Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:30 PM GMT

PDB ID	:	1XJQ
Title	:	ADP Complex OF HUMAN PAPS SYNTHETASE 1
Authors	:	Harjes, S.; Bayer, P.; Scheidig, A.J.
Deposited on	:	2004-09-24
Resolution	:	2.06 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:

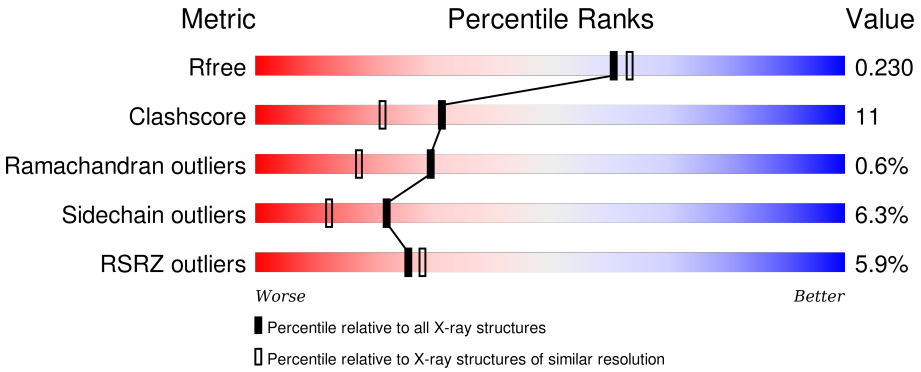
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	630	5% 66% 20% • • 11%
1	B	630	6% 66% 22% 5% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9997 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.

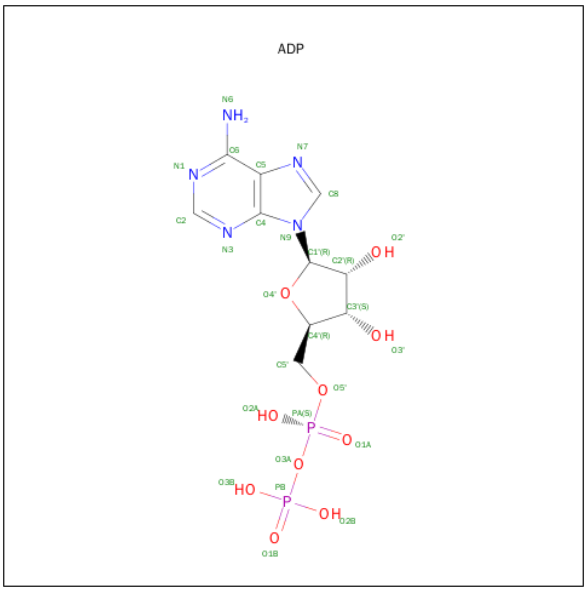
- Molecule 1 is a protein called Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	590	Total	C	N	O	S	0	5	0
			4718	2990	830	867	31			
1	A	563	Total	C	N	O	S	0	8	0
			4514	2864	790	828	32			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	CONFLICT	UNP O43252
B	625	HIS	-	EXPRESSION TAG	UNP O43252
B	626	HIS	-	EXPRESSION TAG	UNP O43252
B	627	HIS	-	EXPRESSION TAG	UNP O43252
B	628	HIS	-	EXPRESSION TAG	UNP O43252
B	629	HIS	-	EXPRESSION TAG	UNP O43252
B	630	HIS	-	EXPRESSION TAG	UNP O43252
A	416	SER	PHE	CONFLICT	UNP O43252
A	625	HIS	-	EXPRESSION TAG	UNP O43252
A	626	HIS	-	EXPRESSION TAG	UNP O43252
A	627	HIS	-	EXPRESSION TAG	UNP O43252
A	628	HIS	-	EXPRESSION TAG	UNP O43252
A	629	HIS	-	EXPRESSION TAG	UNP O43252
A	630	HIS	-	EXPRESSION TAG	UNP O43252

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

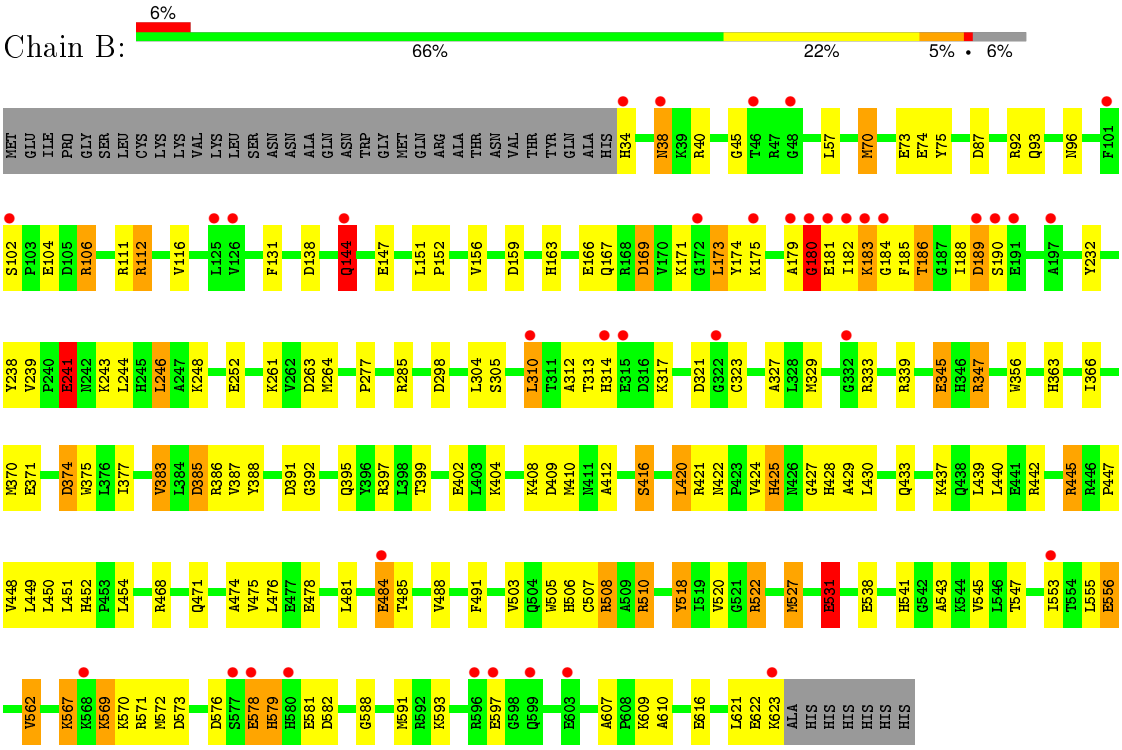
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	361	Total	O	0	0
			361	361		
3	B	323	Total	O	0	0
			323	323		

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.

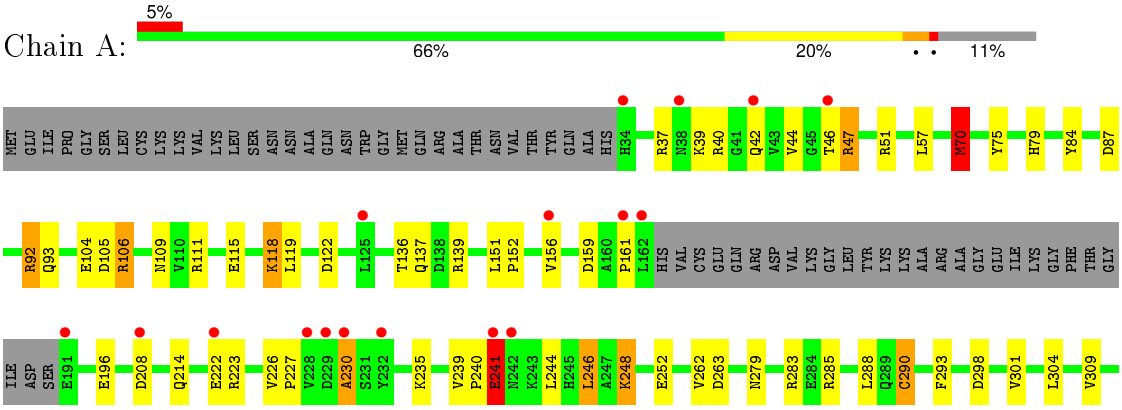
- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1

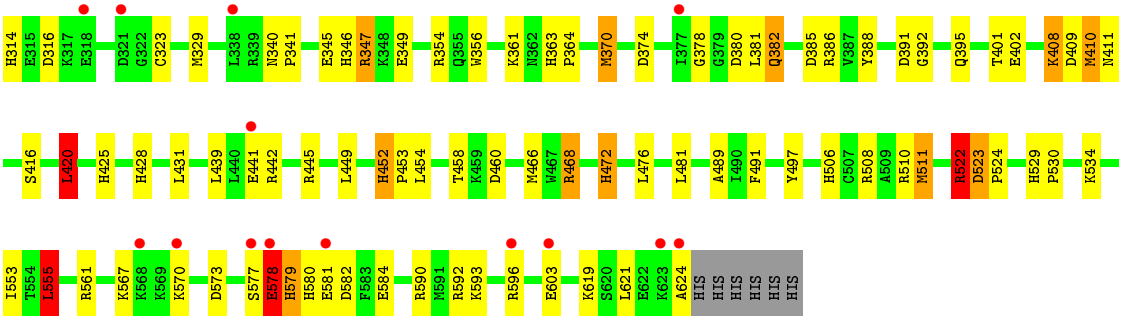
Chain B:



- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1

Chain A:




H314 E315 D316 K317 E318 D321 G322 C323 M329 L338 R339 N340 P341 E345 H346 R347 K348 E349 R354 Q355 W356 K361 N362 H363 P364 M370 D374 I377 G378 G379 D380 L381 Q382 D385 R386 V387 Y388 D391 G392 Q395 T401 E402 K408 D409 N410 N411
S416 L420 H425 H428 L431 L439 L440 E441 R442 R445 L449 H452 P453 L454 T468 K459 D460 M466 W467 R468 H472 L476 L481 A489 I490 F491 Y497 H506 C507 R508 A509 R510 M511 R522 D523 P524 H529 P530 K534
I553 T554 L555 R561 K567 K568 K569 K570 D573 S577 E578 H579 H580 E581 D582 F583 E584 R590 M591 R592 K593 R596 E603 K619 S620 L621 E622 K623 A624 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.50Å 82.50Å 133.00Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.06 19.65 – 2.06	Depositor EDS
% Data completeness (in resolution range)	96.6 (129.10-2.06) 96.7 (19.65-2.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.171 , 0.221 0.181 , 0.230	Depositor DCC
R_{free} test set	4869 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 97370 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9997	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ADP

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	1.54	31/4657 (0.7%)	1.32	56/6314 (0.9%)
1	B	1.55	40/4854 (0.8%)	1.31	42/6574 (0.6%)
All	All	1.54	71/9511 (0.7%)	1.31	98/12888 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	CG-CD	8.74	1.73	1.51
1	B	147	GLU	CD-OE2	8.64	1.35	1.25
1	A	346	HIS	C-O	8.42	1.39	1.23
1	B	518	TYR	CE2-CZ	-7.94	1.28	1.38
1	A	402	GLU	CD-OE2	7.82	1.34	1.25
1	B	345	GLU	CD-OE1	7.54	1.33	1.25
1	B	520	VAL	CB-CG1	-7.34	1.37	1.52
1	A	370	MET	SD-CE	7.27	2.18	1.77
1	B	232	TYR	CE1-CZ	7.25	1.48	1.38
1	A	345	GLU	CD-OE1	-7.06	1.17	1.25
1	B	38	ASN	CB-CG	7.03	1.67	1.51
1	B	356	TRP	CB-CG	6.78	1.62	1.50
1	B	347	ARG	CZ-NH1	6.78	1.41	1.33
1	A	410	MET	CG-SD	6.77	1.98	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	534	LYS	CD-CE	6.58	1.67	1.51
1	A	118	LYS	CD-CE	6.42	1.67	1.51
1	B	616	GLU	CG-CD	6.39	1.61	1.51
1	B	241	GLU	CD-OE2	6.34	1.32	1.25
1	A	401	THR	CB-CG2	6.34	1.73	1.52
1	A	196	GLU	CD-OE2	6.30	1.32	1.25
1	B	484	GLU	CG-CD	6.23	1.61	1.51
1	B	371	GLU	CD-OE2	6.12	1.32	1.25
1	B	531	GLU	CG-CD	6.11	1.61	1.51
1	B	131	PHE	CB-CG	-6.09	1.41	1.51
1	B	545	VAL	CB-CG1	-6.09	1.40	1.52
1	A	293	PHE	CE2-CZ	-6.03	1.25	1.37
1	B	252	GLU	CD-OE2	6.03	1.32	1.25
1	A	39	LYS	CD-CE	5.97	1.66	1.51
1	A	104	GLU	CD-OE1	5.92	1.32	1.25
1	A	301	VAL	CB-CG2	5.87	1.65	1.52
1	A	522	ARG	CG-CD	5.84	1.66	1.51
1	A	84	TYR	CG-CD2	5.84	1.46	1.39
1	B	421	ARG	CZ-NH2	5.83	1.40	1.33
1	B	556	GLU	CD-OE1	5.81	1.32	1.25
1	B	454	LEU	CG-CD1	5.77	1.73	1.51
1	B	505	TRP	CB-CG	5.76	1.60	1.50
1	A	196	GLU	CD-OE1	5.72	1.31	1.25
1	A	111	ARG	NE-CZ	-5.70	1.25	1.33
1	B	527	MET	SD-CE	5.69	2.09	1.77
1	B	74	GLU	CD-OE1	5.67	1.31	1.25
1	B	505	TRP	CE3-CZ3	-5.67	1.28	1.38
1	B	416[A]	SER	CA-CB	-5.63	1.44	1.52
1	B	416[B]	SER	CA-CB	-5.63	1.44	1.52
1	B	383	VAL	CB-CG2	5.60	1.64	1.52
1	A	262	VAL	CA-CB	5.60	1.66	1.54
1	B	518	TYR	CG-CD1	-5.58	1.31	1.39
1	A	382	GLN	CG-CD	5.55	1.63	1.51
1	B	241	GLU	CD-OE1	5.54	1.31	1.25
1	A	290[A]	CYS	CB-SG	-5.54	1.72	1.81
1	A	290[B]	CYS	CB-SG	-5.54	1.72	1.81
1	A	92	ARG	NE-CZ	5.51	1.40	1.33
1	B	144	GLN	CG-CD	5.51	1.63	1.51
1	A	386	ARG	CB-CG	-5.47	1.37	1.52
1	B	70	MET	SD-CE	5.46	2.08	1.77
1	A	70	MET	CG-SD	-5.42	1.67	1.81
1	A	354	ARG	CZ-NH1	-5.34	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CB-CG	-5.31	1.38	1.52
1	A	309	VAL	CA-CB	5.31	1.66	1.54
1	B	106	ARG	CG-CD	5.26	1.65	1.51
1	B	243	LYS	CD-CE	5.25	1.64	1.51
1	B	412	ALA	CA-CB	5.23	1.63	1.52
1	B	104	GLU	CD-OE1	5.22	1.31	1.25
1	B	305	SER	CB-OG	-5.21	1.35	1.42
1	B	327	ALA	CA-CB	5.19	1.63	1.52
1	A	262	VAL	CB-CG1	-5.12	1.42	1.52
1	A	491	PHE	CG-CD2	5.11	1.46	1.38
1	A	241	GLU	CD-OE2	5.10	1.31	1.25
1	B	73	GLU	CD-OE2	-5.08	1.20	1.25
1	B	402	GLU	CD-OE1	5.08	1.31	1.25
1	B	451	LEU	CA-C	-5.06	1.39	1.52
1	B	503	VAL	CA-CB	-5.02	1.44	1.54

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	522	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	B	409	ASP	CB-CG-OD2	11.11	128.30	118.30
1	B	347	ARG	NE-CZ-NH2	-10.41	115.10	120.30
1	B	576	ASP	CB-CG-OD2	10.36	127.62	118.30
1	A	409	ASP	CB-CG-OD2	10.02	127.32	118.30
1	B	159	ASP	CB-CG-OD2	9.32	126.69	118.30
1	A	285	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	B	421	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	B	385	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	285	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	264	MET	CG-SD-CE	-8.34	86.85	100.20
1	B	285	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	391	ASP	CB-CG-OD2	8.10	125.59	118.30
1	A	208	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	380	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	510	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	B	347	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	582	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	316	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	511	MET	CG-SD-CE	-7.62	88.00	100.20
1	A	522	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	A	159	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	466	MET	CG-SD-CE	-7.44	88.29	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	573	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	118	LYS	CD-CE-NZ	7.32	128.54	111.70
1	A	460	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	420	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	523	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	345	GLU	OE1-CD-OE2	7.06	131.78	123.30
1	A	37	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	189	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	87	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	122	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	592	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	138	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	70	MET	CA-CB-CG	6.61	124.54	113.30
1	B	508	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	582	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	468	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	298	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	447	PRO	N-CD-CG	-6.55	93.38	103.20
1	A	573	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	263	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	561	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	B	298	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	420	LEU	CA-CB-CG	6.40	130.02	115.30
1	B	531	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	B	112	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	510	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	571	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	B	339	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	431	LEU	CB-CG-CD1	6.09	121.35	111.00
1	A	47	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	263	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	252	GLU	OE1-CD-OE2	6.00	130.49	123.30
1	B	40	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	561	ARG	CG-CD-NE	5.96	124.31	111.80
1	A	619	LYS	CD-CE-NZ	5.96	125.40	111.70
1	A	442	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	468	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	105	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	92	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	339	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	112	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	442	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	HIS	CB-CA-C	5.73	121.86	110.40
1	A	555[A]	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	555[B]	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	370	MET	CG-SD-CE	5.63	109.21	100.20
1	B	397	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	111	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	522	ARG	CG-CD-NE	5.52	123.40	111.80
1	B	252	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	B	454	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	B	173	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	421	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	223	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	409	ASP	OD1-CG-OD2	-5.32	113.19	123.30
1	A	420	LEU	CB-CG-CD1	5.32	120.04	111.00
1	A	40	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	106	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	449	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	381	LEU	CB-CG-CD1	5.20	119.83	111.00
1	A	139	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	40	ARG	CB-CG-CD	5.18	125.07	111.60
1	A	323[A]	CYS	CA-CB-SG	5.18	123.33	114.00
1	A	323[B]	CYS	CA-CB-SG	5.18	123.33	114.00
1	A	578	GLU	N-CA-C	-5.18	97.02	111.00
1	B	442	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	391	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	410	MET	CB-CA-C	5.08	120.55	110.40
1	A	590	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	458	THR	CA-CB-CG2	-5.05	105.32	112.40
1	B	616	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	592	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	261	LYS	CD-CE-NZ	5.04	123.30	111.70
1	B	285	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	374	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	PRO	Peptide
1	A	230	ALA	Peptide
1	B	102	SER	Peptide
1	B	180	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4514	0	4448	89	0
1	B	4718	0	4650	107	0
2	A	27	0	12	0	0
2	B	54	0	23	6	0
3	A	361	0	0	24	1
3	B	323	0	0	38	1
All	All	9997	0	9133	197	1

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 11.

All (197) 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:591:MET:CE	1:B:591:MET:SD	2.02	1.47
1:A:70:MET:CE	1:A:70:MET:SD	2.05	1.45
1:B:70:MET:CE	1:B:70:MET:SD	2.08	1.39
1:B:527:MET:SD	1:B:527:MET:CE	2.09	1.39
1:A:370:MET:CE	1:A:370:MET:SD	2.18	1.31
1:B:538:GLU:HB3	1:B:541:HIS:CD2	1.73	1.24
1:B:538:GLU:HB3	1:B:541:HIS:HD2	0.90	1.06
1:B:484:GLU:HB2	3:B:1205:HOH:O	1.57	1.02
1:B:404:LYS:HE3	3:B:1190:HOH:O	1.65	0.97
1:B:538:GLU:CB	1:B:541:HIS:HD2	1.81	0.94
1:B:531:GLU:HB3	3:B:1132:HOH:O	1.65	0.93
1:B:541:HIS:CE1	1:A:288:LEU:HD21	2.05	0.91
1:A:452:HIS:HD2	1:A:510:ARG:HE	1.16	0.89
1:B:538:GLU:CB	1:B:541:HIS:CD2	2.56	0.89
1:A:47:ARG:HH11	1:A:230:ALA:HB3	1.38	0.87
1:B:578:GLU:O	1:B:579:HIS:ND1	2.09	0.86
1:A:392:GLY:O	1:A:395:GLN:NE2	2.08	0.86
1:A:279:ASN:HB3	3:A:1252:HOH:O	1.74	0.86
1:A:452:HIS:CD2	1:A:510:ARG:HE	1.93	0.85
1:B:246:LEU:HD12	3:B:1185:HOH:O	1.78	0.82
1:B:370:MET:HE1	3:B:1164:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLN:HG3	3:B:1182:HOH:O	1.81	0.80
1:A:235:LYS:HZ3	1:A:279:ASN:HD21	1.29	0.79
1:B:450:LEU:HD21	1:B:452:HIS:ND1	1.98	0.77
1:B:392:GLY:O	1:B:395:GLN:NE2	2.17	0.76
1:B:34:HIS:N	3:B:1150:HOH:O	2.20	0.75
1:B:506:HIS:HE1	3:B:904:HOH:O	1.68	0.74
1:A:388:TYR:HD1	3:A:1261:HOH:O	1.70	0.74
1:A:214:GLN:HG3	3:A:1240:HOH:O	1.87	0.72
1:B:484:GLU:CB	3:B:1205:HOH:O	2.23	0.70
1:B:395:GLN:HB2	3:B:1184:HOH:O	1.92	0.69
1:B:241:GLU:N	1:B:241:GLU:CD	2.46	0.68
1:B:485:THR:HG23	3:B:1205:HOH:O	1.94	0.68
1:A:621:LEU:O	1:A:624:ALA:HB3	1.94	0.68
1:B:238:TYR:CE1	3:B:1178:HOH:O	2.47	0.68
1:A:314:HIS:HB2	3:A:1209:HOH:O	1.94	0.67
1:B:404:LYS:HG2	3:B:1190:HOH:O	1.94	0.67
1:A:47:ARG:NH2	1:A:79:HIS:O	2.27	0.66
1:A:244:LEU:O	1:A:248:LYS:HG3	1.96	0.65
1:A:388:TYR:CD1	3:A:1261:HOH:O	2.48	0.65
1:A:522:ARG:O	1:A:522:ARG:NH1	2.30	0.64
1:A:235:LYS:NZ	1:A:279:ASN:HD21	1.96	0.64
1:B:144:GLN:HG2	3:B:1173:HOH:O	1.99	0.63
2:B:900:ADP:C8	2:B:900:ADP:H5'2	2.33	0.63
1:B:556:GLU:CD	3:B:1201:HOH:O	2.38	0.62
1:B:185:PHE:HD1	1:B:188:ILE:HD12	1.64	0.62
1:B:399:THR:HG22	3:B:1206:HOH:O	1.99	0.62
1:A:283:ARG:HD2	3:A:1217:HOH:O	2.00	0.61
1:B:386:ARG:HG2	1:B:388:TYR:CE1	2.35	0.61
1:B:433:GLN:OE1	3:B:1177:HOH:O	2.15	0.61
1:A:452:HIS:HD2	1:A:510:ARG:NE	1.95	0.60
1:B:363[B]:HIS:HD2	1:B:366:ILE:H	1.50	0.60
1:B:96:ASN:HD21	1:B:112:ARG:HD2	1.67	0.60
1:A:241:GLU:HB2	3:A:1208:HOH:O	2.01	0.60
1:B:506:HIS:O	1:B:510:ARG:HD3	2.01	0.60
1:B:425:HIS:H	1:B:428:HIS:HD2	1.49	0.60
1:B:541:HIS:ND1	1:A:288:LEU:HD21	2.16	0.60
1:B:484:GLU:CA	3:B:1205:HOH:O	2.50	0.59
1:B:171:LYS:CE	3:B:1210:HOH:O	2.50	0.59
1:B:450:LEU:HD21	1:B:452:HIS:CE1	2.37	0.59
1:A:382:GLN:CD	3:A:1242:HOH:O	2.41	0.59
1:B:184:GLY:HA2	1:B:189:ASP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:N	1:B:241:GLU:OE2	2.36	0.58
1:A:349:GLU:CD	3:A:1227:HOH:O	2.41	0.58
1:B:241:GLU:CD	1:B:241:GLU:H	2.05	0.58
1:A:241:GLU:CD	1:A:241:GLU:H	2.07	0.57
1:B:57:LEU:HD23	1:B:156:VAL:HB	1.86	0.57
1:A:235:LYS:NZ	1:A:279:ASN:ND2	2.53	0.57
1:B:317:LYS:O	1:B:321:ASP:HB2	2.05	0.57
2:B:900:ADP:C8	2:B:900:ADP:C5'	2.88	0.56
1:B:184:GLY:O	1:B:190:SER:OG	2.17	0.56
1:A:214:GLN:CG	3:A:1240:HOH:O	2.49	0.56
1:B:478:GLU:HG3	1:B:607:ALA:HB1	1.87	0.56
1:A:476[A]:LEU:HD23	1:A:481:LEU:HB2	1.87	0.56
1:B:96:ASN:ND2	1:B:112:ARG:HD2	2.20	0.56
1:B:569:LYS:HB3	3:B:1204:HOH:O	2.05	0.55
1:A:578:GLU:O	1:A:579:HIS:CB	2.54	0.55
1:B:468:ARG:HD2	3:B:911:HOH:O	2.06	0.55
1:B:522:ARG:HB3	3:B:1213:HOH:O	2.07	0.55
1:B:541:HIS:HE1	1:A:288:LEU:HD21	1.63	0.54
1:B:174:TYR:CD2	1:B:188:ILE:HD11	2.42	0.54
1:A:476[A]:LEU:CD2	1:A:481:LEU:HB2	2.37	0.54
1:A:468:ARG:O	1:A:472:HIS:ND1	2.41	0.54
1:B:543:ALA:O	1:B:547:THR:HG23	2.07	0.54
1:B:174:TYR:HD2	1:B:188:ILE:HD11	1.73	0.53
1:B:238:TYR:CZ	3:B:1178:HOH:O	2.58	0.53
1:A:87:ASP:HB2	3:A:1118:HOH:O	2.07	0.53
1:B:329:MET:HA	1:B:333:ARG:O	2.08	0.53
1:B:422:ASN:ND2	3:B:992:HOH:O	2.40	0.53
2:B:900:ADP:H8	2:B:900:ADP:H5'2	1.73	0.52
1:A:416[A]:SER:HB2	3:A:1232:HOH:O	2.09	0.52
1:B:171:LYS:NZ	3:B:1210:HOH:O	2.37	0.52
1:B:45:GLY:N	1:A:44:VAL:O	2.34	0.52
1:A:578:GLU:O	1:A:579:HIS:ND1	2.43	0.52
1:B:395:GLN:CB	3:B:1184:HOH:O	2.56	0.51
1:A:75:TYR:C	1:A:75:TYR:CD1	2.84	0.51
1:B:588:GLY:HA2	1:B:591:MET:CE	2.41	0.51
1:B:347:ARG:N	3:B:1162:HOH:O	2.43	0.51
1:B:345:GLU:HB3	3:B:1168:HOH:O	2.11	0.50
1:A:579:HIS:O	1:A:580:HIS:C	2.50	0.50
1:B:425:HIS:H	1:B:428:HIS:CD2	2.27	0.50
1:A:578:GLU:O	1:A:579:HIS:CG	2.65	0.50
2:B:900:ADP:C5'	2:B:900:ADP:H8	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:GLY:HA2	1:B:591:MET:HE3	1.94	0.50
1:A:363[B]:HIS:HE1	1:A:497:TYR:O	1.94	0.50
1:B:445:ARG:HD3	3:B:1222:HOH:O	2.11	0.50
1:B:186:THR:HA	1:B:190:SER:HB2	1.93	0.50
1:A:382:GLN:NE2	3:A:1242:HOH:O	2.45	0.50
1:A:118:LYS:NZ	3:A:1105:HOH:O	2.43	0.49
1:B:474:ALA:HB2	3:B:1192:HOH:O	2.12	0.49
1:A:70:MET:CE	1:A:70:MET:CG	2.88	0.49
1:A:452:HIS:HE1	3:A:923:HOH:O	1.96	0.49
1:B:395:GLN:CG	3:B:1184:HOH:O	2.60	0.49
1:B:553:ILE:HD13	3:B:1090:HOH:O	2.13	0.49
1:A:374:ASP:CG	3:A:1255:HOH:O	2.51	0.49
1:A:51:ARG:HD2	3:A:1060:HOH:O	2.12	0.49
1:A:388:TYR:HB3	3:A:1177:HOH:O	2.12	0.49
1:A:241:GLU:CB	3:A:1208:HOH:O	2.60	0.49
1:A:578:GLU:O	1:A:579:HIS:HB2	2.12	0.49
1:B:507:CYS:HA	1:B:518:TYR:CE1	2.48	0.49
1:B:476:LEU:HD23	1:B:481:LEU:HB2	1.95	0.48
1:A:420:LEU:HD13	1:A:453:PRO:HA	1.95	0.48
1:B:92:ARG:HH21	1:B:93:GLN:HG3	1.79	0.48
1:A:416[A]:SER:OG	1:A:439:LEU:HD11	2.14	0.48
1:A:239[B]:VAL:HG23	1:A:240:PRO:HD2	1.96	0.48
1:B:399:THR:CG2	3:B:1206:HOH:O	2.59	0.47
1:A:106:ARG:O	1:A:109:ASN:HB3	2.15	0.47
1:B:476:LEU:HD11	1:B:488:VAL:HG21	1.96	0.47
1:B:567:LYS:HB2	1:B:567:LYS:HE2	1.56	0.47
1:A:340:ASN:N	1:A:341:PRO:CD	2.77	0.47
1:A:341:PRO:HA	1:A:378:GLY:O	2.14	0.47
1:A:454:LEU:C	1:A:454:LEU:HD23	2.35	0.47
1:B:427:GLY:N	1:B:572:MET:HG3	2.30	0.47
1:A:578:GLU:C	1:A:579:HIS:ND1	2.68	0.47
1:B:424:VAL:HA	1:B:428:HIS:HD2	1.79	0.46
1:A:93:GLN:HE21	1:A:93:GLN:HA	1.80	0.46
1:B:416[A]:SER:OG	1:B:439:LEU:HD11	2.14	0.46
1:B:238:TYR:HE1	3:B:1178:HOH:O	1.90	0.46
1:A:593:LYS:CG	3:A:1253:HOH:O	2.63	0.46
1:A:340:ASN:N	1:A:341:PRO:HD3	2.30	0.46
1:B:313:THR:HA	3:B:1111:HOH:O	2.15	0.46
1:B:179:ALA:O	1:B:180:GLY:O	2.33	0.46
2:B:900:ADP:H2'	2:B:900:ADP:H5'1	1.76	0.46
1:A:395:GLN:CD	1:A:395:GLN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363[B]:HIS:CD2	1:A:364:PRO:HD2	2.51	0.45
1:B:476:LEU:HD11	1:B:488:VAL:CG2	2.46	0.45
1:B:410:MET:HE2	1:B:448:VAL:CG2	2.45	0.45
1:B:410:MET:HE2	1:B:448:VAL:HG21	1.99	0.45
1:B:450:LEU:CD2	1:B:452:HIS:ND1	2.76	0.45
1:B:314:HIS:CD2	1:B:375:TRP:HE1	2.35	0.45
1:A:523:ASP:N	1:A:524:PRO:CD	2.80	0.45
1:A:92:ARG:NH1	3:A:1066:HOH:O	2.49	0.44
1:A:506:HIS:O	1:A:510:ARG:HD3	2.17	0.44
1:A:115:GLU:O	1:A:119:LEU:HG	2.17	0.44
1:B:452:HIS:CD2	1:B:491:PHE:HB2	2.52	0.44
1:A:468:ARG:HB3	1:A:472:HIS:CE1	2.51	0.44
1:A:453:PRO:HD2	1:A:489:ALA:O	2.16	0.44
1:B:609:LYS:HD2	3:B:1203:HOH:O	2.17	0.44
1:A:57:LEU:HD23	1:A:156:VAL:HB	1.99	0.44
1:B:310[A]:LEU:HD13	1:B:377:ILE:HD12	1.99	0.44
1:B:248:LYS:NZ	1:B:385:ASP:OD1	2.46	0.44
1:A:567:LYS:HE2	1:A:584:GLU:HB2	2.00	0.44
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.80	0.44
1:A:452:HIS:CD2	1:A:510:ARG:NE	2.73	0.43
1:B:163:HIS:CE1	3:B:1166:HOH:O	2.70	0.43
1:A:356:TRP:CD1	1:A:363[B]:HIS:CE1	3.05	0.43
1:A:136:THR:O	1:A:137:GLN:C	2.56	0.43
1:B:607:ALA:O	1:B:610:ALA:N	2.52	0.43
1:A:329:MET:HG2	3:A:976:HOH:O	2.19	0.43
1:B:312:ALA:HB2	1:B:377:ILE:HD11	2.01	0.43
1:A:408:LYS:O	1:A:411:ASN:N	2.41	0.43
1:A:593:LYS:HG3	3:A:1253:HOH:O	2.19	0.42
1:B:562:VAL:HA	2:B:900:ADP:C2	2.53	0.42
1:A:385:ASP:CG	3:A:1259:HOH:O	2.56	0.42
1:B:386:ARG:HG3	1:B:387:VAL:N	2.34	0.42
1:A:425:HIS:O	1:A:428:HIS:HB2	2.19	0.42
1:A:151:LEU:HA	1:A:152:PRO:HD3	1.92	0.42
1:B:166:GLU:O	1:B:169:ASP:HB2	2.20	0.42
1:A:529:HIS:HA	1:A:530:PRO:HD3	1.93	0.42
1:B:239:VAL:HG12	1:B:383:VAL:O	2.20	0.41
1:B:112:ARG:O	1:B:116:VAL:HG23	2.21	0.41
1:A:511:MET:SD	1:A:555[A]:LEU:HD22	2.61	0.41
1:B:244:LEU:O	1:B:248:LYS:HG3	2.20	0.41
1:B:471:GLN:O	1:B:475:VAL:HG23	2.21	0.41
1:B:171:LYS:HE2	3:B:1210:HOH:O	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:VAL:HA	1:A:227:PRO:HD3	1.91	0.41
1:B:151:LEU:HA	1:B:152:PRO:HD3	1.90	0.41
1:A:356:TRP:NE1	1:A:363[A]:HIS:CE1	2.89	0.40
1:B:75:TYR:CD1	1:B:75:TYR:C	2.95	0.40
1:A:347:ARG:HH11	1:A:347:ARG:HD2	1.73	0.40
1:B:429:ALA:O	1:B:430:LEU:C	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1218:HOH:O	3:A:1007:HOH:O[1_455]	2.00	0.20

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	566/630 (90%)	551 (97%)	14 (2%)	1 (0%)	52 43
1	B	592/630 (94%)	567 (96%)	19 (3%)	6 (1%)	19 8
All	All	1158/1260 (92%)	1118 (96%)	33 (3%)	7 (1%)	30 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	GLY
1	B	183	LYS
1	B	579	HIS
1	A	579	HIS
1	B	597	GLU
1	B	169	ASP
1	B	181	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	489/538 (91%)	460 (94%)	29 (6%)	24 14
1	B	508/538 (94%)	472 (93%)	36 (7%)	18 9
All	All	997/1076 (93%)	932 (94%)	65 (6%)	22 12

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
1	B	106	ARG
1	B	144	GLN
1	B	167	GLN
1	B	173	LEU
1	B	175	LYS
1	B	182	ILE
1	B	183	LYS
1	B	186	THR
1	B	241	GLU
1	B	246	LEU
1	B	277	PRO
1	B	304	LEU
1	B	310[A]	LEU
1	B	310[B]	LEU
1	B	323	CYS
1	B	374	ASP
1	B	408	LYS
1	B	420	LEU
1	B	425	HIS
1	B	437	LYS
1	B	445	ARG
1	B	508	ARG
1	B	522	ARG
1	B	531	GLU
1	B	555	LEU
1	B	562	VAL

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Mol	Chain	Res	Type
1	B	567	LYS
1	B	569	LYS
1	B	570	LYS
1	B	578	GLU
1	B	581	GLU
1	B	593	LYS
1	B	621	LEU
1	B	622	GLU
1	B	623	LYS
1	A	42	GLN
1	A	46	THR
1	A	70	MET
1	A	222	GLU
1	A	241	GLU
1	A	246[A]	LEU
1	A	246[B]	LEU
1	A	248	LYS
1	A	304	LEU
1	A	347	ARG
1	A	361	LYS
1	A	408	LYS
1	A	410	MET
1	A	420	LEU
1	A	441	GLU
1	A	445	ARG
1	A	452	HIS
1	A	472	HIS
1	A	508	ARG
1	A	522	ARG
1	A	553	ILE
1	A	555[A]	LEU
1	A	555[B]	LEU
1	A	570	LYS
1	A	577	SER
1	A	578	GLU
1	A	581	GLU
1	A	596	ARG
1	A	603	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
1	B	109	ASN
1	B	210	ASN
1	B	314	HIS
1	B	422	ASN
1	B	428	HIS
1	B	506	HIS
1	B	541	HIS
1	B	599	GLN
1	A	93	GLN
1	A	140	ASN
1	A	279	ASN
1	A	422	ASN
1	A	452	HIS

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

3 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	ADP	A	900	-	22,29,29	1.54	4 (18%)	27,45,45	2.79	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	B	800	-	22,29,29	1.61	5 (22%)	27,45,45	1.90	4 (14%)
2	ADP	B	900	-	22,29,29	1.86	5 (22%)	27,45,45	3.65	13 (48%)

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	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	800	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	ADP	O5'-C5'	-4.17	1.27	1.44
2	B	900	ADP	PB-O3B	-3.95	1.40	1.54
2	B	800	ADP	O2'-C2'	-2.96	1.35	1.43
2	B	900	ADP	O4'-C4'	-2.79	1.38	1.45
2	A	900	ADP	O2'-C2'	-2.53	1.36	1.43
2	B	800	ADP	O4'-C4'	-2.38	1.39	1.45
2	B	800	ADP	PA-O2A	-2.11	1.45	1.54
2	B	900	ADP	PB-O1B	-2.04	1.44	1.51
2	A	900	ADP	PB-O2B	-2.03	1.47	1.54
2	A	900	ADP	C2-N1	2.35	1.38	1.33
2	B	800	ADP	C2-N1	2.57	1.38	1.33
2	B	900	ADP	C2-N1	3.07	1.39	1.33
2	A	900	ADP	O4'-C1'	3.86	1.46	1.41
2	B	800	ADP	C2-N3	4.85	1.40	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	ADP	N3-C2-N1	-11.48	120.10	128.89
2	A	900	ADP	N3-C2-N1	-10.34	120.97	128.89
2	B	800	ADP	N3-C2-N1	-6.88	123.63	128.89
2	B	900	ADP	O4'-C4'-C5'	-6.35	86.60	109.32
2	B	900	ADP	O2B-PB-O1B	-4.34	96.61	110.58
2	B	900	ADP	O5'-PA-O1A	-3.08	97.67	109.62
2	A	900	ADP	O4'-C1'-N9	-2.88	102.07	108.10
2	A	900	ADP	C1'-N9-C4	-2.62	122.99	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	ADP	O2A-PA-O3A	-2.26	94.84	105.09
2	B	800	ADP	O2A-PA-O5'	2.02	118.65	108.46
2	B	800	ADP	O4'-C1'-N9	2.02	112.33	108.10
2	A	900	ADP	C2'-C1'-N9	2.11	117.52	114.29
2	A	900	ADP	O2A-PA-O3A	2.74	117.51	105.09
2	B	900	ADP	C4'-O4'-C1'	2.80	112.79	109.72
2	B	900	ADP	C4-C5-N7	2.95	112.19	109.48
2	B	900	ADP	O3B-PB-O1B	3.09	120.53	110.58
2	B	900	ADP	O2'-C2'-C3'	3.17	122.15	111.83
2	B	900	ADP	N6-C6-N1	3.20	126.08	119.20
2	A	900	ADP	C2-N1-C6	3.26	124.59	118.77
2	B	800	ADP	O2B-PB-O1B	3.43	121.61	110.58
2	A	900	ADP	C4'-O4'-C1'	3.59	113.66	109.72
2	A	900	ADP	O3A-PA-O5'	3.94	113.39	102.94
2	B	900	ADP	O3B-PB-O2B	4.38	124.05	107.38
2	B	900	ADP	C2'-C1'-N9	4.51	121.19	114.29
2	A	900	ADP	O3B-PB-O2B	4.89	126.00	107.38
2	B	900	ADP	O2A-PA-O5'	7.33	145.42	108.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	ADP	6	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	563/630 (89%)	0.16	31 (5%)	29	31	22, 37, 67, 90	3 (0%)
1	B	590/630 (93%)	0.26	37 (6%)	23	25	23, 39, 72, 104	0
All	All	1153/1260 (91%)	0.21	68 (5%)	26	28	22, 38, 69, 104	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	GLU	7.0
1	A	624	ALA	6.3
1	B	184	GLY	5.5
1	B	180	GLY	4.8
1	B	179	ALA	4.7
1	B	175	LYS	4.4
1	A	46	THR	4.4
1	B	183	LYS	4.3
1	B	189	ASP	4.3
1	A	161	PRO	4.0
1	A	162	LEU	3.9
1	B	48	GLY	3.7
1	B	577	SER	3.6
1	A	578	GLU	3.5
1	B	603	GLU	3.4
1	A	228	VAL	3.4
1	A	596	ARG	3.3
1	A	568	LYS	3.1
1	A	232	TYR	3.1
1	B	126	VAL	3.1
1	B	322	GLY	3.1
1	B	484	GLU	3.0
1	B	578	GLU	3.0
1	B	102	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	596	ARG	3.0
1	B	597	GLU	3.0
1	A	577	SER	3.0
1	A	241	GLU	2.9
1	B	46	THR	2.9
1	A	38	ASN	2.9
1	B	190	SER	2.9
1	B	599	GLN	2.8
1	A	321	ASP	2.8
1	B	580	HIS	2.7
1	B	182	ILE	2.7
1	B	172	GLY	2.7
1	B	332	GLY	2.6
1	A	338	LEU	2.6
1	B	623	LYS	2.6
1	A	191	GLU	2.5
1	B	191	GLU	2.5
1	B	101	PHE	2.5
1	B	315	GLU	2.5
1	A	242	ASN	2.4
1	A	229	ASP	2.4
1	A	156	VAL	2.4
1	B	144	GLN	2.4
1	A	570	LYS	2.4
1	A	603	GLU	2.4
1	A	208	ASP	2.4
1	A	125	LEU	2.4
1	B	314	HIS	2.3
1	A	581	GLU	2.3
1	B	310[A]	LEU	2.3
1	A	230	ALA	2.3
1	B	197	ALA	2.3
1	A	222	GLU	2.3
1	A	441	GLU	2.3
1	A	34	HIS	2.3
1	B	34	HIS	2.2
1	A	42	GLN	2.1
1	A	318	GLU	2.1
1	B	553	ILE	2.1
1	A	623	LYS	2.1
1	B	38	ASN	2.1
1	B	568	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	125	LEU	2.0
1	A	377	ILE	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	ADP	B	900	27/27	0.98	0.07	-1.40	33,38,46,48	0
2	ADP	A	900	27/27	0.99	0.07	-1.55	30,33,39,41	0
2	ADP	B	800	27/27	0.98	0.07	-1.61	37,41,43,49	0

6.5 Other polymers (i)

There are no such residues in this entry.