WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1AD5
Title : SRC FAMILY KINASE HCK-AMP-PNP COMPLEX
Authors : Sicheri, F.; Moarefi, I.; Kuriyan, J.
Deposited on : 1997-02-20
Resolution : 2.60 Å(reported)

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		2.2%
Sidechain outliers		10.3%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
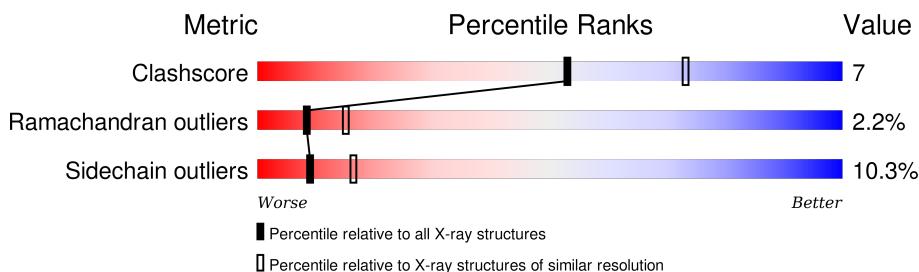
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	72% 23% · ·
1	B	438	69% 25% 5% ·
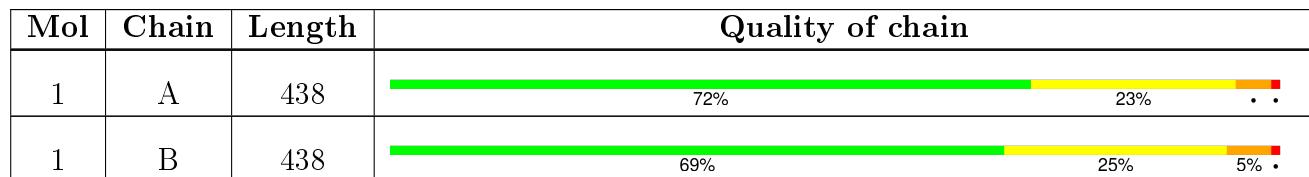
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8572 atoms, of which 1536 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 HAEMATOPOETIC CELL KINASE HCK.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	438	Total 4253	C 2232	H 768	N 585	O 647	P 1	S 20	0	0	0
1	B	438	Total 4253	C 2232	H 768	N 585	O 647	P 1	S 20	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP P08631
A	?	-	GLU	DELETION	UNP P08631
A	?	-	ASP	DELETION	UNP P08631
A	?	-	ASN	DELETION	UNP P08631
A	?	-	GLU	DELETION	UNP P08631
A	?	-	TYR	DELETION	UNP P08631
A	?	-	THR	DELETION	UNP P08631
A	?	-	ALA	DELETION	UNP P08631
A	?	-	ARG	DELETION	UNP P08631
A	?	-	GLU	DELETION	UNP P08631
A	527	PTR	TYR	MODIFIED RESIDUE	UNP P08631
B	?	-	ILE	DELETION	UNP P08631
B	?	-	GLU	DELETION	UNP P08631
B	?	-	ASP	DELETION	UNP P08631
B	?	-	ASN	DELETION	UNP P08631
B	?	-	GLU	DELETION	UNP P08631
B	?	-	TYR	DELETION	UNP P08631
B	?	-	THR	DELETION	UNP P08631
B	?	-	ALA	DELETION	UNP P08631
B	?	-	ARG	DELETION	UNP P08631
B	?	-	GLU	DELETION	UNP P08631
B	527	PTR	TYR	MODIFIED RESIDUE	UNP P08631

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Ca 2	0	0
2	A	2	Total 2	Ca 2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
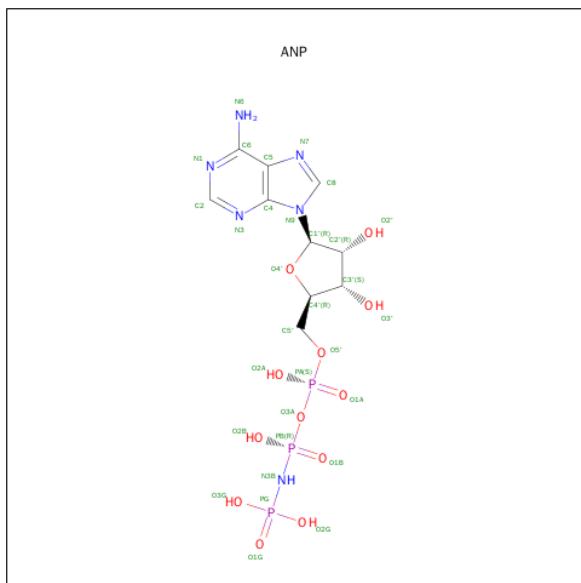
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: HAEMATOPOETIC CELL KINASE HCK

Chain A:

- Molecule 1: HAEMATOPOETIC CELL KINASE HCK

Chain B:
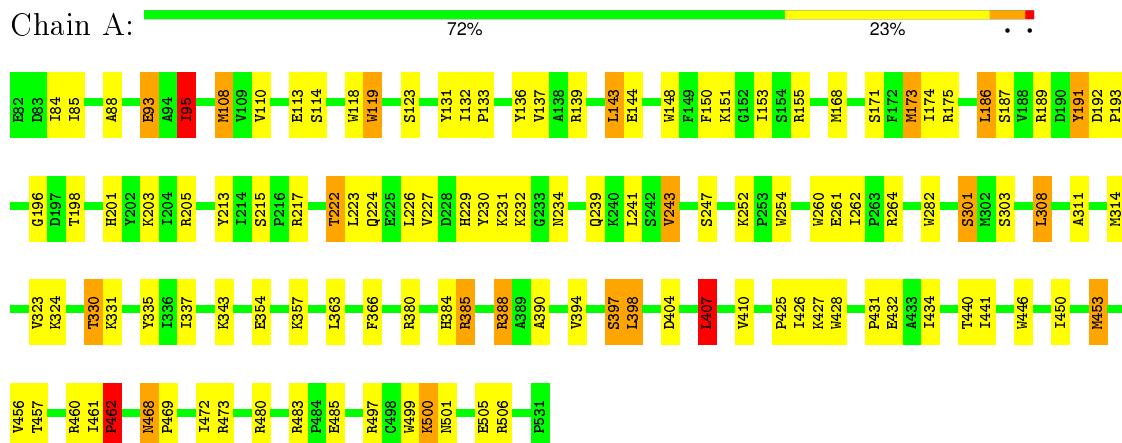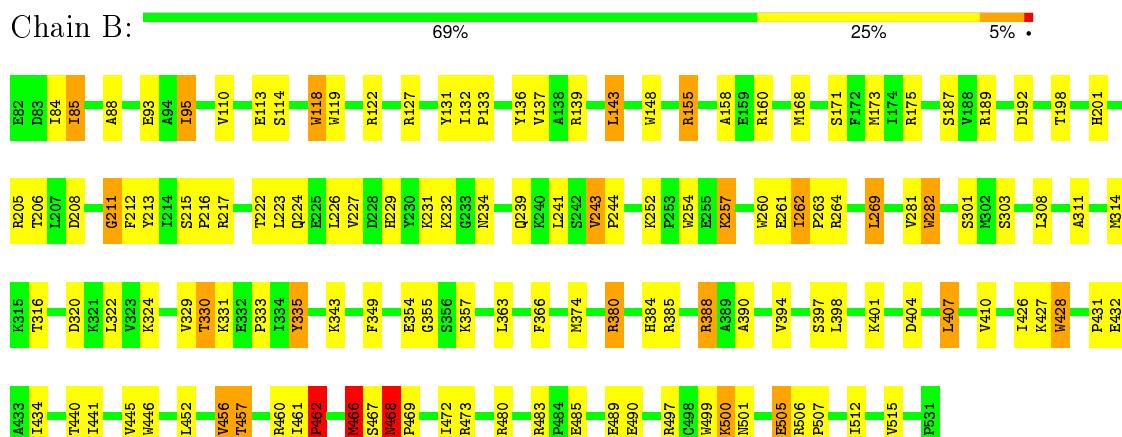
4　Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.77Å　92.36Å　178.29Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	18.00　–　2.60	Depositor
% Data completeness (in resolution range)	79.4 (18.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.239　,　0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ANP, PTR

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	0.92	0/3552	1.62	61/4799 (1.3%)
1	B	0.93	0/3552	1.64	68/4799 (1.4%)
All	All	0.93	0/7104	1.63	129/9598 (1.3%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	A	118	TRP	CD1-CG-CD2	9.27	113.72	106.30
1	B	260	TRP	CD1-CG-CD2	9.19	113.65	106.30
1	B	499	TRP	CD1-CG-CD2	9.08	113.57	106.30
1	B	282	TRP	CD1-CG-CD2	9.02	113.52	106.30
1	A	380	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	428	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	155	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	B	119	TRP	CD1-CG-CD2	8.58	113.16	106.30
1	B	497	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	254	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	B	260	TRP	CE2-CD2-CG	-8.54	100.47	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	A	260	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	497	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	380	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	260	TRP	CE2-CD2-CG	-8.34	100.63	107.30
1	A	380	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	282	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	118	TRP	CE2-CD2-CG	-8.11	100.82	107.30
1	B	155	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	499	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	A	254	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	B	175	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	499	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	B	148	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	B	497	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	254	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A	155	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	119	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	B	407	LEU	CA-C-N	-7.56	100.57	117.20
1	A	428	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	388	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	466	MET	CA-CB-CG	7.41	125.89	113.30
1	B	119	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	282	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	B	118	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	428	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	B	282	TRP	CE2-CD2-CG	-7.23	101.51	107.30
1	B	428	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	A	468	ASN	CA-C-N	7.10	136.99	117.10
1	B	457	THR	CA-CB-CG2	-7.05	102.53	112.40
1	B	335	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	A	148	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	323	VAL	CG1-CB-CG2	-6.98	99.74	110.90
1	A	148	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	407	LEU	CA-C-N	-6.79	102.26	117.20
1	B	324	LYS	CA-CB-CG	6.79	128.34	113.40
1	A	499	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	A	410	VAL	CA-C-N	6.77	129.73	116.20
1	A	264	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	148	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	B	260	TRP	CG-CD2-CE3	6.68	139.91	133.90
1	A	175	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	TRP	CD1-CG-CD2	6.64	111.61	106.30
1	A	254	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	A	324	LYS	CA-CB-CG	6.55	127.81	113.40
1	A	118	TRP	CG-CD2-CE3	6.43	139.69	133.90
1	A	260	TRP	CB-CG-CD1	-6.42	118.66	127.00
1	B	206	THR	N-CA-CB	-6.39	98.15	110.30
1	A	175	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	506	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	260	TRP	CG-CD2-CE3	6.32	139.59	133.90
1	B	374	MET	CG-SD-CE	6.31	110.30	100.20
1	B	446	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	B	303	SER	N-CA-CB	-6.26	101.11	110.50
1	A	483	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	446	TRP	CD1-CG-CD2	6.23	111.28	106.30
1	B	175	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	446	TRP	CE2-CD2-CG	-6.17	102.37	107.30
1	B	410	VAL	CA-C-N	6.16	128.51	116.20
1	B	260	TRP	CB-CG-CD1	-6.14	119.02	127.00
1	B	380	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	118	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	A	497	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	428	TRP	CB-CG-CD1	-6.06	119.12	127.00
1	B	483	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	473	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	118	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	186	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	473	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	160	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	483	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	428	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	B	155	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	148	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	B	384	HIS	CA-C-N	5.72	129.78	117.20
1	A	303	SER	N-CA-CB	-5.70	101.95	110.50
1	A	254	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	B	499	TRP	CG-CD2-CE3	5.68	139.01	133.90
1	B	282	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	335	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	446	TRP	CD1-CG-CD2	5.62	110.80	106.30
1	B	127	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	173	MET	CA-CB-CG	5.58	122.78	113.30
1	A	139	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	468	ASN	CA-C-O	-5.49	108.56	120.10
1	A	118	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	A	95	ILE	N-CA-CB	-5.47	98.22	110.80
1	A	282	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	B	515	VAL	CG1-CB-CG2	-5.45	102.17	110.90
1	B	468	ASN	CA-C-N	5.45	132.36	117.10
1	B	388	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	131	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	B	473	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	301	SER	N-CA-C	5.39	125.57	111.00
1	B	506	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	260	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	428	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	385	ARG	CA-C-N	5.32	128.91	117.20
1	B	122	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	384	HIS	CA-C-N	5.30	128.86	117.20
1	B	456	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	A	456	VAL	CG1-CB-CG2	-5.25	102.51	110.90
1	B	428	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	B	490	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	B	118	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	B	428	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	B	445	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	B	173	MET	CA-CB-CG	5.16	122.07	113.30
1	B	95	ILE	N-CA-CB	-5.14	98.97	110.80
1	B	499	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	B	211	GLY	CA-C-N	-5.12	105.94	117.20
1	B	148	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	B	254	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	B	322	LEU	CA-CB-CG	5.06	126.95	115.30
1	B	139	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	388	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASP	Peptide
1	B	192	ASP	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	3485	768	3422	45	0
1	B	3485	768	3421	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	2	0
All	All	7036	1536	6869	92	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 7.

All (92) 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:427:LYS:HD3	1:B:462:PRO:HB2	1.60	0.82
1:A:203:LYS:HD3	1:B:489:GLU:HG3	1.62	0.82
1:A:427:LYS:HD3	1:A:462:PRO:HB2	1.64	0.78
1:B:457:THR:HB	1:B:460:ARG:HB3	1.78	0.64
1:A:457:THR:HB	1:A:460:ARG:HB3	1.80	0.63
1:A:191:TYR:HE1	1:A:193:PRO:HA	1.64	0.62
1:B:452:LEU:O	1:B:456:VAL:HG23	1.99	0.61
1:A:330:THR:HB	1:A:331:LYS:HD2	1.81	0.60
1:B:224:GLN:O	1:B:227:VAL:HG22	2.02	0.60
1:B:88:ALA:HA	1:B:137:VAL:HG12	1.84	0.59
1:B:231:LYS:HA	1:B:241:LEU:O	2.03	0.59
1:A:133:PRO:HB2	1:A:136:TYR:CD1	2.38	0.59
1:B:426:ILE:HG12	1:B:468:ASN:ND2	2.18	0.58
1:A:354:GLU:HA	1:A:357:LYS:HD2	1.85	0.58
1:A:388:ARG:HG3	1:A:390:ALA:HB3	1.85	0.57
1:B:316:THR:HG22	1:B:380:ARG:NH2	2.18	0.57
1:B:311:ALA:HA	1:B:314:MET:HB2	1.86	0.57
1:B:330:THR:HB	1:B:331:LYS:HD2	1.87	0.56
1:A:144:GLU:HG2	1:A:151:LYS:HD3	1.88	0.56
1:A:224:GLN:O	1:A:227:VAL:HG22	2.06	0.55
1:A:191:TYR:CE1	1:A:193:PRO:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:HG3	1:B:390:ALA:HB3	1.88	0.55
1:B:187:SER:OG	1:B:201:HIS:HD2	1.92	0.53
1:B:133:PRO:HB2	1:B:136:TYR:CD1	2.42	0.53
1:B:343:LYS:HB2	1:B:394:VAL:HB	1.89	0.53
1:B:143:LEU:HD23	1:B:143:LEU:H	1.73	0.53
1:B:354:GLU:HA	1:B:357:LYS:HD2	1.91	0.52
1:A:205:ARG:HH12	1:B:489:GLU:HG2	1.74	0.51
1:A:215:SER:HB3	1:A:217:ARG:HD3	1.92	0.51
1:B:226:LEU:O	1:B:229:HIS:HB3	2.11	0.51
1:B:223:LEU:O	1:B:226:LEU:HB3	2.10	0.50
1:A:187:SER:OG	1:A:201:HIS:HD2	1.94	0.50
1:A:223:LEU:O	1:A:227:VAL:HG13	2.10	0.50
1:A:450:ILE:O	1:A:453:MET:HB3	2.11	0.50
1:A:469:PRO:HA	1:A:472:ILE:HG12	1.93	0.50
1:B:223:LEU:O	1:B:227:VAL:HG13	2.12	0.50
1:A:231:LYS:HA	1:A:241:LEU:O	2.12	0.49
1:A:93:GLU:HG2	1:A:95:ILE:HD12	1.94	0.49
1:B:469:PRO:HA	1:B:472:ILE:HG12	1.93	0.49
1:A:363:LEU:O	1:A:366:PHE:HB2	2.13	0.49
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.95	0.48
1:B:316:THR:HG22	1:B:380:ARG:HH22	1.78	0.48
1:A:223:LEU:H	1:A:223:LEU:HD12	1.79	0.48
3:B:532:ANP:H5'1	3:B:532:ANP:O3G	2.14	0.48
1:B:215:SER:HB3	1:B:217:ARG:HD3	1.97	0.47
1:A:143:LEU:HD23	1:A:143:LEU:H	1.78	0.47
1:B:426:ILE:HG12	1:B:468:ASN:CG	2.35	0.47
1:A:88:ALA:HA	1:A:137:VAL:HG12	1.96	0.47
1:B:426:ILE:HD12	1:B:427:LYS:H	1.79	0.47
1:A:174:ILE:HG12	1:A:186:LEU:HD23	1.97	0.47
1:B:349:PHE:O	1:B:355:GLY:HA3	2.15	0.47
1:A:132:ILE:HA	1:A:133:PRO:HD3	1.78	0.46
1:A:426:ILE:HD12	1:A:427:LYS:H	1.80	0.45
1:B:132:ILE:HA	1:B:133:PRO:HD3	1.82	0.45
1:B:461:ILE:HA	1:B:462:PRO:HD3	1.92	0.45
1:A:500:LYS:HE2	1:A:505:GLU:HB3	1.99	0.45
1:B:281:VAL:HG11	3:B:532:ANP:C8	2.46	0.45
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.78	0.45
1:A:407:LEU:HA	1:A:407:LEU:HD13	1.61	0.45
1:B:507:PRO:HG2	1:B:512:ILE:HD11	1.98	0.44
1:A:205:ARG:HH22	1:B:489:GLU:HG2	1.83	0.44
1:A:131:TYR:O	1:A:132:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LYS:NZ	1:A:505:GLU:HG2	2.33	0.43
1:A:226:LEU:O	1:A:229:HIS:HB3	2.18	0.43
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.53	0.43
1:A:150:PHE:CD1	1:A:173:MET:HB2	2.53	0.43
1:A:153:ILE:HA	1:A:153:ILE:HD13	1.79	0.43
1:B:269:LEU:HD13	1:B:282:TRP:HB2	1.99	0.43
1:B:205:ARG:O	1:B:212:PHE:HA	2.18	0.43
1:B:205:ARG:HB2	1:B:213:TYR:CE1	2.54	0.43
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.93	0.43
1:B:500:LYS:HE2	1:B:505:GLU:HB3	2.01	0.43
1:A:230:TYR:HB3	1:A:241:LEU:HG	2.00	0.42
1:A:343:LYS:HB2	1:A:394:VAL:HB	2.02	0.42
1:A:311:ALA:HA	1:A:314:MET:HB2	2.01	0.42
1:B:264:ARG:NH2	1:B:333:PRO:O	2.52	0.42
1:A:397:SER:O	1:A:398:LEU:HB2	2.20	0.42
1:B:213:TYR:CE2	1:B:216:PRO:HG3	2.54	0.42
1:B:426:ILE:HD13	1:B:427:LYS:HG3	2.01	0.42
1:A:108:MET:HB3	1:A:123:SER:HA	2.02	0.41
1:B:363:LEU:O	1:B:366:PHE:HB2	2.20	0.41
1:A:337:ILE:HD12	1:A:337:ILE:N	2.35	0.41
1:A:461:ILE:HA	1:A:462:PRO:HD3	1.95	0.41
1:B:426:ILE:CD1	1:B:427:LYS:HG3	2.51	0.41
1:A:203:LYS:HG2	1:A:205:ARG:CZ	2.51	0.41
1:B:155:ARG:O	1:B:158:ALA:HB3	2.21	0.41
1:B:118:TRP:CD1	1:B:257:LYS:HG2	2.56	0.40
1:B:171:SER:HA	1:B:243:VAL:O	2.21	0.40
1:A:119:TRP:HB2	1:A:132:ILE:HG22	2.02	0.40
1:B:320:ASP:O	1:B:401:LYS:HE3	2.21	0.40
1:B:85:ILE:O	1:B:85:ILE:HG13	2.21	0.40
1:A:171:SER:HA	1:A:243:VAL:O	2.22	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	433/438 (99%)	392 (90%)	32 (7%)	9 (2%)	9	16
1	B	433/438 (99%)	390 (90%)	33 (8%)	10 (2%)	8	14
All	All	866/876 (99%)	782 (90%)	65 (8%)	19 (2%)	8	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	A	468	ASN
1	A	501	ASN
1	B	208	ASP
1	B	462	PRO
1	B	468	ASN
1	B	501	ASN
1	B	211	GLY
1	B	301	SER
1	B	467	SER
1	A	196	GLY
1	A	234	ASN
1	A	404	ASP
1	B	234	ASN
1	A	301	SER
1	B	404	ASP
1	B	466	MET
1	A	222	THR
1	A	425	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/382 (97%)	331 (90%)	38 (10%)	9	16
1	B	369/382 (97%)	331 (90%)	38 (10%)	9	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	738/764 (97%)	662 (90%)	76 (10%)	9 16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	85	ILE
1	A	93	GLU
1	A	95	ILE
1	A	108	MET
1	A	110	VAL
1	A	113	GLU
1	A	114	SER
1	A	143	LEU
1	A	168	MET
1	A	189	ARG
1	A	191	TYR
1	A	198	THR
1	A	213	TYR
1	A	222	THR
1	A	232	LYS
1	A	239	GLN
1	A	243	VAL
1	A	247	SER
1	A	252	LYS
1	A	261	GLU
1	A	262	ILE
1	A	308	LEU
1	A	330	THR
1	A	385	ARG
1	A	397	SER
1	A	398	LEU
1	A	407	LEU
1	A	431	PRO
1	A	432	GLU
1	A	434	ILE
1	A	440	THR
1	A	441	ILE
1	A	453	MET
1	A	462	PRO
1	A	480	ARG
1	A	485	GLU

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Mol	Chain	Res	Type
1	A	500	LYS
1	B	84	ILE
1	B	85	ILE
1	B	93	GLU
1	B	95	ILE
1	B	110	VAL
1	B	113	GLU
1	B	114	SER
1	B	143	LEU
1	B	168	MET
1	B	189	ARG
1	B	198	THR
1	B	222	THR
1	B	232	LYS
1	B	239	GLN
1	B	243	VAL
1	B	244	PRO
1	B	252	LYS
1	B	257	LYS
1	B	261	GLU
1	B	262	ILE
1	B	269	LEU
1	B	308	LEU
1	B	330	THR
1	B	385	ARG
1	B	397	SER
1	B	398	LEU
1	B	407	LEU
1	B	431	PRO
1	B	432	GLU
1	B	434	ILE
1	B	440	THR
1	B	441	ILE
1	B	462	PRO
1	B	466	MET
1	B	480	ARG
1	B	485	GLU
1	B	500	LYS
1	B	505	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	201	HIS
1	A	391	ASN
1	B	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	PTR	A	527	1,2	14,16,17	1.08	1 (7%)	18,22,24	1.18	0
1	PTR	B	527	1,2	14,16,17	0.95	1 (7%)	18,22,24	1.21	1 (5%)

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
1	PTR	A	527	1,2	-	0/9/11/13	0/1/1/1
1	PTR	B	527	1,2	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	PTR	P-O3P	-2.25	1.46	1.54
1	A	527	PTR	OH-CZ	2.36	1.46	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	527	PTR	CE2-CZ-CE1	2.17	123.72	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ANP	A	1	2	27,33,33	1.50	5 (18%)	30,52,52	1.82	8 (26%)
3	ANP	B	532	2	27,33,33	1.49	6 (22%)	30,52,52	1.89	9 (30%)

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
3	ANP	A	1	2	-	0/12/38/38	0/3/3/3
3	ANP	B	532	2	-	1/12/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ANP	PB-O3A	-3.32	1.54	1.59
3	B	532	ANP	PB-O2B	-2.78	1.48	1.56
3	A	1	ANP	PG-O3G	-2.72	1.49	1.56
3	B	532	ANP	PG-O2G	-2.65	1.49	1.56
3	A	1	ANP	PG-O2G	-2.60	1.49	1.56
3	B	532	ANP	PG-O3G	-2.52	1.49	1.56
3	A	1	ANP	PB-O2B	-2.44	1.49	1.56
3	B	532	ANP	C8-N7	-2.39	1.30	1.34
3	B	532	ANP	PB-O3A	-2.39	1.56	1.59
3	A	1	ANP	PG-O1G	3.11	1.49	1.46
3	B	532	ANP	PG-O1G	3.13	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	532	ANP	O1G-PG-N3B	-5.58	103.35	111.90
3	A	1	ANP	O1G-PG-N3B	-5.56	103.36	111.90
3	B	532	ANP	O3A-PB-N3B	-2.86	98.57	106.44
3	B	532	ANP	O1B-PB-N3B	-2.76	107.66	111.90
3	A	1	ANP	O1B-PB-N3B	-2.47	108.10	111.90
3	A	1	ANP	O3A-PA-O5'	-2.39	96.59	102.94
3	A	1	ANP	O3A-PB-N3B	-2.38	99.90	106.44
3	B	532	ANP	O3A-PA-O5'	-2.32	96.77	102.94
3	A	1	ANP	O3'-C3'-C4'	-2.00	105.04	111.05
3	B	532	ANP	C4-C5-N7	2.08	111.39	109.48
3	B	532	ANP	PA-O3A-PB	2.13	139.81	132.67
3	B	532	ANP	C4'-O4'-C1'	2.29	112.24	109.72
3	A	1	ANP	C4'-O4'-C1'	2.35	112.30	109.72
3	A	1	ANP	O3G-PG-O2G	2.44	114.82	107.58
3	B	532	ANP	O3G-PG-O2G	2.52	115.06	107.58
3	A	1	ANP	O2B-PB-O1B	4.09	118.53	110.00
3	B	532	ANP	O2B-PB-O1B	4.34	119.05	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	532	ANP	O1G-PG-N3B-PB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	532	ANP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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