXPRESSION TAG	UNP P30566
B	-16	HIS	-	EXPRESSION TAG	UNP P30566
B	-15	HIS	-	EXPRESSION TAG	UNP P30566
B	-14	SER	-	EXPRESSION TAG	UNP P30566
B	-13	SER	-	EXPRESSION TAG	UNP P30566
B	-12	GLY	-	EXPRESSION TAG	UNP P30566
B	-11	VAL	-	EXPRESSION TAG	UNP P30566
B	-10	ASP	-	EXPRESSION TAG	UNP P30566
B	-9	LEU	-	EXPRESSION TAG	UNP P30566
B	-8	GLY	-	EXPRESSION TAG	UNP P30566
B	-7	THR	-	EXPRESSION TAG	UNP P30566
B	-6	GLU	-	EXPRESSION TAG	UNP P30566
B	-5	ASN	-	EXPRESSION TAG	UNP P30566
B	-4	LEU	-	EXPRESSION TAG	UNP P30566
B	-3	TYR	-	EXPRESSION TAG	UNP P30566
B	-2	PHE	-	EXPRESSION TAG	UNP P30566
B	-1	GLN	-	EXPRESSION TAG	UNP P30566
B	0	SER	-	EXPRESSION TAG	UNP P30566
C	-21	MET	-	EXPRESSION TAG	UNP P30566
C	-20	HIS	-	EXPRESSION TAG	UNP P30566
C	-19	HIS	-	EXPRESSION TAG	UNP P30566
C	-18	HIS	-	EXPRESSION TAG	UNP P30566
C	-17	HIS	-	EXPRESSION TAG	UNP P30566
C	-16	HIS	-	EXPRESSION TAG	UNP P30566
C	-15	HIS	-	EXPRESSION TAG	UNP P30566
C	-14	SER	-	EXPRESSION TAG	UNP P30566
C	-13	SER	-	EXPRESSION TAG	UNP P30566
C	-12	GLY	-	EXPRESSION TAG	UNP P30566
C	-11	VAL	-	EXPRESSION TAG	UNP P30566
C	-10	ASP	-	EXPRESSION TAG	UNP P30566
C	-9	LEU	-	EXPRESSION TAG	UNP P30566
C	-8	GLY	-	EXPRESSION TAG	UNP P30566
C	-7	THR	-	EXPRESSION TAG	UNP P30566
C	-6	GLU	-	EXPRESSION TAG	UNP P30566
C	-5	ASN	-	EXPRESSION TAG	UNP P30566
C	-4	LEU	-	EXPRESSION TAG	UNP P30566
C	-3	TYR	-	EXPRESSION TAG	UNP P30566

Continued on next page...

Continued from previous page...

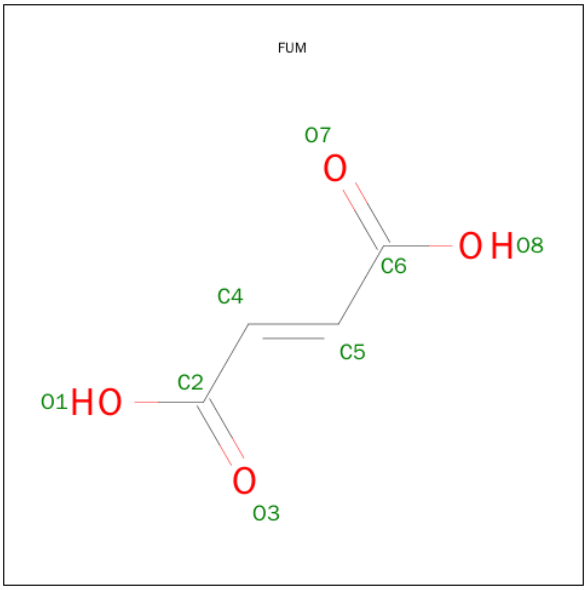
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	EXPRESSION TAG	UNP P30566
C	-1	GLN	-	EXPRESSION TAG	UNP P30566
C	0	SER	-	EXPRESSION TAG	UNP P30566
D	-21	MET	-	EXPRESSION TAG	UNP P30566
D	-20	HIS	-	EXPRESSION TAG	UNP P30566
D	-19	HIS	-	EXPRESSION TAG	UNP P30566
D	-18	HIS	-	EXPRESSION TAG	UNP P30566
D	-17	HIS	-	EXPRESSION TAG	UNP P30566
D	-16	HIS	-	EXPRESSION TAG	UNP P30566
D	-15	HIS	-	EXPRESSION TAG	UNP P30566
D	-14	SER	-	EXPRESSION TAG	UNP P30566
D	-13	SER	-	EXPRESSION TAG	UNP P30566
D	-12	GLY	-	EXPRESSION TAG	UNP P30566
D	-11	VAL	-	EXPRESSION TAG	UNP P30566
D	-10	ASP	-	EXPRESSION TAG	UNP P30566
D	-9	LEU	-	EXPRESSION TAG	UNP P30566
D	-8	GLY	-	EXPRESSION TAG	UNP P30566
D	-7	THR	-	EXPRESSION TAG	UNP P30566
D	-6	GLU	-	EXPRESSION TAG	UNP P30566
D	-5	ASN	-	EXPRESSION TAG	UNP P30566
D	-4	LEU	-	EXPRESSION TAG	UNP P30566
D	-3	TYR	-	EXPRESSION TAG	UNP P30566
D	-2	PHE	-	EXPRESSION TAG	UNP P30566
D	-1	GLN	-	EXPRESSION TAG	UNP P30566
D	0	SER	-	EXPRESSION TAG	UNP P30566

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



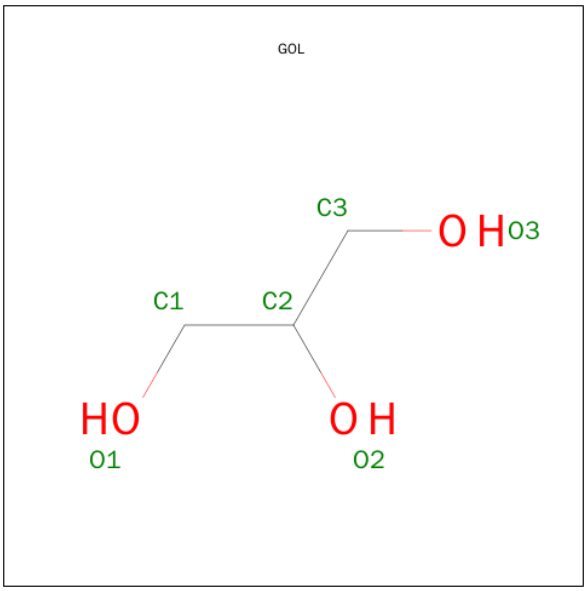
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



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

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

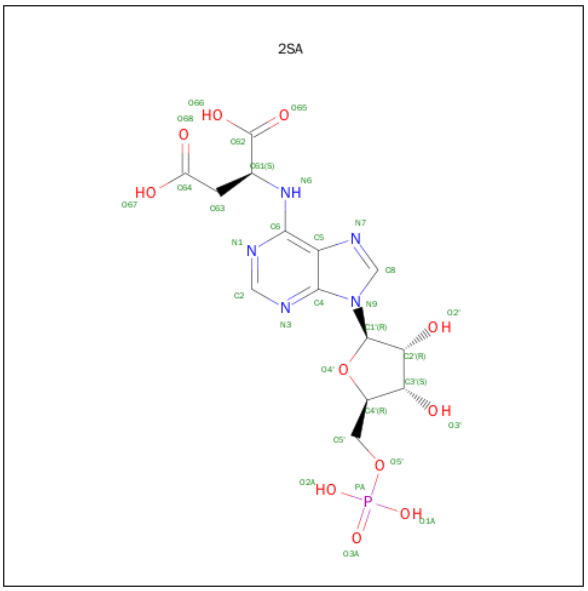


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Cl 2 2	0	0
5	A	2	Total Cl 2 2	0	0
5	D	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is 2-[9-(3,4-DIHYDROXY-5-PHOSPHONOOXYMETHYL-TETRAHYDRO-FURAN-2-YL)-9H-PURIN-6-YLAMINO]-SUCCINIC ACID (three-letter code: 2SA) (formula: $C_{14}H_{18}N_5O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			31	14	5	11	1		
6	D	1	Total	C	N	O	P	0	0
			31	14	5	11	1		

- Molecule 7 is water.

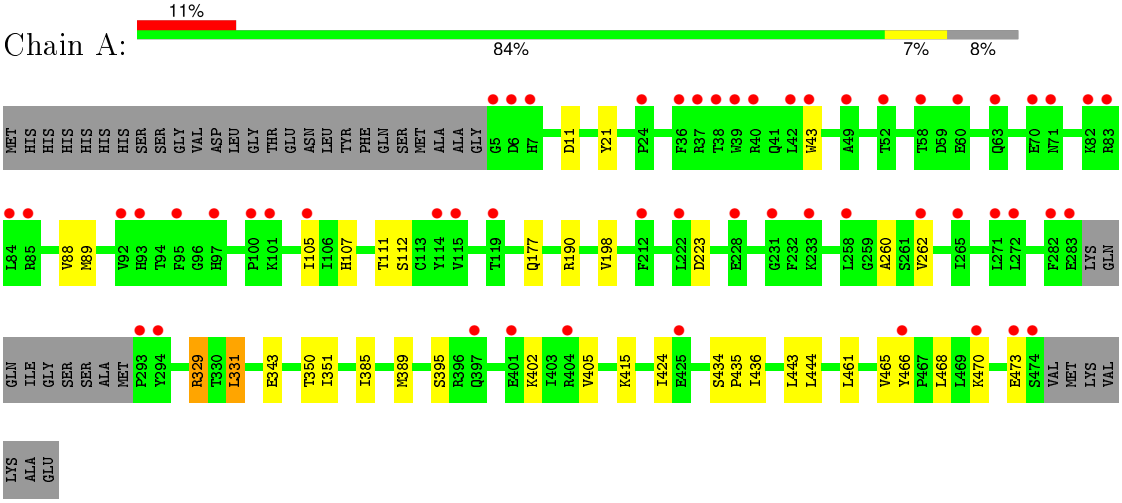
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	247	Total	O	0	0
			247	247		
7	B	158	Total	O	0	0
			158	158		
7	C	235	Total	O	0	0
			235	235		
7	D	240	Total	O	0	0
			240	240		

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.

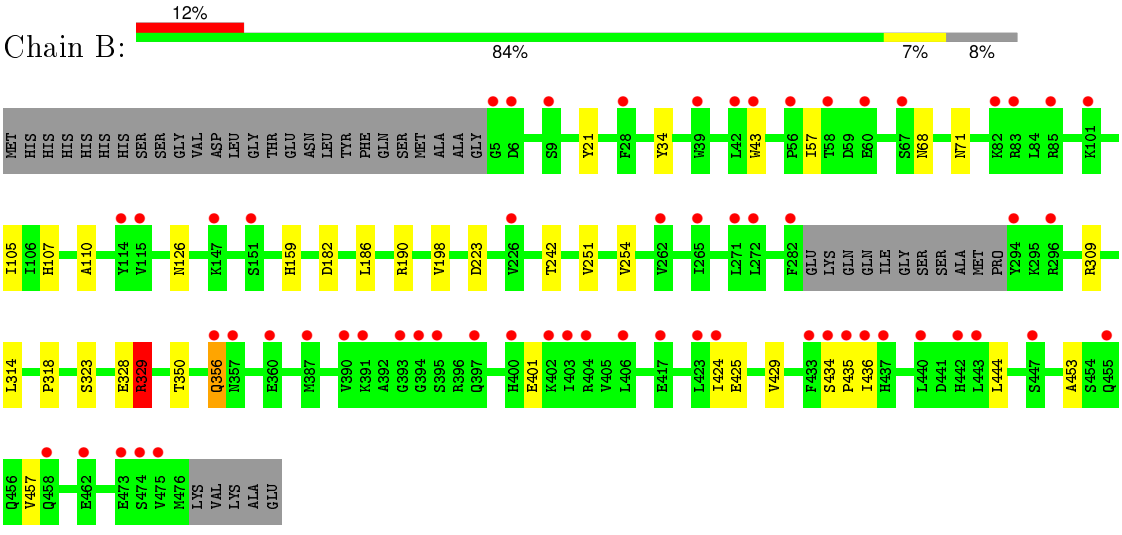
- Molecule 1: ADENYLOSUCCINATE LYASE

Chain A:



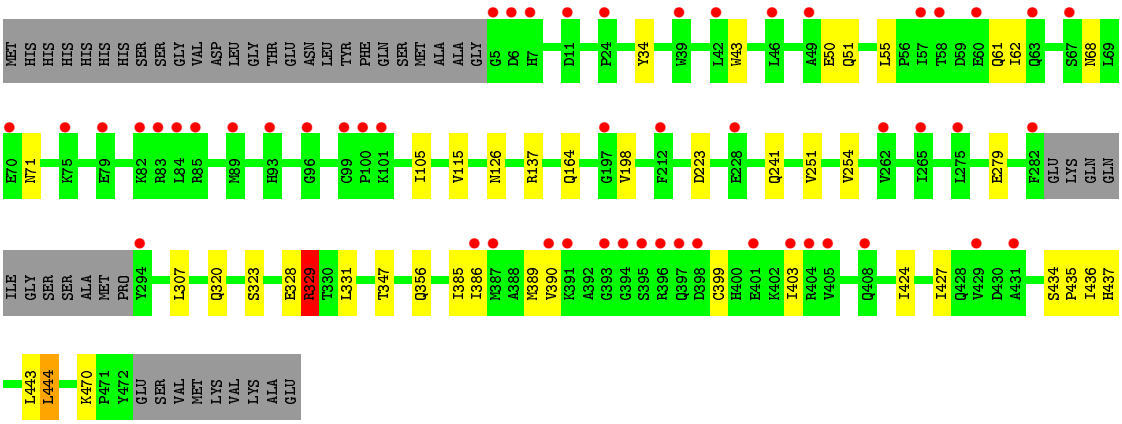
- Molecule 1: ADENYLOSUCCINATE LYASE

Chain B:



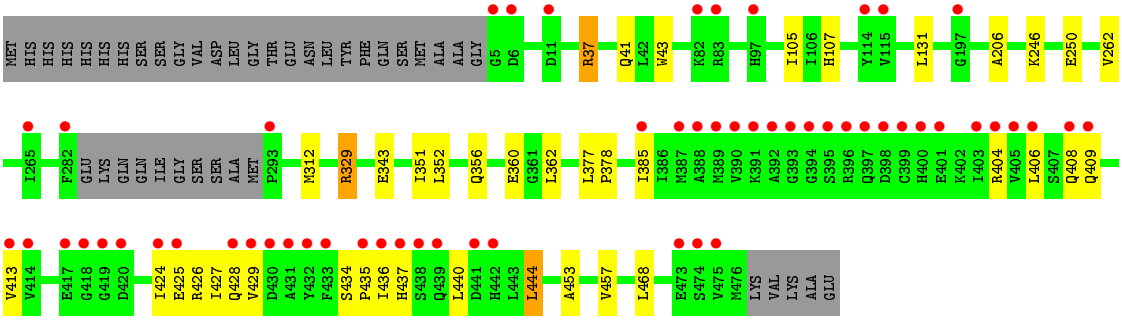
- Molecule 1: ADENYLOSUCCINATE LYASE

Chain C:



- Molecule 1: ADENYLOSUCCINATE LYASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.30Å 128.10Å 190.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 24.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.00) 99.8 (24.83-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.192 , 0.229 0.197 , 0.232	Depositor DCC
R_{free} test set	7207 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 144135 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15817	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.375 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, AMP, FUM, 2SA, CL

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	0.45	0/3778	0.58	0/5101
1	B	0.38	0/3756	0.53	0/5071
1	C	0.45	2/3752 (0.1%)	0.58	0/5066
1	D	0.40	0/3779	0.57	0/5102
All	All	0.42	2/15065 (0.0%)	0.56	0/20340

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	GLN	CD-OE1	6.87	1.39	1.24
1	C	61	GLN	CD-NE2	5.36	1.46	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3706	0	3711	31	0
1	B	3685	0	3698	28	0
1	C	3681	0	3689	30	0
1	D	3704	0	3718	27	0
2	A	23	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	23	0	12	3	0
3	A	8	0	2	2	0
3	C	8	0	2	2	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	B	31	0	14	1	0
6	D	31	0	14	1	0
7	A	247	0	0	3	0
7	B	158	0	0	0	0
7	C	235	0	0	0	0
7	D	240	0	0	1	0
All	All	15817	0	14912	114	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 (114) 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:328:GLU:O	1:B:329:ARG:HB2	1.64	0.98
1:B:424:ILE:CD1	1:B:444:LEU:HD11	2.04	0.88
1:D:424:ILE:HD12	1:D:444:LEU:HD21	1.58	0.86
1:A:424:ILE:HD12	1:A:444:LEU:HD11	1.60	0.84
1:A:331:LEU:HD13	1:B:159:HIS:CE1	2.16	0.81
1:B:424:ILE:HD12	1:B:444:LEU:HD11	1.61	0.80
1:A:424:ILE:CD1	1:A:444:LEU:HD11	2.16	0.76
1:B:57:ILE:HG23	1:B:105:ILE:HD13	1.68	0.75
1:C:164[B]:GLN:NE2	1:D:206:ALA:HB3	2.04	0.72
1:A:385:ILE:HG23	1:A:436:ILE:CD1	2.20	0.72
1:C:385:ILE:HG23	1:C:436:ILE:CD1	2.26	0.65
1:A:343:GLU:OE2	1:D:343:GLU:OE2	2.15	0.64
1:D:43:TRP:HE1	1:D:107:HIS:CD2	2.17	0.62
1:B:424:ILE:HD11	1:B:444:LEU:HD11	1.80	0.61
1:D:43:TRP:HE1	1:D:107:HIS:HD2	1.49	0.61
1:B:424:ILE:CD1	1:B:444:LEU:CD1	2.78	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:GLU:O	1:D:429:VAL:HG22	2.04	0.58
1:D:385:ILE:HD13	1:D:427:ILE:HD13	1.85	0.58
1:C:34:TYR:OH	1:C:126:ASN:ND2	2.37	0.57
1:C:403:ILE:HD11	1:C:427:ILE:HD11	1.86	0.56
1:D:37:ARG:HH12	1:D:41:GLN:HE21	1.54	0.56
1:D:406:LEU:HD22	1:D:426:ARG:HB3	1.88	0.55
1:B:424:ILE:HD12	1:B:444:LEU:CD1	2.33	0.55
1:A:111:THR:HG22	7:A:2054:HOH:O	2.05	0.55
1:B:68:ASN:ND2	1:B:71:ASN:HD22	2.05	0.54
1:A:415:LYS:NZ	1:C:279:GLU:OE2	2.32	0.54
1:A:105:ILE:HD12	1:A:105:ILE:C	2.29	0.53
1:C:403:ILE:HD11	1:C:427:ILE:CD1	2.39	0.52
1:B:43:TRP:HE1	1:B:107:HIS:CD2	2.27	0.52
1:B:242:THR:HG23	1:B:329:ARG:HG3	1.91	0.51
1:A:385:ILE:HG23	1:A:436:ILE:HD11	1.92	0.51
2:C:1000:AMP:N6	3:C:1001:FUM:C4	2.73	0.51
1:C:328:GLU:O	1:C:329:ARG:HB3	2.10	0.51
1:A:88:VAL:HG21	1:A:112:SER:HB3	1.94	0.49
1:A:331:LEU:HD13	1:B:159:HIS:NE2	2.27	0.49
1:D:429:VAL:O	1:D:429:VAL:HG23	2.11	0.49
1:A:88:VAL:HG12	1:A:89[B]:MET:HE2	1.94	0.49
1:D:424:ILE:CD1	1:D:444:LEU:HD21	2.37	0.49
1:A:385:ILE:HG23	1:A:436:ILE:HD12	1.92	0.48
1:A:389:MET:HG2	1:A:436:ILE:HD13	1.95	0.48
1:C:389:MET:HG2	1:C:436:ILE:HD13	1.96	0.48
1:A:402:LYS:O	1:A:405:VAL:HG22	2.14	0.48
1:D:105:ILE:C	1:D:105:ILE:HD12	2.35	0.47
1:C:385:ILE:HG23	1:C:436:ILE:HD12	1.93	0.47
1:C:424:ILE:HD12	1:C:444:LEU:CD1	2.43	0.47
1:B:198:VAL:HG22	1:B:223:ASP:HA	1.96	0.47
1:C:68:ASN:ND2	1:C:71:ASN:HD22	2.13	0.47
1:A:466:TYR:HE1	7:A:2247:HOH:O	1.97	0.47
1:C:251:VAL:O	1:C:254:VAL:HG22	2.15	0.47
1:B:107:HIS:CD2	1:B:110:ALA:HB3	2.50	0.47
6:B:1002:2SA:H61	6:B:1002:2SA:N7	2.30	0.47
2:C:1000:AMP:N6	3:C:1001:FUM:C5	2.78	0.46
1:D:409:GLN:O	1:D:413:VAL:HG23	2.15	0.46
1:D:468:LEU:HD23	7:D:2236:HOH:O	2.14	0.46
1:C:137:ARG:HD2	1:C:356[A]:GLN:NE2	2.30	0.46
1:C:434:SER:N	1:C:435:PRO:CD	2.78	0.46
1:D:404:ARG:O	1:D:408:GLN:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:GLN:HG3	1:D:440:LEU:HD13	1.98	0.46
2:A:1000:AMP:N6	3:A:1001:FUM:C4	2.79	0.45
1:D:434:SER:N	1:D:435:PRO:CD	2.79	0.45
1:D:246:LYS:O	1:D:250:GLU:HG2	2.16	0.45
1:A:385:ILE:HD12	1:A:443:LEU:HD13	1.98	0.45
1:A:260:ALA:HA	1:B:323[B]:SER:OG	2.17	0.45
1:B:436:ILE:O	1:B:436:ILE:HG23	2.16	0.45
1:D:262:VAL:HG11	1:D:351:ILE:CG2	2.48	0.44
1:C:385:ILE:HD13	1:C:443:LEU:HD13	2.00	0.44
1:B:34:TYR:OH	1:B:126:ASN:ND2	2.46	0.43
6:D:1002:2SA:N7	6:D:1002:2SA:H61	2.33	0.43
1:C:434:SER:HA	1:C:437:HIS:ND1	2.34	0.43
1:C:424:ILE:HD12	1:C:444:LEU:HD13	2.01	0.43
1:D:434:SER:HA	1:D:437:HIS:ND1	2.34	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
1:D:436:ILE:C	1:D:436:ILE:HD12	2.39	0.43
1:C:43:TRP:CE2	1:C:115:VAL:HG11	2.54	0.43
1:C:105:ILE:HD12	1:C:105:ILE:C	2.39	0.43
1:A:21:TYR:HB3	1:A:350:THR:HG21	2.00	0.42
1:C:389:MET:HG3	1:C:399:CYS:SG	2.59	0.42
1:C:198:VAL:HG22	1:C:223:ASP:HA	2.00	0.42
1:B:309:ARG:HD3	1:C:320:GLN:HB2	2.01	0.42
1:C:386:ILE:O	1:C:390:VAL:HG23	2.20	0.42
1:A:111:THR:HG22	1:A:112:SER:N	2.34	0.42
1:B:436:ILE:O	1:B:436:ILE:CG2	2.66	0.42
2:A:1000:AMP:N6	3:A:1001:FUM:C5	2.83	0.42
1:D:377:LEU:N	1:D:378:PRO:CD	2.83	0.42
1:B:425:GLU:O	1:B:429:VAL:HG22	2.19	0.42
1:A:177:GLN:NE2	7:A:2096:HOH:O	2.53	0.42
1:A:111:THR:HG22	1:A:112:SER:H	1.85	0.42
1:D:356[A]:GLN:NE2	1:D:360:GLU:OE2	2.52	0.42
1:D:131:LEU:HD22	1:D:352:LEU:HD12	2.02	0.42
1:A:461:LEU:HD23	1:A:465:VAL:HG21	2.01	0.42
1:A:424:ILE:CD1	1:A:444:LEU:CD1	2.95	0.41
1:B:182:ASP:O	1:B:186:LEU:HD13	2.19	0.41
1:A:331:LEU:HD21	2:A:1000:AMP:C4	2.54	0.41
1:A:43:TRP:HE1	1:A:107:HIS:CD2	2.37	0.41
1:B:314:LEU:O	1:B:318:PRO:HD2	2.21	0.41
1:D:453:ALA:O	1:D:457:VAL:HG23	2.20	0.41
1:A:43:TRP:HE1	1:A:107:HIS:HD2	1.68	0.41
1:C:50:GLU:HB3	1:C:55:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ARG:HH12	1:D:41:GLN:NE2	2.19	0.41
1:A:262:VAL:HG11	1:A:351:ILE:CG2	2.50	0.41
1:C:307:LEU:HB3	1:C:347:THR:HG23	2.03	0.41
1:B:453:ALA:O	1:B:457:VAL:HG23	2.20	0.41
1:A:198:VAL:HG22	1:A:223:ASP:HA	2.02	0.41
1:B:251:VAL:O	1:B:254:VAL:HG22	2.20	0.41
1:A:88:VAL:HG12	1:A:89[B]:MET:CE	2.51	0.41
1:A:434[B]:SER:N	1:A:435:PRO:CD	2.83	0.41
1:C:331:LEU:HD21	2:C:1000:AMP:C6	2.56	0.40
1:C:51:GLN:OE1	1:C:62:ILE:HD12	2.20	0.40
1:B:242:THR:HG23	1:B:329:ARG:CG	2.52	0.40
1:C:328:GLU:O	1:C:329:ARG:CB	2.69	0.40
1:C:323[B]:SER:OG	1:D:312:MET:SD	2.79	0.40
1:B:21:TYR:HB3	1:B:350:THR:HG21	2.04	0.40
1:B:356:GLN:HA	1:B:356:GLN:HE21	1.87	0.40
1:C:241:GLN:HB3	1:C:329:ARG:HG2	2.04	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	461/503 (92%)	450 (98%)	9 (2%)	2 (0%)	39	33
1	B	458/503 (91%)	449 (98%)	8 (2%)	1 (0%)	52	48
1	C	457/503 (91%)	451 (99%)	5 (1%)	1 (0%)	52	48
1	D	461/503 (92%)	450 (98%)	10 (2%)	1 (0%)	52	48
All	All	1837/2012 (91%)	1800 (98%)	32 (2%)	5 (0%)	46	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	329	ARG
1	C	329	ARG
1	D	329	ARG
1	A	473	GLU

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	408/438 (93%)	401 (98%)	7 (2%)	68	71
1	B	405/438 (92%)	401 (99%)	4 (1%)	82	85
1	C	404/438 (92%)	401 (99%)	3 (1%)	88	91
1	D	408/438 (93%)	404 (99%)	4 (1%)	82	85
All	All	1625/1752 (93%)	1607 (99%)	18 (1%)	80	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	190	ARG
1	A	329	ARG
1	A	331	LEU
1	A	395	SER
1	A	468	LEU
1	A	470	LYS
1	B	190	ARG
1	B	329	ARG
1	B	356	GLN
1	B	401	GLU
1	C	329	ARG
1	C	444	LEU
1	C	470	LYS
1	D	37	ARG
1	D	329	ARG
1	D	362	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	444	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	107	HIS
1	A	164	GLN
1	A	177	GLN
1	A	408	GLN
1	B	68	ASN
1	B	107	HIS
1	B	177	GLN
1	B	356	GLN
1	B	455	GLN
1	C	68	ASN
1	C	97	HIS
1	C	126	ASN
1	D	41	GLN
1	D	107	HIS
1	D	126	ASN
1	D	210	GLN
1	D	375	GLN
1	D	408	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	1000	-	20,25,25	1.09	2 (10%)	22,38,38	2.12	2 (9%)
3	FUM	A	1001	-	1,7,7	0.36	0	0,8,8	0.00	-
4	GOL	A	1003	-	5,5,5	0.23	0	5,5,5	0.26	0
6	2SA	B	1002	-	21,33,33	0.70	0	24,49,49	2.72	5 (20%)
4	GOL	B	1003	-	5,5,5	0.24	0	5,5,5	0.39	0
4	GOL	B	1004	-	5,5,5	0.36	0	5,5,5	0.60	0
2	AMP	C	1000	-	20,25,25	1.06	2 (10%)	22,38,38	2.10	2 (9%)
3	FUM	C	1001	-	1,7,7	0.55	0	0,8,8	0.00	-
4	GOL	C	1003	-	5,5,5	0.37	0	5,5,5	0.20	0
6	2SA	D	1002	-	21,33,33	0.81	0	24,49,49	2.93	6 (25%)
4	GOL	D	1003	-	5,5,5	0.28	0	5,5,5	0.32	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
2	AMP	A	1000	-	-	0/6/26/26	0/3/3/3
3	FUM	A	1001	-	-	0/0/5/5	0/0/0/0
4	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
6	2SA	B	1002	-	-	0/11/38/38	0/3/3/3
4	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
2	AMP	C	1000	-	-	0/6/26/26	0/3/3/3
3	FUM	C	1001	-	-	0/0/5/5	0/0/0/0
4	GOL	C	1003	-	-	0/4/4/4	0/0/0/0
6	2SA	D	1002	-	-	0/11/38/38	0/3/3/3
4	GOL	D	1003	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	AMP	O4'-C1'	2.45	1.44	1.41
2	A	1000	AMP	C5-C4	2.51	1.46	1.40
2	C	1000	AMP	O4'-C1'	2.56	1.44	1.41
2	C	1000	AMP	C5-C4	2.68	1.46	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1002	2SA	N3-C2-N1	-10.23	121.06	128.89
6	B	1002	2SA	N3-C2-N1	-9.80	121.39	128.89
2	A	1000	AMP	N3-C2-N1	-8.02	122.75	128.89
2	C	1000	AMP	N3-C2-N1	-7.96	122.80	128.89
6	D	1002	2SA	C63-C61-C62	-3.42	104.22	111.55
6	B	1002	2SA	C63-C61-C62	-2.86	105.41	111.55
2	C	1000	AMP	C1'-N9-C4	-2.69	122.88	126.94
2	A	1000	AMP	C1'-N9-C4	-2.62	122.98	126.94
6	B	1002	2SA	C4-C5-N7	-2.52	107.16	109.48
6	D	1002	2SA	C1'-N9-C4	-2.49	123.19	126.94
6	D	1002	2SA	C4-C5-N7	-2.13	107.52	109.48
6	D	1002	2SA	C4'-O4'-C1'	-2.08	107.43	109.72
6	B	1002	2SA	O4'-C1'-N9	2.58	113.51	108.10
6	B	1002	2SA	C2-N1-C6	6.70	121.31	116.48
6	D	1002	2SA	C2-N1-C6	7.90	122.17	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	AMP	3	0
3	A	1001	FUM	2	0
6	B	1002	2SA	1	0
2	C	1000	AMP	3	0
3	C	1001	FUM	2	0
6	D	1002	2SA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	461/503 (91%)	0.74	54 (11%) 6 7	27, 34, 44, 55	0
1	B	461/503 (91%)	0.87	60 (13%) 5 5	28, 34, 44, 50	0
1	C	457/503 (90%)	0.77	52 (11%) 7 7	28, 33, 50, 61	0
1	D	462/503 (91%)	0.80	58 (12%) 5 5	27, 33, 53, 63	0
All	All	1841/2012 (91%)	0.79	224 (12%) 5 6	27, 34, 47, 63	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	9.5
1	D	397	GLN	8.7
1	C	5	GLY	8.1
1	B	282	PHE	7.8
1	D	5	GLY	7.2
1	A	5	GLY	6.9
1	D	396	ARG	6.3
1	C	391	LYS	5.9
1	D	395	SER	5.9
1	A	474	SER	5.8
1	B	387	MET	5.8
1	D	282	PHE	5.7
1	D	391	LYS	5.6
1	D	6	ASP	5.5
1	A	293	PRO	5.5
1	C	6	ASP	5.4
1	D	392	ALA	5.4
1	C	397	GLN	5.4
1	D	419	GLY	5.2
1	D	475	VAL	5.2
1	C	404	ARG	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	4.7
1	B	391	LYS	4.7
1	C	394	GLY	4.6
1	D	436	ILE	4.6
1	D	401	GLU	4.5
1	D	429	VAL	4.5
1	D	417	GLU	4.5
1	D	432	TYR	4.5
1	B	442	HIS	4.4
1	B	85	ARG	4.2
1	C	93	HIS	4.1
1	D	433	PHE	4.1
1	D	435	PRO	4.1
1	A	473	GLU	4.1
1	D	394	GLY	4.0
1	D	405	VAL	4.0
1	D	387	MET	4.0
1	D	393	GLY	4.0
1	C	60	GLU	3.9
1	B	424	ILE	3.9
1	D	413	VAL	3.9
1	D	400	HIS	3.8
1	B	423	LEU	3.8
1	B	294	TYR	3.8
1	C	63	GLN	3.8
1	C	96	GLY	3.8
1	C	85	ARG	3.7
1	A	115	VAL	3.7
1	B	406	LEU	3.7
1	C	84	LEU	3.7
1	D	404	ARG	3.7
1	B	390	VAL	3.7
1	D	398	ASP	3.6
1	A	105	ILE	3.6
1	B	475	VAL	3.6
1	B	397	GLN	3.5
1	A	42	LEU	3.4
1	C	431	ALA	3.4
1	D	431	ALA	3.4
1	A	85	ARG	3.4
1	A	93	HIS	3.4
1	D	390	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	399	CYS	3.3
1	A	233	LYS	3.3
1	D	82	LYS	3.3
1	D	438	SER	3.3
1	B	83	ARG	3.3
1	C	83	ARG	3.3
1	B	400	HIS	3.2
1	C	7	HIS	3.2
1	A	43	TRP	3.2
1	C	282	PHE	3.2
1	B	440	LEU	3.1
1	B	394	GLY	3.1
1	B	436	ILE	3.1
1	C	79	GLU	3.1
1	A	52	THR	3.1
1	D	418	GLY	3.0
1	B	393	GLY	3.0
1	B	265	ILE	3.0
1	C	396	ARG	3.0
1	A	39	TRP	3.0
1	C	395	SER	3.0
1	A	58	THR	3.0
1	A	272	LEU	3.0
1	A	114	TYR	3.0
1	C	390	VAL	3.0
1	D	11	ASP	3.0
1	D	474	SER	2.9
1	A	83	ARG	2.9
1	B	404	ARG	2.9
1	D	409	GLN	2.9
1	A	466	TYR	2.9
1	C	101	LYS	2.9
1	B	403	ILE	2.8
1	A	283	GLU	2.8
1	C	398	ASP	2.8
1	A	294	TYR	2.8
1	A	71	ASN	2.8
1	C	429	VAL	2.8
1	B	114	TYR	2.8
1	B	43	TRP	2.8
1	A	60	GLU	2.8
1	C	42	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	393	GLY	2.8
1	B	9	SER	2.8
1	D	114	TYR	2.7
1	D	437	HIS	2.7
1	D	441	ASP	2.7
1	A	70	GLU	2.7
1	D	473	GLU	2.7
1	C	401	GLU	2.7
1	B	458	GLN	2.7
1	C	67	SER	2.7
1	B	417	GLU	2.7
1	D	83	ARG	2.7
1	A	7	HIS	2.7
1	B	395	SER	2.7
1	A	82	LYS	2.6
1	D	403	ILE	2.6
1	D	293	PRO	2.6
1	D	424	ILE	2.6
1	A	97	HIS	2.6
1	B	462	GLU	2.6
1	D	428	GLN	2.6
1	A	265	ILE	2.6
1	C	58	THR	2.5
1	B	115	VAL	2.5
1	A	282	PHE	2.5
1	C	99	CYS	2.5
1	D	406	LEU	2.5
1	B	101	LYS	2.5
1	A	228	GLU	2.5
1	B	433	PHE	2.5
1	C	89	MET	2.5
1	A	24	PRO	2.5
1	C	57	ILE	2.5
1	D	442	HIS	2.5
1	B	226	VAL	2.5
1	D	408	GLN	2.5
1	C	39	TRP	2.5
1	C	82	LYS	2.5
1	D	389	MET	2.4
1	C	46	LEU	2.4
1	A	470	LYS	2.4
1	B	39	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	75	LYS	2.4
1	B	272	LEU	2.4
1	D	420	ASP	2.4
1	C	49	ALA	2.4
1	A	63	GLN	2.4
1	A	404	ARG	2.4
1	C	403	ILE	2.4
1	C	100	PRO	2.4
1	C	294	TYR	2.4
1	D	97	HIS	2.4
1	C	228	GLU	2.4
1	B	6	ASP	2.3
1	B	455	GLN	2.3
1	B	402	LYS	2.3
1	D	414	VAL	2.3
1	B	434	SER	2.3
1	D	265	ILE	2.3
1	B	82	LYS	2.3
1	A	95	PHE	2.3
1	A	212	PHE	2.3
1	B	357	ASN	2.3
1	B	447	SER	2.3
1	D	425	GLU	2.3
1	B	147	LYS	2.3
1	C	387	MET	2.3
1	A	38	THR	2.3
1	C	265	ILE	2.3
1	D	385	ILE	2.3
1	B	473	GLU	2.3
1	C	275	LEU	2.3
1	C	197	GLY	2.2
1	A	262	VAL	2.2
1	C	386	ILE	2.2
1	D	388	ALA	2.2
1	C	212	PHE	2.2
1	A	231	GLY	2.2
1	B	67	SER	2.2
1	B	56	PRO	2.2
1	C	24	PRO	2.2
1	A	101	LYS	2.2
1	D	439	GLN	2.2
1	C	11	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	2.2
1	A	258	LEU	2.2
1	B	28	PHE	2.2
1	A	397	GLN	2.2
1	B	356	GLN	2.2
1	D	115	VAL	2.2
1	B	42	LEU	2.1
1	A	92	VAL	2.1
1	C	262	VAL	2.1
1	A	37	ARG	2.1
1	A	84	LEU	2.1
1	A	119	THR	2.1
1	B	271	LEU	2.1
1	B	262	VAL	2.1
1	D	430	ASP	2.1
1	B	474	SER	2.1
1	B	151	SER	2.1
1	A	40	ARG	2.1
1	C	408	GLN	2.1
1	A	271	LEU	2.1
1	B	437	HIS	2.1
1	B	360	GLU	2.1
1	B	435	PRO	2.1
1	A	36	PHE	2.1
1	C	405	VAL	2.1
1	A	401	GLU	2.0
1	A	425	GLU	2.0
1	C	70	GLU	2.0
1	B	443	LEU	2.0
1	A	49	ALA	2.0
1	B	296	ARG	2.0
1	B	58	THR	2.0
1	A	100	PRO	2.0
1	B	60	GLU	2.0
1	D	197	GLY	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	B	1004	6/6	0.82	0.22	3.54	49,50,51,51	0
5	CL	C	2002	1/1	0.98	0.27	2.81	38,38,38,38	0
4	GOL	C	1003	6/6	0.81	0.25	2.57	49,50,52,53	0
3	FUM	A	1001	8/8	0.88	0.19	1.72	41,41,42,43	0
5	CL	A	2002	1/1	0.98	0.21	0.98	35,35,35,35	0
4	GOL	A	1003	6/6	0.90	0.17	0.30	43,43,43,44	0
3	FUM	C	1001	8/8	0.89	0.14	0.03	41,42,43,44	0
2	AMP	C	1000	23/23	0.94	0.13	-0.32	37,41,41,41	0
2	AMP	A	1000	23/23	0.95	0.13	-0.34	26,36,37,37	0
6	2SA	B	1002	31/31	0.97	0.12	-0.37	22,24,26,29	0
6	2SA	D	1002	31/31	0.97	0.12	-0.47	18,20,22,24	0
4	GOL	B	1003	6/6	0.91	0.14	-0.67	39,40,40,40	0
4	GOL	D	1003	6/6	0.91	0.14	-0.90	33,35,35,36	0
5	CL	B	2002	1/1	0.99	0.08	-1.85	25,25,25,25	0
5	CL	D	2002	1/1	1.00	0.01	-3.37	18,18,18,18	0
5	CL	B	2001	1/1	0.99	0.15	-	31,31,31,31	0
5	CL	A	2001	1/1	0.90	0.12	-	55,55,55,55	0
5	CL	D	2001	1/1	0.99	0.13	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.