Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:17 AM GMT

PDB ID	:	3LGX
Title	:	Structure of probable D-alanine-poly(phosphoribitol) ligase subunit-1 from Streptococcus pyogenes with ATP
Authors	:	Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-01-21
Resolution	:	2.60 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:

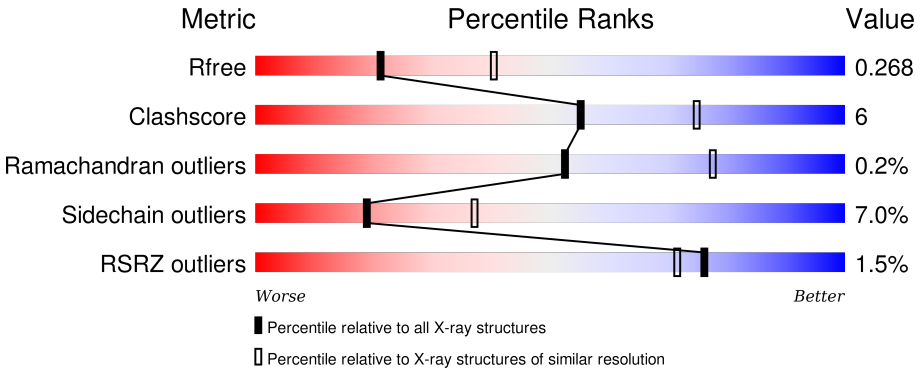
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	521	2% 81% 15%
1	B	521	2% 78% 18%
1	C	521	2% 79% 17%
1	D	521	% 79% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16060 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--poly(phosphoribitol) ligase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			3969	2554	632	766	17			
1	B	507	Total	C	N	O	S	0	3	0
			3986	2564	640	765	17			
1	C	508	Total	C	N	O	S	0	1	0
			3969	2553	636	763	17			
1	D	508	Total	C	N	O	S	0	0	0
			3964	2551	632	764	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q99ZA6
A	-3	SER	-	expression tag	UNP Q99ZA6
A	-2	LEU	-	expression tag	UNP Q99ZA6
A	509	GLU	-	expression tag	UNP Q99ZA6
A	510	GLY	-	expression tag	UNP Q99ZA6
A	511	HIS	-	expression tag	UNP Q99ZA6
A	512	HIS	-	expression tag	UNP Q99ZA6
A	513	HIS	-	expression tag	UNP Q99ZA6
A	514	HIS	-	expression tag	UNP Q99ZA6
A	515	HIS	-	expression tag	UNP Q99ZA6
A	516	HIS	-	expression tag	UNP Q99ZA6
B	-4	MET	-	expression tag	UNP Q99ZA6
B	-3	SER	-	expression tag	UNP Q99ZA6
B	-2	LEU	-	expression tag	UNP Q99ZA6
B	509	GLU	-	expression tag	UNP Q99ZA6
B	510	GLY	-	expression tag	UNP Q99ZA6
B	511	HIS	-	expression tag	UNP Q99ZA6
B	512	HIS	-	expression tag	UNP Q99ZA6
B	513	HIS	-	expression tag	UNP Q99ZA6
B	514	HIS	-	expression tag	UNP Q99ZA6
B	515	HIS	-	expression tag	UNP Q99ZA6

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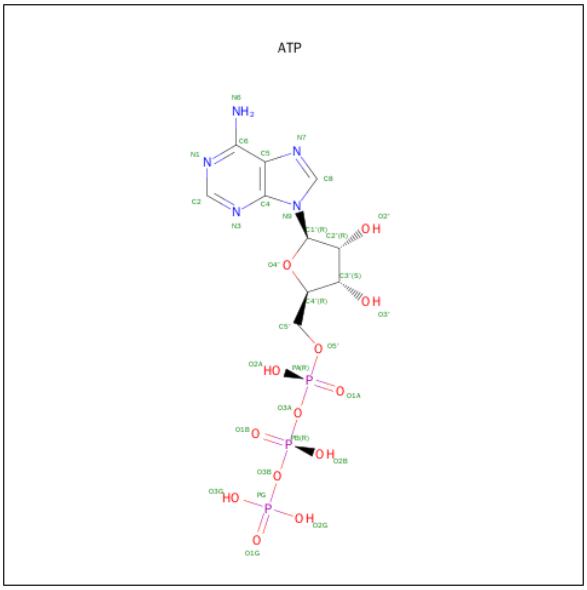
Chain	Residue	Modelled	Actual	Comment	Reference
B	516	HIS	-	expression tag	UNP Q99ZA6
C	-4	MET	-	expression tag	UNP Q99ZA6
C	-3	SER	-	expression tag	UNP Q99ZA6
C	-2	LEU	-	expression tag	UNP Q99ZA6
C	509	GLU	-	expression tag	UNP Q99ZA6
C	510	GLY	-	expression tag	UNP Q99ZA6
C	511	HIS	-	expression tag	UNP Q99ZA6
C	512	HIS	-	expression tag	UNP Q99ZA6
C	513	HIS	-	expression tag	UNP Q99ZA6
C	514	HIS	-	expression tag	UNP Q99ZA6
C	515	HIS	-	expression tag	UNP Q99ZA6
C	516	HIS	-	expression tag	UNP Q99ZA6
D	-4	MET	-	expression tag	UNP Q99ZA6
D	-3	SER	-	expression tag	UNP Q99ZA6
D	-2	LEU	-	expression tag	UNP Q99ZA6
D	509	GLU	-	expression tag	UNP Q99ZA6
D	510	GLY	-	expression tag	UNP Q99ZA6
D	511	HIS	-	expression tag	UNP Q99ZA6
D	512	HIS	-	expression tag	UNP Q99ZA6
D	513	HIS	-	expression tag	UNP Q99ZA6
D	514	HIS	-	expression tag	UNP Q99ZA6
D	515	HIS	-	expression tag	UNP Q99ZA6
D	516	HIS	-	expression tag	UNP Q99ZA6

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

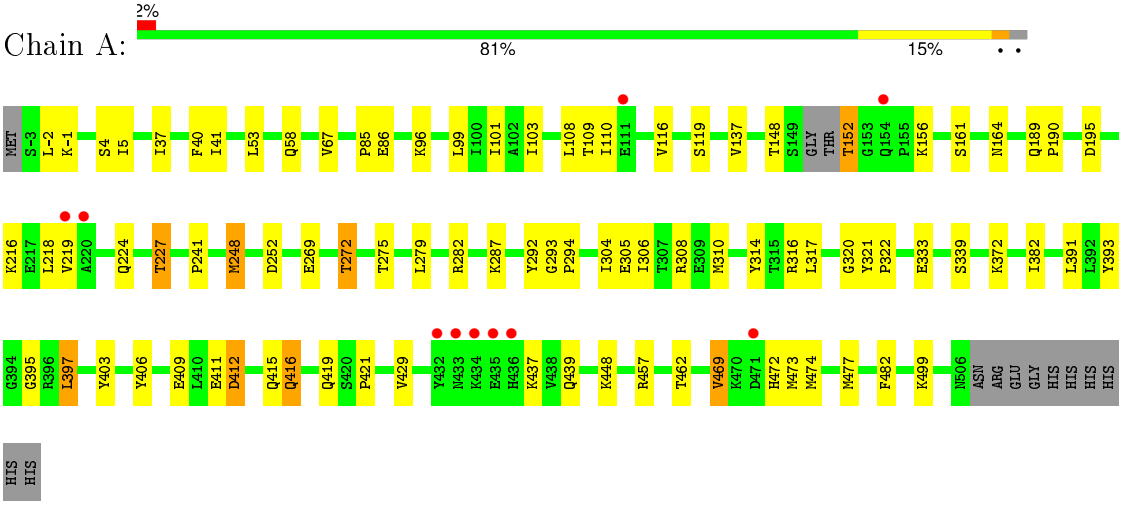
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	17	Total	O	0	0
			17	17		
3	C	9	Total	O	0	0
			9	9		
3	D	11	Total	O	0	0
			11	11		

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.

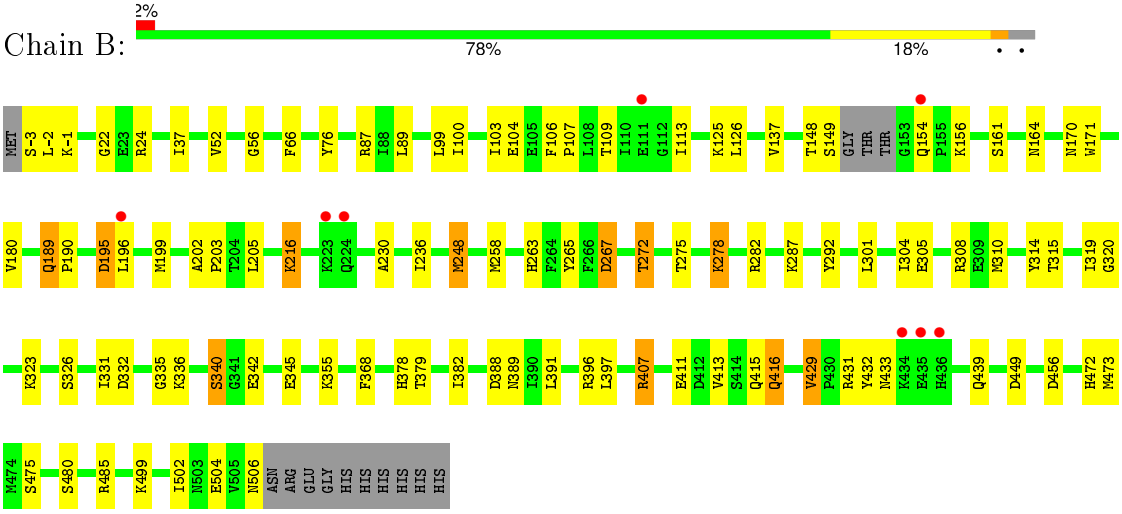
- Molecule 1: D-alanine--poly(phosphoribitol) ligase subunit 1

Chain A:



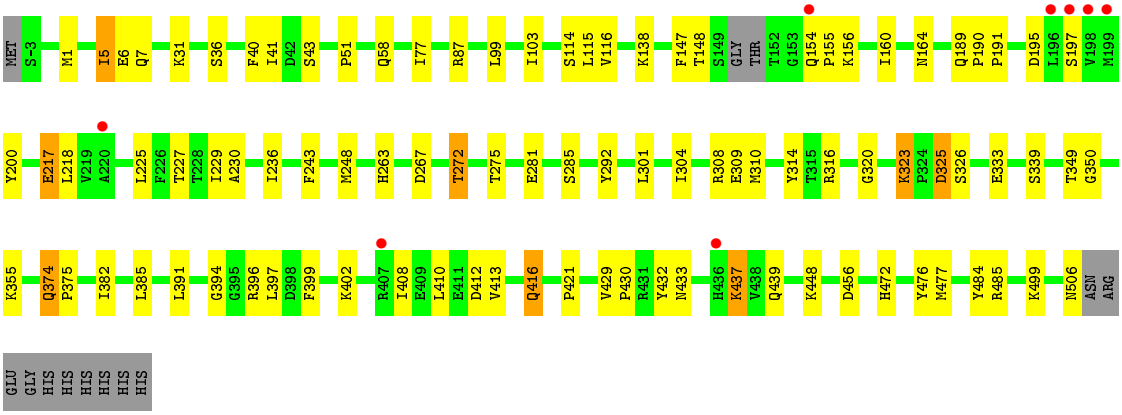
- Molecule 1: D-alanine--poly(phosphoribitol) ligase subunit 1

Chain B:

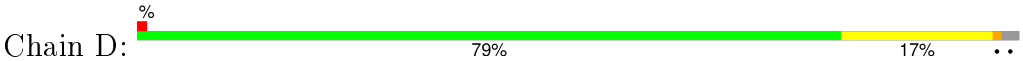


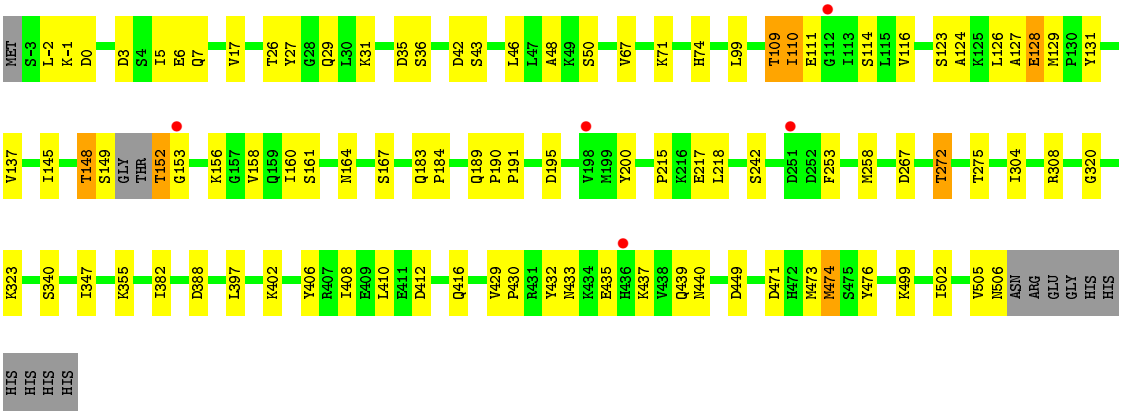
- Molecule 1: D-alanine--poly(phosphoribitol) ligase subunit 1

Chain C:



- Molecule 1: D-alanine--poly(phosphoribitol) ligase subunit 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.41Å 174.41Å 176.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 34.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.8 (34.32-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.218 , 0.276 0.211 , 0.268	Depositor DCC
R_{free} test set	4149 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.2	EDS
Estimated twinning fraction	0.035 for -h,l,k 0.032 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 83021 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16060	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: ATP

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	0.70	0/4060	0.75	2/5519 (0.0%)
1	B	0.74	0/4077	0.77	2/5540 (0.0%)
1	C	0.70	0/4060	0.77	2/5518 (0.0%)
1	D	0.70	0/4055	0.74	1/5512 (0.0%)
All	All	0.71	0/16252	0.76	7/22089 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	B	267	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	412	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	267	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	267	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	391	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	195	ASP	CB-CG-OD2	5.18	122.96	118.30

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	3969	0	3928	38	0
1	B	3986	0	3944	56	0
1	C	3969	0	3921	52	0
1	D	3964	0	3920	54	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	11	0	0	0	0
3	B	17	0	0	0	0
3	C	9	0	0	0	0
3	D	11	0	0	0	0
All	All	16060	0	15761	200	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 (200) 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:D:474:MET:HG2	1:D:476:TYR:CE1	1.83	1.13
1:C:382:ILE:HD11	1:C:397:LEU:HD13	1.19	1.12
1:B:407:ARG:HH11	1:B:407:ARG:HG3	1.10	1.09
1:C:485[B]:ARG:HG2	1:C:485[B]:ARG:HH11	1.16	1.07
1:D:382:ILE:HD11	1:D:397:LEU:HD12	1.39	1.03
1:D:474:MET:HG2	1:D:476:TYR:CZ	2.05	0.92
1:C:272:THR:HG22	1:C:275:THR:H	1.35	0.90
1:B:272:THR:HG22	1:B:275:THR:H	1.36	0.89
1:A:161:SER:H	1:A:164:ASN:HD22	1.22	0.86
1:B:407:ARG:NH1	1:B:407:ARG:HG3	1.89	0.86
1:A:416:GLN:HG2	1:A:473:MET:HG2	1.58	0.85
1:B:161:SER:H	1:B:164:ASN:HD22	1.21	0.84
1:C:485[B]:ARG:HG2	1:C:485[B]:ARG:NH1	1.94	0.82
1:D:272:THR:HG22	1:D:275:THR:H	1.45	0.81
1:C:154:GLN:HE21	1:C:155:PRO:HD2	1.47	0.79
1:A:272:THR:HG22	1:A:275:THR:H	1.48	0.79
1:D:148:THR:HG22	1:D:156:LYS:H	1.47	0.78
1:D:253:PHE:HA	1:D:258:MET:CE	2.14	0.77
1:B:161:SER:H	1:B:164:ASN:ND2	1.82	0.77
1:D:161:SER:H	1:D:164:ASN:ND2	1.83	0.77
1:D:382:ILE:CD1	1:D:397:LEU:HD12	2.14	0.76
1:C:382:ILE:CD1	1:C:397:LEU:HD13	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:SER:H	1:D:164:ASN:HD22	1.31	0.76
1:D:31:LYS:O	1:D:35:ASP:OD1	2.06	0.74
1:A:152:THR:N	1:A:499:LYS:HE3	2.04	0.71
1:B:416:GLN:HG2	1:B:473:MET:HG2	1.74	0.69
1:A:241:PRO:HG2	1:A:269:GLU:HG3	1.75	0.69
1:B:382:ILE:HD11	1:B:397:LEU:HD13	1.73	0.69
1:C:413:VAL:HG22	1:C:477:MET:HG2	1.75	0.69
1:D:416:GLN:HG3	1:D:473:MET:HG2	1.73	0.68
1:C:272:THR:CG2	1:C:275:THR:H	2.06	0.67
1:D:36:SER:OG	1:D:124:ALA:O	2.13	0.67
1:A:161:SER:H	1:A:164:ASN:ND2	1.90	0.66
1:C:160:ILE:HA	1:C:164:ASN:HD22	1.61	0.66
1:D:148:THR:HG23	1:D:149:SER:N	2.08	0.66
1:C:350:GLY:HA2	1:C:374:GLN:HG2	1.78	0.65
1:C:421:PRO:O	1:C:448:LYS:HE2	1.96	0.65
1:B:433:ASN:HD22	1:B:439:GLN:HE21	1.45	0.65
1:D:432:TYR:H	1:D:506:ASN:HD21	1.44	0.65
1:A:189:GLN:HB3	1:A:190:PRO:HD3	1.78	0.64
1:C:382:ILE:HD11	1:C:397:LEU:CD1	2.12	0.64
1:D:304:ILE:HB	1:D:320:GLY:HA2	1.80	0.63
1:C:58:GLN:HE21	1:C:191:PRO:HA	1.64	0.62
1:B:485[A]:ARG:NH2	1:B:504:GLU:OE1	2.32	0.62
1:C:304:ILE:HB	1:C:320:GLY:HA2	1.82	0.61
1:C:99:LEU:HD11	1:C:116:VAL:HG23	1.83	0.61
1:B:379:THR:O	1:B:396[B]:ARG:NH1	2.34	0.61
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.98	0.61
1:A:316:ARG:HD3	1:A:415:GLN:HG3	1.83	0.60
1:D:429:VAL:HG22	1:D:502:ILE:HG12	1.84	0.59
1:A:304:ILE:HB	1:A:320:GLY:HA2	1.85	0.59
1:D:17:VAL:HG23	1:D:27:TYR:CZ	2.38	0.59
1:A:310:MET:HG3	1:A:314:TYR:CE2	2.38	0.58
1:D:99:LEU:HD11	1:D:116:VAL:HG23	1.84	0.58
1:B:432:TYR:H	1:B:506:ASN:HD21	1.52	0.58
1:D:50:SER:O	1:D:74:HIS:HD2	1.86	0.58
1:B:304:ILE:HB	1:B:320:GLY:HA2	1.86	0.57
1:C:323:LYS:HG3	1:C:326:SER:HB2	1.85	0.57
1:C:408:ILE:HD11	1:C:476:TYR:CE2	2.39	0.57
1:D:0:ASP:HB3	1:D:3:ASP:HB2	1.86	0.57
1:C:333:GLU:CD	1:C:333:GLU:H	2.08	0.57
1:B:52:VAL:HG13	1:B:99:LEU:HB3	1.86	0.57
1:D:190:PRO:HD2	1:D:200:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLN:CG	1:D:473:MET:HG2	2.35	0.56
1:A:248:MET:O	1:A:282:ARG:NH2	2.38	0.56
1:D:26:THR:OG1	1:D:29:GLN:HG3	2.05	0.55
1:D:253:PHE:HA	1:D:258:MET:HE1	1.88	0.55
1:D:474:MET:CG	1:D:476:TYR:CE1	2.76	0.55
1:B:287:LYS:HD2	1:B:305:GLU:OE2	2.07	0.55
1:D:347:ILE:C	1:D:347:ILE:HD12	2.28	0.54
1:B:189:GLN:HB3	1:B:190:PRO:HD3	1.89	0.54
1:D:110:ILE:HD13	1:D:110:ILE:N	2.22	0.54
1:B:433:ASN:HB3	1:B:439:GLN:HG2	1.88	0.54
1:C:6:GLU:OE1	1:C:31:LYS:NZ	2.27	0.54
1:C:316:ARG:NH2	1:C:394:GLY:O	2.41	0.54
1:B:22:GLY:O	1:B:24:ARG:HG3	2.08	0.54
1:D:161:SER:N	1:D:164:ASN:HD22	2.04	0.53
1:C:154:GLN:HE21	1:C:155:PRO:CD	2.21	0.53
1:D:5:ILE:HD11	1:D:67:VAL:HG11	1.89	0.53
1:A:101:ILE:HG22	1:A:103:ILE:HG12	1.89	0.53
1:B:310:MET:HG2	1:B:314:TYR:CE2	2.44	0.53
1:C:432:TYR:HA	1:C:437:LYS:O	2.08	0.52
1:C:154:GLN:NE2	1:C:155:PRO:HD2	2.21	0.52
1:D:253:PHE:HA	1:D:258:MET:HE3	1.92	0.52
1:C:484:TYR:O	1:C:485[B]:ARG:HG2	2.09	0.52
1:C:408:ILE:HD11	1:C:476:TYR:HE2	1.71	0.52
1:D:402:LYS:HA	1:D:406:TYR:O	2.10	0.52
1:A:85:PRO:HB3	1:A:108:LEU:HD21	1.92	0.52
1:C:225:LEU:HD21	1:C:229:ILE:HD11	1.91	0.52
1:D:190:PRO:HD2	1:D:200:TYR:HE2	1.74	0.51
1:B:416:GLN:CG	1:B:473:MET:HG2	2.40	0.51
1:A:409:GLU:O	1:A:412:ASP:HB2	2.11	0.51
1:B:171:TRP:CE3	1:B:323:LYS:HD3	2.46	0.51
1:C:416:GLN:HG3	1:C:472:HIS:HD2	1.75	0.50
1:B:196:LEU:HD13	1:B:267:ASP:HB3	1.93	0.50
1:B:248:MET:HG2	1:B:278:LYS:HG2	1.92	0.50
1:B:432:TYR:H	1:B:506:ASN:ND2	2.09	0.50
1:B:248:MET:O	1:B:282:ARG:NH2	2.39	0.49
1:B:161:SER:N	1:B:164:ASN:HD22	1.99	0.49
1:C:189:GLN:HB3	1:C:190:PRO:HD3	1.93	0.49
1:D:50:SER:O	1:D:74:HIS:CD2	2.64	0.48
1:D:145:ILE:HA	1:D:158:VAL:O	2.13	0.48
1:C:432:TYR:H	1:C:506:ASN:HD21	1.61	0.48
1:C:433:ASN:HB3	1:C:439:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:C	1:B:301:LEU:HD12	2.34	0.48
1:B:407:ARG:NH1	1:B:407:ARG:CG	2.66	0.48
1:A:382:ILE:HG13	1:A:397:LEU:HD13	1.96	0.48
1:B:99:LEU:HG	1:B:100:ILE:N	2.28	0.48
1:C:310:MET:HG2	1:C:314:TYR:CE2	2.49	0.48
1:D:429:VAL:CG1	1:D:505:VAL:HG21	2.44	0.47
1:D:433:ASN:HD22	1:D:439:GLN:HE21	1.62	0.47
1:C:301:LEU:C	1:C:301:LEU:HD12	2.33	0.47
1:B:148:THR:CG2	1:B:149:SER:N	2.77	0.47
1:A:469:VAL:HG12	1:A:472:HIS:HD2	1.80	0.47
1:D:148:THR:CG2	1:D:149:SER:N	2.77	0.47
1:D:42:ASP:OD2	1:D:131:TYR:HE1	1.98	0.47
1:B:199:MET:O	1:B:203:PRO:HG3	2.15	0.47
1:C:325:ASP:C	1:C:325:ASP:OD1	2.53	0.46
1:B:382:ILE:HD11	1:B:397:LEU:CD1	2.40	0.46
1:D:215:PRO:HD2	1:D:218:LEU:HD12	1.97	0.46
1:B:388:ASP:O	1:B:389:ASN:HB3	2.16	0.46
1:C:189:GLN:HG3	1:C:243:PHE:CE1	2.51	0.46
1:A:403:TYR:O	1:A:406:TYR:HB2	2.15	0.46
1:A:393:TYR:CZ	1:A:395:GLY:HA2	2.50	0.46
1:A:473:MET:CE	1:A:477:MET:HB3	2.45	0.46
1:C:217:GLU:O	1:C:218:LEU:HD12	2.16	0.46
1:C:349:THR:HA	1:C:375:PRO:O	2.16	0.45
1:B:202:ALA:N	1:B:203:PRO:HD2	2.32	0.45
1:B:37:ILE:HD11	1:B:125:LYS:HG2	1.98	0.45
1:A:287:LYS:HD3	1:A:305:GLU:OE2	2.16	0.45
1:B:416:GLN:HG3	1:B:472:HIS:HD2	1.82	0.45
1:B:382:ILE:CD1	1:B:397:LEU:HD13	2.43	0.45
1:B:230:ALA:HA	1:B:258:MET:HE2	1.99	0.45
1:A:421:PRO:O	1:A:448:LYS:HE2	2.16	0.45
1:C:51:PRO:HB2	1:C:77:ILE:HD11	1.98	0.45
1:B:331:ILE:HD12	1:B:335:GLY:HA2	1.97	0.45
1:B:413:VAL:HG13	1:B:473:MET:HE1	1.99	0.44
1:B:319:ILE:HG13	1:B:391:LEU:HB3	1.98	0.44
1:C:236:ILE:HG12	1:C:263:HIS:HB2	1.99	0.44
1:B:180:VAL:HG22	1:B:265:TYR:OH	2.18	0.44
1:C:225:LEU:C	1:C:225:LEU:HD23	2.37	0.44
1:B:-3:SER:HB2	1:B:170:ASN:OD1	2.17	0.44
1:B:429:VAL:HG22	1:B:502:ILE:HG12	1.99	0.44
1:D:355:LYS:HB3	1:D:355:LYS:HE3	1.78	0.44
1:C:484:TYR:O	1:C:485[B]:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLU:OE2	1:B:378:HIS:HB3	2.17	0.43
1:C:304:ILE:HB	1:C:320:GLY:CA	2.46	0.43
1:B:236:ILE:HG12	1:B:263:HIS:HB2	2.00	0.43
1:A:292:TYR:CG	1:A:293:GLY:N	2.86	0.43
1:C:147:PHE:HA	1:C:156:LYS:O	2.17	0.43
1:A:416:GLN:CG	1:A:473:MET:HG2	2.38	0.43
1:D:190:PRO:HA	1:D:191:PRO:HD3	1.84	0.43
1:A:53:LEU:C	1:A:53:LEU:HD23	2.38	0.43
1:C:396:ARG:O	1:C:399:PHE:N	2.47	0.43
1:B:332:ASP:OD2	1:B:336:LYS:HB2	2.18	0.43
1:D:433:ASN:HB3	1:D:439:GLN:HG2	2.00	0.43
1:C:103:ILE:H	1:C:103:ILE:HD12	1.84	0.43
1:C:103:ILE:HD12	1:C:103:ILE:N	2.34	0.43
1:B:106:PHE:HA	1:B:107:PRO:HD3	1.78	0.43
1:A:416:GLN:O	1:A:419:GLN:HB2	2.19	0.42
1:A:411:GLU:O	1:A:415:GLN:HG2	2.18	0.42
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.76	0.42
1:D:126:LEU:C	1:D:128:GLU:H	2.22	0.42
1:A:224:GLN:HA	1:A:224:GLN:OE1	2.18	0.42
1:C:429:VAL:HA	1:C:430:PRO:HD3	1.94	0.42
1:D:46:LEU:HD11	1:D:99:LEU:HD22	2.01	0.42
1:C:1:MET:O	1:C:5:ILE:HG23	2.20	0.42
1:B:433:ASN:HB3	1:B:439:GLN:HE21	1.85	0.42
1:B:323:LYS:HE3	1:B:326:SER:OG	2.20	0.42
1:C:385:LEU:HD13	1:C:391:LEU:HD13	2.01	0.42
1:B:66:PHE:HB3	1:B:76:TYR:CE1	2.54	0.42
1:C:197:SER:HA	1:C:200:TYR:CE2	2.54	0.42
1:A:227:THR:HG23	1:A:252:ASP:OD1	2.20	0.42
1:D:408:ILE:HD11	1:D:476:TYR:HE2	1.85	0.42
1:A:306:ILE:HD12	1:A:317:LEU:HD13	2.02	0.42
1:D:160:ILE:HA	1:D:164:ASN:HD22	1.85	0.42
1:C:40:PHE:HD2	1:C:41:ILE:HD12	1.84	0.41
1:D:164:ASN:O	1:D:167:SER:HB3	2.19	0.41
1:A:-2:LEU:HA	1:A:-2:LEU:HD12	1.90	0.41
1:A:333:GLU:HG3	1:A:333:GLU:H	1.73	0.41
1:A:310:MET:HG2	1:A:314:TYR:CD2	2.55	0.41
1:B:368:PHE:CD1	1:B:368:PHE:N	2.88	0.41
1:D:109:THR:C	1:D:110:ILE:HD13	2.41	0.41
1:A:321:TYR:HA	1:A:322:PRO:HD3	1.93	0.41
1:D:152:THR:HB	1:D:153:GLY:H	1.56	0.41
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:THR:O	1:C:230:ALA:HB3	2.20	0.41
1:A:294:PRO:HA	2:A:600:ATP:H5'1	2.03	0.41
1:D:410:LEU:HD23	1:D:410:LEU:HA	1.80	0.41
1:A:37:ILE:O	1:A:40:PHE:HB3	2.21	0.41
1:A:5:ILE:HD11	1:A:67:VAL:HG11	2.02	0.40
1:D:429:VAL:HA	1:D:430:PRO:HD3	1.92	0.40
1:A:99:LEU:HD11	1:A:116:VAL:HG23	2.03	0.40
1:B:431:ARG:HA	1:B:506:ASN:HD21	1.87	0.40
1:D:67:VAL:HG12	1:D:71:LYS:HE3	2.04	0.40
1:B:56:GLY:HA2	1:B:104:GLU:HG2	2.04	0.40
1:B:411:GLU:O	1:B:415:GLN:HG2	2.20	0.40
1:D:127:ALA:O	1:D:129:MET:N	2.54	0.40
1:A:462:THR:HG23	1:A:482:PHE:CD2	2.57	0.40
1:D:183:GLN:N	1:D:184:PRO:CD	2.85	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	504/521 (97%)	477 (95%)	27 (5%)	0	100	100
1	B	506/521 (97%)	485 (96%)	19 (4%)	2 (0%)	39	65
1	C	505/521 (97%)	478 (95%)	27 (5%)	0	100	100
1	D	504/521 (97%)	474 (94%)	28 (6%)	2 (0%)	39	65
All	All	2019/2084 (97%)	1914 (95%)	101 (5%)	4 (0%)	52	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	GLU

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Mol	Chain	Res	Type
1	B	216	LYS
1	B	340	SER
1	D	48	ALA

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	432/447 (97%)	400 (93%)	32 (7%)	17	34
1	B	432/447 (97%)	401 (93%)	31 (7%)	18	35
1	C	430/447 (96%)	402 (94%)	28 (6%)	21	42
1	D	431/447 (96%)	401 (93%)	30 (7%)	19	37
All	All	1725/1788 (96%)	1604 (93%)	121 (7%)	19	37

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	LYS
1	A	4	SER
1	A	58	GLN
1	A	86	GLU
1	A	96	LYS
1	A	109	THR
1	A	110	ILE
1	A	119	SER
1	A	137	VAL
1	A	148	THR
1	A	152	THR
1	A	156	LYS
1	A	195	ASP
1	A	216	LYS
1	A	218	LEU
1	A	219	VAL
1	A	227	THR
1	A	248	MET

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Mol	Chain	Res	Type
1	A	272	THR
1	A	279	LEU
1	A	308	ARG
1	A	339	SER
1	A	372	LYS
1	A	397	LEU
1	A	412	ASP
1	A	416	GLN
1	A	429	VAL
1	A	437	LYS
1	A	439	GLN
1	A	457	ARG
1	A	469	VAL
1	A	474	MET
1	B	-2	LEU
1	B	-1	LYS
1	B	87	ARG
1	B	89	LEU
1	B	103	ILE
1	B	109	THR
1	B	113	ILE
1	B	126	LEU
1	B	137	VAL
1	B	154	GLN
1	B	156	LYS
1	B	189	GLN
1	B	195	ASP
1	B	216	LYS
1	B	248	MET
1	B	272	THR
1	B	278	LYS
1	B	292	TYR
1	B	308	ARG
1	B	315	THR
1	B	340	SER
1	B	342	GLU
1	B	355	LYS
1	B	407	ARG
1	B	416	GLN
1	B	429	VAL
1	B	449	ASP
1	B	456	ASP

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Mol	Chain	Res	Type
1	B	475	SER
1	B	480	SER
1	B	499	LYS
1	C	5	ILE
1	C	7	GLN
1	C	36	SER
1	C	43	SER
1	C	87	ARG
1	C	114	SER
1	C	115	LEU
1	C	138	LYS
1	C	148	THR
1	C	195	ASP
1	C	217	GLU
1	C	248	MET
1	C	272	THR
1	C	281	GLU
1	C	285	SER
1	C	292	TYR
1	C	308	ARG
1	C	309	GLU
1	C	323	LYS
1	C	325	ASP
1	C	339	SER
1	C	355	LYS
1	C	374	GLN
1	C	402	LYS
1	C	416	GLN
1	C	437	LYS
1	C	456	ASP
1	C	499	LYS
1	D	-2	LEU
1	D	-1	LYS
1	D	6	GLU
1	D	7	GLN
1	D	43	SER
1	D	109	THR
1	D	110	ILE
1	D	111	GLU
1	D	114	SER
1	D	123	SER
1	D	137	VAL

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Mol	Chain	Res	Type
1	D	148	THR
1	D	152	THR
1	D	189	GLN
1	D	195	ASP
1	D	217	GLU
1	D	242	SER
1	D	272	THR
1	D	308	ARG
1	D	323	LYS
1	D	340	SER
1	D	388	ASP
1	D	412	ASP
1	D	435	GLU
1	D	437	LYS
1	D	440	ASN
1	D	449	ASP
1	D	471	ASP
1	D	474	MET
1	D	499	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	164	ASN
1	A	189	GLN
1	A	472	HIS
1	A	503	ASN
1	B	154	GLN
1	B	164	ASN
1	B	189	GLN
1	B	255	GLN
1	B	359	ASN
1	B	416	GLN
1	B	439	GLN
1	B	472	HIS
1	B	503	ASN
1	B	506	ASN
1	C	58	GLN
1	C	74	HIS
1	C	154	GLN
1	C	164	ASN

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Mol	Chain	Res	Type
1	C	189	GLN
1	C	359	ASN
1	C	503	ASN
1	C	506	ASN
1	D	74	HIS
1	D	154	GLN
1	D	164	ASN
1	D	189	GLN
1	D	224	GLN
1	D	359	ASN
1	D	439	GLN
1	D	503	ASN
1	D	506	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	ATP	A	600	-	24,33,33	0.85	0	31,52,52	2.05	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ATP	B	600	-	24,33,33	1.03	2 (8%)	31,52,52	1.98	8 (25%)
2	ATP	C	600	-	24,33,33	0.83	1 (4%)	31,52,52	2.22	5 (16%)
2	ATP	D	600	-	24,33,33	1.10	2 (8%)	31,52,52	1.48	3 (9%)

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	ATP	A	600	-	-	0/18/38/38	0/3/3/3
2	ATP	B	600	-	-	0/18/38/38	0/3/3/3
2	ATP	C	600	-	-	0/18/38/38	0/3/3/3
2	ATP	D	600	-	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ATP	C2-N3	2.02	1.35	1.32
2	D	600	ATP	O4'-C1'	2.31	1.44	1.41
2	C	600	ATP	C5-C4	2.61	1.46	1.40
2	B	600	ATP	C5-C4	2.87	1.47	1.40
2	D	600	ATP	C5-C4	3.35	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	ATP	N3-C2-N1	-9.63	121.52	128.89
2	A	600	ATP	N3-C2-N1	-8.89	122.09	128.89
2	B	600	ATP	N3-C2-N1	-8.07	122.72	128.89
2	D	600	ATP	N3-C2-N1	-5.70	124.53	128.89
2	A	600	ATP	C4-C5-N7	-4.05	105.75	109.48
2	C	600	ATP	PB-O3B-PG	-3.48	121.01	132.67
2	C	600	ATP	C4-C5-N7	-3.36	106.39	109.48
2	A	600	ATP	PB-O3B-PG	-2.98	122.67	132.67
2	C	600	ATP	C2'-C1'-N9	-2.96	109.77	114.29
2	B	600	ATP	PB-O3B-PG	-2.64	123.80	132.67
2	D	600	ATP	PB-O3B-PG	-2.50	124.27	132.67
2	D	600	ATP	C2'-C1'-N9	-2.18	110.96	114.29
2	B	600	ATP	C2'-C1'-N9	-2.17	110.98	114.29
2	B	600	ATP	PA-O3A-PB	-2.14	126.71	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	ATP	C1'-N9-C4	-2.12	123.73	126.94
2	B	600	ATP	C4'-O4'-C1'	-2.08	107.43	109.72
2	A	600	ATP	O2B-PB-O1B	2.03	123.51	112.53
2	B	600	ATP	O2A-PA-O1A	2.04	123.56	112.53
2	B	600	ATP	O3G-PG-O2G	2.17	115.63	107.38
2	A	600	ATP	O3G-PG-O2G	2.34	116.28	107.38
2	C	600	ATP	C2-N1-C6	2.37	123.01	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ATP	1	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, 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	508/521 (97%)	-0.10	10 (1%)	68	63	30, 52, 80, 97	0
1	B	507/521 (97%)	-0.15	8 (1%)	74	69	26, 45, 66, 82	0
1	C	508/521 (97%)	-0.13	8 (1%)	74	69	33, 49, 73, 86	0
1	D	508/521 (97%)	-0.18	5 (0%)	84	81	32, 49, 70, 86	0
All	All	2031/2084 (97%)	-0.14	31 (1%)	76	71	26, 49, 74, 97	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	GLU	3.5
1	B	434	LYS	3.3
1	A	436	HIS	3.3
1	A	435	GLU	3.2
1	A	220	ALA	3.2
1	A	434	LYS	3.2
1	C	220	ALA	2.9
1	B	436	HIS	2.9
1	C	436	HIS	2.8
1	B	223	LYS	2.8
1	D	198	VAL	2.8
1	A	433	ASN	2.7
1	C	199	MET	2.7
1	B	111	GLU	2.7
1	A	219	VAL	2.7
1	D	153	GLY	2.6
1	A	111	GLU	2.4
1	A	471	ASP	2.4
1	C	198	VAL	2.3
1	D	436	HIS	2.3
1	D	112	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	154	GLN	2.3
1	B	224	GLN	2.2
1	D	251	ASP	2.2
1	A	154	GLN	2.2
1	C	407	ARG	2.1
1	B	154	GLN	2.1
1	B	196	LEU	2.1
1	A	432	TYR	2.1
1	C	197	SER	2.1
1	C	196	LEU	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
2	ATP	D	600	31/31	0.97	0.19	0.12	26,41,66,67	0
2	ATP	A	600	31/31	0.97	0.18	0.03	22,39,67,67	0
2	ATP	B	600	31/31	0.98	0.16	-0.36	23,34,58,59	0
2	ATP	C	600	31/31	0.97	0.17	-0.46	30,41,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.