



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KRM
Title : Crystal structure of bovine adenosine deaminase complexed with 6-hydroxyl-1,6-dihydropurine riboside
Authors : Kinoshita, T.
Deposited on : 2002-01-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

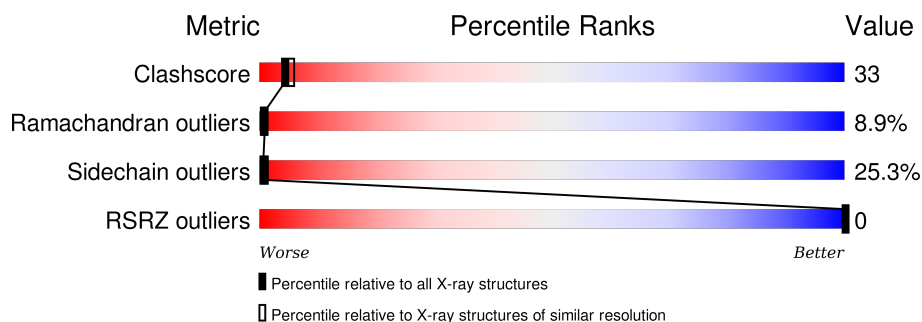
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3298 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 adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2788	1773	470	533	12	0	0	0

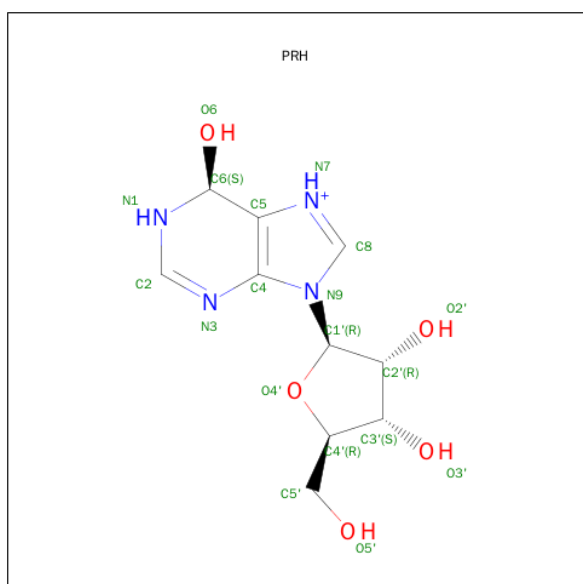
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	GLN	CONFLICT	UNP P56658

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-HYDROXY-1,6-DIHYDRO PURINE NUCLEOSIDE (three-letter code: PRH) (formula: C₁₀H₁₅N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	4	5		

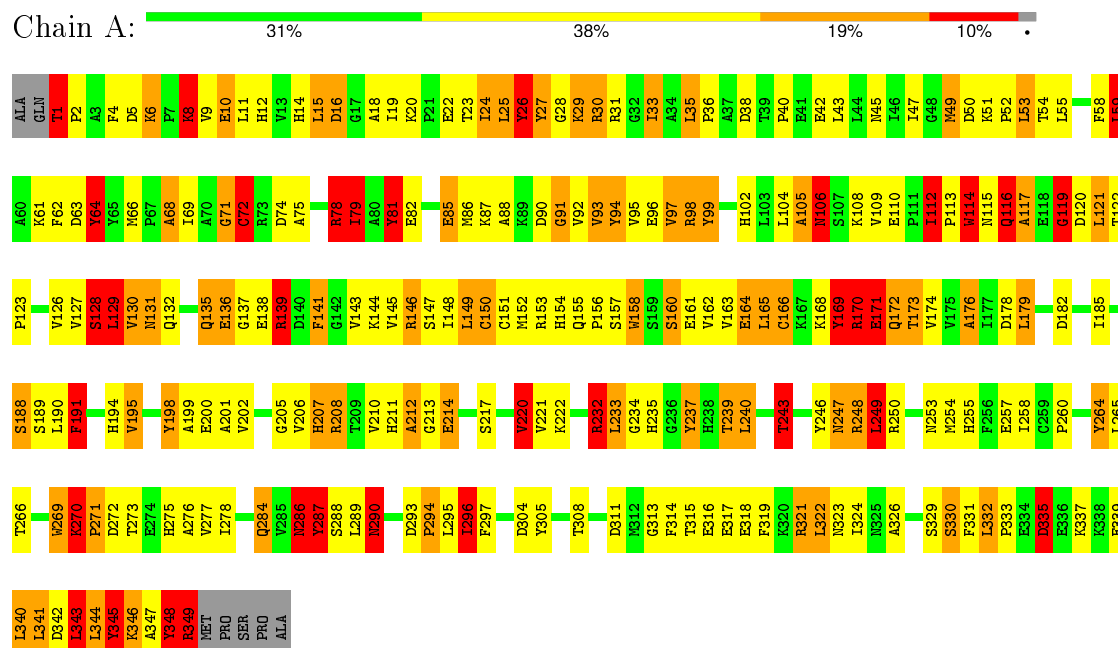
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	490	Total	O	0	0
			490	490		

3 Residue-property plots

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

- Molecule 1: adenosine deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.03Å 80.03Å 141.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 53.04 – 1.93	Depositor EDS
% Data completeness (in resolution range)	75.4 (8.00-2.50) 49.4 (53.04-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.94Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.198 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 1184.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 17387 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3298	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PRH

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	1.06	0/2852	2.04	92/3866 (2.4%)

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	24

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	TYR	CB-CG-CD2	-11.81	113.91	121.00
1	A	72	CYS	CA-CB-SG	-10.68	94.77	114.00
1	A	27	TYR	CB-CG-CD1	-9.84	115.10	121.00
1	A	78	ARG	CD-NE-CZ	-9.58	110.19	123.60
1	A	72	CYS	N-CA-C	9.10	135.56	111.00
1	A	198	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	A	78	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	170	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	182	ASP	CB-CA-C	-7.99	94.42	110.40
1	A	239	THR	CA-CB-CG2	-7.88	101.37	112.40
1	A	152	MET	CG-SD-CE	-7.80	87.72	100.20
1	A	98	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	191	PHE	CB-CG-CD2	-7.64	115.45	120.80
1	A	98	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	A	269	TRP	C-N-CA	-7.46	103.05	121.70
1	A	270	LYS	CB-CA-C	7.34	125.08	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	345	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	A	170	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	335	ASP	N-CA-CB	-7.14	97.75	110.60
1	A	8	LYS	CB-CA-C	-6.99	96.42	110.40
1	A	158	TRP	CB-CA-C	-6.98	96.44	110.40
1	A	248	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	119	GLY	C-N-CA	-6.87	104.53	121.70
1	A	78	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	348	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	A	49	MET	C-N-CA	-6.66	105.04	121.70
1	A	284	GLN	CA-CB-CG	6.29	127.24	113.40
1	A	330	SER	CB-CA-C	-6.23	98.27	110.10
1	A	146	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	27	TYR	CD1-CG-CD2	6.05	124.55	117.90
1	A	8	LYS	N-CA-C	6.03	127.27	111.00
1	A	150	CYS	CB-CA-C	-6.02	98.36	110.40
1	A	116	GLN	CB-CA-C	6.00	122.40	110.40
1	A	220	VAL	CA-CB-CG2	5.98	119.87	110.90
1	A	290	ASN	C-N-CA	-5.94	106.86	121.70
1	A	321	ARG	C-N-CA	-5.87	107.03	121.70
1	A	50	ASP	N-CA-C	5.86	126.82	111.00
1	A	188	SER	CB-CA-C	-5.83	99.02	110.10
1	A	152	MET	N-CA-CB	-5.83	100.11	110.60
1	A	308	THR	CA-CB-CG2	-5.82	104.25	112.40
1	A	27	TYR	CG-CD2-CE2	-5.81	116.65	121.30
1	A	249	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	79	ILE	CA-CB-CG1	5.76	121.95	111.00
1	A	117	ALA	N-CA-C	5.72	126.45	111.00
1	A	91	GLY	N-CA-C	5.67	127.28	113.10
1	A	248	ARG	C-N-CA	-5.65	107.58	121.70
1	A	232	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	171	GLU	N-CA-C	5.59	126.10	111.00
1	A	182	ASP	CA-CB-CG	5.58	125.68	113.40
1	A	94	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	40	PRO	C-N-CA	-5.54	107.85	121.70
1	A	59	LEU	CA-CB-CG	-5.52	102.61	115.30
1	A	114	TRP	N-CA-C	5.51	125.88	111.00
1	A	271	PRO	C-N-CA	-5.50	107.95	121.70
1	A	93	VAL	CB-CA-C	-5.49	100.97	111.40
1	A	135	GLN	CA-CB-CG	-5.48	101.33	113.40
1	A	332	LEU	CA-CB-CG	5.48	127.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	CA-CB-CG2	5.45	119.08	110.90
1	A	222	LYS	CA-CB-CG	5.45	125.39	113.40
1	A	237	TYR	CD1-CG-CD2	5.45	123.89	117.90
1	A	26	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	272	ASP	CA-CB-CG	-5.40	101.52	113.40
1	A	249	LEU	N-CA-CB	5.39	121.17	110.40
1	A	212	ALA	C-N-CA	-5.33	111.11	122.30
1	A	81	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	A	18	ALA	CB-CA-C	-5.29	102.16	110.10
1	A	220	VAL	CA-CB-CG1	-5.29	102.97	110.90
1	A	116	GLN	CA-CB-CG	5.25	124.96	113.40
1	A	94	TYR	CG-CD1-CE1	-5.25	117.10	121.30
1	A	121	LEU	N-CA-C	5.21	125.06	111.00
1	A	139	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	176	ALA	CB-CA-C	-5.19	102.31	110.10
1	A	296	ILE	CA-CB-CG1	5.19	120.86	111.00
1	A	272	ASP	N-CA-C	5.19	125.00	111.00
1	A	166	CYS	CB-CA-C	-5.16	100.08	110.40
1	A	35	LEU	N-CA-CB	-5.16	100.09	110.40
1	A	99	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	266	THR	CB-CA-C	-5.14	97.71	111.60
1	A	74	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	69	ILE	C-N-CA	-5.12	108.89	121.70
1	A	88	ALA	CB-CA-C	-5.12	102.42	110.10
1	A	232	ARG	CA-CB-CG	5.11	124.65	113.40
1	A	94	TYR	CD1-CG-CD2	5.11	123.52	117.90
1	A	45	ASN	CA-CB-CG	-5.09	102.21	113.40
1	A	105	ALA	O-C-N	-5.07	114.59	122.70
1	A	170	ARG	C-N-CA	5.05	134.32	121.70
1	A	198	TYR	CD1-CG-CD2	5.05	123.45	117.90
1	A	106	ASN	CA-CB-CG	-5.05	102.30	113.40
1	A	151	CYS	CA-CB-SG	-5.05	104.92	114.00
1	A	169	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	97	VAL	CB-CA-C	-5.03	101.84	111.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	THR	Peptide
1	A	128	SER	Peptide
1	A	141	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	169	TYR	Sidechain
1	A	172	GLN	Peptide
1	A	191	PHE	Sidechain
1	A	199	ALA	Peptide
1	A	205	GLY	Peptide
1	A	232	ARG	Sidechain
1	A	26	TYR	Sidechain
1	A	287	TYR	Sidechain
1	A	289	LEU	Peptide
1	A	30	ARG	Sidechain
1	A	345	TYR	Sidechain
1	A	348	TYR	Sidechain,Peptide
1	A	349	ARG	Sidechain
1	A	49	MET	Peptide
1	A	64	TYR	Sidechain
1	A	71	GLY	Peptide
1	A	78	ARG	Sidechain
1	A	81	TYR	Sidechain
1	A	90	ASP	Peptide
1	A	99	TYR	Sidechain

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	2788	0	2749	183	0
2	A	1	0	0	0	0
3	A	19	0	14	1	0
4	A	490	0	0	15	0
All	All	3298	0	2763	183	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 33.

All (183) 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:A:221:VAL:HG13	1:A:233:LEU:HD11	1.58	0.85
1:A:316:GLU:HA	1:A:319:PHE:HD1	1.45	0.80
1:A:171:GLU:O	1:A:173:THR:HA	1.84	0.78
1:A:26:TYR:CE1	1:A:30:ARG:HG3	2.21	0.76
1:A:169:TYR:O	1:A:174:VAL:HG22	1.90	0.72
1:A:264:TYR:HB2	1:A:269:TRP:CE3	2.26	0.70
1:A:154:HIS:CD2	1:A:155:GLN:HG2	2.28	0.69
1:A:185:ILE:HB	1:A:188:SER:OG	1.92	0.69
1:A:104:LEU:HB3	1:A:126:VAL:HG11	1.74	0.69
1:A:221:VAL:HG21	1:A:239:THR:HG22	1.75	0.68
1:A:258:ILE:HD12	1:A:287:TYR:HB2	1.77	0.67
1:A:155:GLN:HG3	1:A:158:TRP:CZ2	2.31	0.66
1:A:51:LYS:O	1:A:53:LEU:HD13	1.96	0.65
1:A:258:ILE:HG21	1:A:277:VAL:HB	1.78	0.65
1:A:287:TYR:HD1	1:A:287:TYR:H	1.45	0.64
1:A:264:TYR:HB2	1:A:269:TRP:HE3	1.61	0.64
1:A:81:TYR:CE2	1:A:141:PHE:HE1	2.17	0.63
1:A:28:GLY:HA3	1:A:35:LEU:HD22	1.82	0.62
1:A:138:GLU:OE2	1:A:144:LYS:HG3	1.99	0.61
1:A:19:ILE:HG12	1:A:79:ILE:HG13	1.83	0.60
1:A:344:LEU:HD22	1:A:344:LEU:H	1.66	0.59
1:A:10:GLU:HG2	1:A:95:VAL:HG13	1.84	0.59
1:A:81:TYR:CE2	1:A:141:PHE:CE1	2.90	0.59
1:A:153:ARG:HH12	1:A:189:SER:HB3	1.66	0.59
1:A:22:GLU:H	1:A:22:GLU:CD	2.06	0.59
1:A:114:TRP:HD1	1:A:116:GLN:HE21	1.51	0.59
1:A:52:PRO:HG3	1:A:264:TYR:CE1	2.38	0.57
1:A:148:ILE:HG12	1:A:176:ALA:HB3	1.86	0.57
1:A:232:ARG:HD3	1:A:257:GLU:OE2	2.04	0.57
1:A:332:LEU:HD13	4:A:850:HOH:O	2.05	0.57
1:A:179:LEU:HB3	1:A:210:VAL:HG13	1.87	0.57
1:A:206:VAL:HG11	4:A:858:HOH:O	2.04	0.57
1:A:105:ALA:HA	1:A:106:ASN:HB2	1.88	0.56
1:A:207:HIS:HD2	1:A:331:PHE:CD1	2.24	0.56
1:A:246:TYR:O	1:A:250:ARG:HG3	2.06	0.56
1:A:206:VAL:HG12	1:A:206:VAL:O	2.06	0.55
1:A:198:TYR:O	1:A:201:ALA:HB3	2.06	0.55
1:A:61:LYS:O	1:A:64:TYR:HB2	2.07	0.55
1:A:136:GLU:O	1:A:139:ARG:HB2	2.08	0.54
1:A:341:LEU:HD23	1:A:345:TYR:CE2	2.42	0.54
1:A:106:ASN:OD1	1:A:119:GLY:HA2	2.06	0.54
1:A:113:PRO:C	1:A:115:ASN:HA	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	1:A:344:LEU:HD22	2.08	0.54
1:A:269:TRP:CZ2	1:A:275:HIS:HB2	2.43	0.54
1:A:275:HIS:ND1	1:A:277:VAL:HG12	2.23	0.54
1:A:221:VAL:HG12	4:A:887:HOH:O	2.08	0.53
1:A:20:LYS:HG3	4:A:662:HOH:O	2.08	0.53
1:A:232:ARG:HG3	1:A:255:HIS:HB3	1.89	0.53
1:A:1:THR:OG1	1:A:2:PRO:HD3	2.08	0.53
1:A:23:THR:O	1:A:27:TYR:HD2	1.92	0.53
1:A:232:ARG:HB2	1:A:255:HIS:HB3	1.91	0.53
1:A:344:LEU:HB3	1:A:348:TYR:CE1	2.44	0.53
1:A:212:ALA:HB3	1:A:233:LEU:HD21	1.91	0.53
1:A:340:LEU:HD22	1:A:340:LEU:O	2.09	0.52
1:A:221:VAL:HG11	1:A:239:THR:HG21	1.91	0.52
1:A:14:HIS:CE1	3:A:401:PRH:C8	2.92	0.52
1:A:185:ILE:HB	1:A:188:SER:HG	1.74	0.52
1:A:35:LEU:HD11	1:A:68:ALA:HB2	1.90	0.52
1:A:25:LEU:HD21	1:A:38:ASP:O	2.10	0.51
1:A:113:PRO:O	1:A:116:GLN:HB3	2.10	0.51
1:A:128:SER:HA	1:A:131:ASN:OD1	2.11	0.51
1:A:104:LEU:O	1:A:126:VAL:HG21	2.10	0.51
1:A:81:TYR:HE2	1:A:141:PHE:CE1	2.28	0.51
1:A:96:GLU:HA	1:A:146:ARG:O	2.10	0.51
1:A:114:TRP:N	1:A:115:ASN:HA	2.26	0.51
1:A:255:HIS:CE1	1:A:288:SER:HB3	2.46	0.51
1:A:221:VAL:HG21	1:A:239:THR:CG2	2.40	0.50
1:A:253:ASN:HA	4:A:931:HOH:O	2.12	0.49
1:A:188:SER:HA	1:A:191:PHE:CE1	2.47	0.49
1:A:294:PRO:HG2	4:A:688:HOH:O	2.12	0.49
1:A:82:GLU:O	1:A:85:GLU:HB2	2.12	0.49
1:A:147:SER:OG	1:A:174:VAL:HG12	2.11	0.49
1:A:31:ARG:NE	1:A:72:CYS:HB2	2.26	0.49
1:A:19:ILE:HG23	1:A:23:THR:HG22	1.93	0.49
1:A:154:HIS:HD2	1:A:155:GLN:HG2	1.76	0.49
1:A:102:HIS:HA	4:A:696:HOH:O	2.12	0.49
1:A:253:ASN:HB3	4:A:1076:HOH:O	2.13	0.48
1:A:178:ASP:OD2	1:A:179:LEU:N	2.46	0.48
1:A:55:LEU:HG	1:A:59:LEU:HD12	1.95	0.48
1:A:106:ASN:HB3	1:A:121:LEU:HB2	1.95	0.48
1:A:116:GLN:HG2	1:A:117:ALA:H	1.77	0.48
1:A:58:PHE:CE1	1:A:297:PHE:CZ	3.02	0.48
1:A:92:VAL:HG12	1:A:94:TYR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HG2	1:A:174:VAL:O	2.13	0.48
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.52	0.48
1:A:146:ARG:HE	1:A:171:GLU:HG3	1.79	0.48
1:A:202:VAL:HG22	1:A:208:ARG:NE	2.29	0.48
1:A:255:HIS:CD2	1:A:257:GLU:HG2	2.49	0.47
1:A:270:LYS:HA	1:A:271:PRO:HD3	1.84	0.47
1:A:127:VAL:HG11	1:A:169:TYR:CD2	2.50	0.47
1:A:104:LEU:HD21	4:A:866:HOH:O	2.15	0.47
1:A:95:VAL:HB	4:A:867:HOH:O	2.14	0.47
1:A:81:TYR:HE2	1:A:141:PHE:CZ	2.32	0.47
1:A:35:LEU:HG	1:A:36:PRO:HD2	1.97	0.47
1:A:258:ILE:HD13	1:A:277:VAL:HG23	1.97	0.46
1:A:293:ASP:HB2	1:A:297:PHE:CE2	2.51	0.46
1:A:247:ASN:OD1	1:A:247:ASN:N	2.48	0.46
1:A:258:ILE:O	1:A:290:ASN:HB2	2.16	0.46
1:A:158:TRP:O	1:A:161:GLU:HB2	2.16	0.46
1:A:305:TYR:HD2	1:A:319:PHE:CE2	2.34	0.46
1:A:286:ASN:OD1	1:A:286:ASN:C	2.54	0.46
1:A:129:LEU:O	1:A:130:VAL:C	2.52	0.46
1:A:316:GLU:HA	1:A:319:PHE:CD1	2.36	0.45
1:A:207:HIS:CD2	1:A:331:PHE:CD1	3.04	0.45
1:A:105:ALA:HB3	4:A:696:HOH:O	2.17	0.45
1:A:11:LEU:HD11	1:A:326:ALA:HB1	1.97	0.45
1:A:333:PRO:HB2	1:A:335:ASP:HB3	1.99	0.45
1:A:305:TYR:CD2	1:A:319:PHE:CD2	3.05	0.45
1:A:264:TYR:CD1	1:A:265:LEU:HD12	2.52	0.45
1:A:314:PHE:O	1:A:315:THR:C	2.56	0.45
1:A:233:LEU:HD12	4:A:901:HOH:O	2.17	0.45
1:A:322:LEU:HD22	1:A:323:ASN:N	2.31	0.45
1:A:166:CYS:O	1:A:170:ARG:HB2	2.17	0.45
1:A:93:VAL:O	1:A:93:VAL:HG12	2.17	0.44
1:A:315:THR:O	1:A:319:PHE:CD1	2.71	0.44
1:A:19:ILE:HG23	1:A:23:THR:CG2	2.47	0.44
1:A:249:LEU:O	1:A:250:ARG:C	2.55	0.44
1:A:221:VAL:HG11	1:A:239:THR:CG2	2.47	0.44
1:A:166:CYS:HA	1:A:174:VAL:HG21	1.99	0.44
1:A:121:LEU:HD22	1:A:126:VAL:HG22	1.98	0.44
1:A:239:THR:HG23	1:A:239:THR:H	1.58	0.44
1:A:149:LEU:HB3	1:A:162:VAL:HG13	2.00	0.44
1:A:120:ASP:HB2	4:A:1038:HOH:O	2.17	0.44
1:A:324:ILE:HD11	1:A:348:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:HA	1:A:234:GLY:O	2.17	0.44
1:A:165:LEU:O	1:A:166:CYS:C	2.53	0.44
1:A:130:VAL:O	1:A:131:ASN:C	2.54	0.44
1:A:12:HIS:CE1	1:A:211:HIS:NE2	2.86	0.44
1:A:42:GLU:O	1:A:43:LEU:C	2.55	0.44
1:A:264:TYR:HD1	1:A:265:LEU:HD12	1.83	0.43
1:A:25:LEU:HD12	1:A:29:LYS:HD3	1.99	0.43
1:A:198:TYR:N	1:A:198:TYR:CD1	2.86	0.43
1:A:305:TYR:HD2	1:A:319:PHE:CD2	2.37	0.43
1:A:319:PHE:HA	1:A:322:LEU:HD13	1.99	0.43
1:A:275:HIS:CG	1:A:277:VAL:HG12	2.53	0.43
1:A:264:TYR:HB2	1:A:269:TRP:CZ3	2.53	0.43
1:A:137:GLY:O	1:A:141:PHE:HD1	2.02	0.43
1:A:108:LYS:O	1:A:109:VAL:C	2.56	0.43
1:A:31:ARG:CZ	1:A:72:CYS:H	2.32	0.43
1:A:93:VAL:HG11	1:A:343:LEU:HD12	2.01	0.43
1:A:258:ILE:HD12	1:A:287:TYR:HD2	1.84	0.43
1:A:33:ILE:HG21	1:A:68:ALA:N	2.33	0.43
1:A:243:THR:O	1:A:247:ASN:OD1	2.36	0.43
1:A:346:LYS:HE3	1:A:346:LYS:HB2	1.54	0.43
1:A:58:PHE:O	1:A:61:LYS:HB2	2.19	0.42
1:A:237:TYR:O	1:A:240:LEU:HG	2.19	0.42
1:A:121:LEU:HD22	1:A:126:VAL:CG2	2.49	0.42
1:A:92:VAL:O	1:A:143:VAL:HG23	2.19	0.42
1:A:160:SER:O	1:A:163:VAL:HG12	2.19	0.42
1:A:15:LEU:HD22	4:A:868:HOH:O	2.19	0.42
1:A:278:ILE:HG13	1:A:314:PHE:CE1	2.54	0.42
1:A:161:GLU:O	1:A:164:GLU:HG3	2.20	0.42
1:A:136:GLU:O	1:A:139:ARG:N	2.52	0.42
1:A:146:ARG:NE	1:A:171:GLU:HG3	2.35	0.42
1:A:75:ALA:O	1:A:79:ILE:HG23	2.18	0.42
1:A:54:THR:O	1:A:55:LEU:C	2.58	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HG21	1.85	0.42
1:A:345:TYR:O	1:A:349:ARG:HB3	2.20	0.42
1:A:318:GLU:O	1:A:319:PHE:C	2.58	0.41
1:A:71:GLY:CA	1:A:121:LEU:HD12	2.50	0.41
1:A:337:LYS:O	1:A:341:LEU:HB2	2.20	0.41
1:A:324:ILE:HD11	1:A:348:TYR:HD1	1.85	0.41
1:A:171:GLU:C	1:A:173:THR:HA	2.40	0.41
1:A:112:ILE:HA	1:A:113:PRO:HD3	1.85	0.41
1:A:248:ARG:HD3	1:A:248:ARG:HH21	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:O	1:A:59:LEU:HD12	2.19	0.41
1:A:295:LEU:HG	1:A:296:ILE:N	2.35	0.41
1:A:26:TYR:O	1:A:30:ARG:HB2	2.21	0.41
1:A:255:HIS:HD2	1:A:257:GLU:HG2	1.85	0.41
1:A:47:ILE:O	1:A:61:LYS:HD2	2.21	0.41
1:A:217:SER:O	1:A:220:VAL:HG23	2.21	0.41
1:A:146:ARG:HG3	4:A:850:HOH:O	2.20	0.41
1:A:135:GLN:O	1:A:138:GLU:HB3	2.20	0.41
1:A:4:PHE:HB3	1:A:8:LYS:NZ	2.36	0.41
1:A:143:VAL:O	1:A:143:VAL:HG13	2.21	0.41
1:A:275:HIS:O	1:A:276:ALA:C	2.60	0.41
1:A:156:PRO:HG3	1:A:191:PHE:HD2	1.86	0.40
1:A:98:ARG:HA	1:A:148:ILE:O	2.21	0.40
1:A:170:ARG:HB3	1:A:170:ARG:HH11	1.85	0.40
1:A:6:LYS:HB2	1:A:348:TYR:HE2	1.86	0.40
1:A:255:HIS:ND1	1:A:286:ASN:OD1	2.54	0.40
1:A:8:LYS:HB2	1:A:92:VAL:HG22	2.02	0.40
1:A:213:GLY:O	1:A:214:GLU:C	2.60	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	347/356 (98%)	238 (69%)	78 (22%)	31 (9%)	1 1

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	16	ASP
1	A	33	ILE

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Mol	Chain	Res	Type
1	A	62	PHE
1	A	106	ASN
1	A	129	LEU
1	A	207	HIS
1	A	235	HIS
1	A	313	GLY
1	A	330	SER
1	A	335	ASP
1	A	347	ALA
1	A	24	ILE
1	A	72	CYS
1	A	112	ILE
1	A	114	TRP
1	A	243	THR
1	A	68	ALA
1	A	286	ASN
1	A	343	LEU
1	A	81	TYR
1	A	194	HIS
1	A	260	PRO
1	A	26	TYR
1	A	91	GLY
1	A	119	GLY
1	A	165	LEU
1	A	214	GLU
1	A	130	VAL
1	A	66	MET
1	A	294	PRO

5.3.2 Protein sidechains ⓘ

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	304/309 (98%)	227 (75%)	77 (25%)	1 1

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	5	ASP
1	A	6	LYS
1	A	9	VAL
1	A	10	GLU
1	A	15	LEU
1	A	16	ASP
1	A	25	LEU
1	A	29	LYS
1	A	53	LEU
1	A	59	LEU
1	A	63	ASP
1	A	72	CYS
1	A	78	ARG
1	A	79	ILE
1	A	81	TYR
1	A	85	GLU
1	A	86	MET
1	A	97	VAL
1	A	106	ASN
1	A	110	GLU
1	A	112	ILE
1	A	116	GLN
1	A	122	THR
1	A	123	PRO
1	A	128	SER
1	A	129	LEU
1	A	131	ASN
1	A	132	GLN
1	A	136	GLU
1	A	139	ARG
1	A	145	VAL
1	A	149	LEU
1	A	150	CYS
1	A	157	SER
1	A	160	SER
1	A	164	GLU
1	A	168	LYS
1	A	170	ARG
1	A	171	GLU
1	A	172	GLN
1	A	173	THR
1	A	179	LEU

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Mol	Chain	Res	Type
1	A	190	LEU
1	A	195	VAL
1	A	200	GLU
1	A	208	ARG
1	A	220	VAL
1	A	232	ARG
1	A	233	LEU
1	A	240	LEU
1	A	243	THR
1	A	247	ASN
1	A	249	LEU
1	A	254	MET
1	A	264	TYR
1	A	270	LYS
1	A	273	THR
1	A	284	GLN
1	A	286	ASN
1	A	287	TYR
1	A	290	ASN
1	A	296	ILE
1	A	304	ASP
1	A	311	ASP
1	A	317	GLU
1	A	321	ARG
1	A	322	LEU
1	A	329	SER
1	A	339	GLU
1	A	340	LEU
1	A	341	LEU
1	A	342	ASP
1	A	343	LEU
1	A	344	LEU
1	A	346	LYS
1	A	349	ARG

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	154	HIS
1	A	194	HIS
1	A	207	HIS
1	A	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PRH	A	401	2	13,21,21	1.86	4 (30%)	13,31,31	2.69	6 (46%)

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	PRH	A	401	2	-	0/2/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PRH	O4'-C4'	-2.72	1.38	1.45
3	A	401	PRH	O5'-C5'	2.15	1.51	1.42
3	A	401	PRH	O2'-C2'	2.84	1.49	1.43
3	A	401	PRH	C2-N1	4.02	1.42	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	PRH	O2'-C2'-C3'	-3.77	99.56	111.83
3	A	401	PRH	O4'-C4'-C3'	-3.54	98.02	105.15
3	A	401	PRH	O3'-C3'-C4'	-2.80	102.65	111.05
3	A	401	PRH	O6-C6-C5	-2.67	106.27	111.63
3	A	401	PRH	O3'-C3'-C2'	2.21	119.00	111.83
3	A	401	PRH	C2'-C1'-N9	5.94	124.71	114.17

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
3	A	401	PRH	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/356 (98%)	-0.53	0 100 100	13, 23, 32, 42	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PRH	A	401	19/19	0.94	0.11	-0.06	19,23,27,27	0
2	ZN	A	501	1/1	0.99	0.02	-3.49	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.