Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1NDW
Title	:	Crystal Structure of Adenosine Deaminase Complexed with FR221647
Authors	:	Kinoshita, T.
Deposited on	:	2002-12-09
Resolution	:	2.00 Å(reported)

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

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

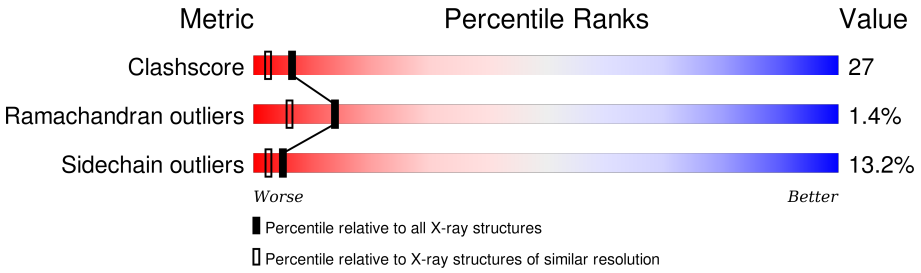
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	356	38% 39% 15% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3288 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
1	A	349	Total	C	N	O	S	0	0	0
			2788	1772	471	533	12			

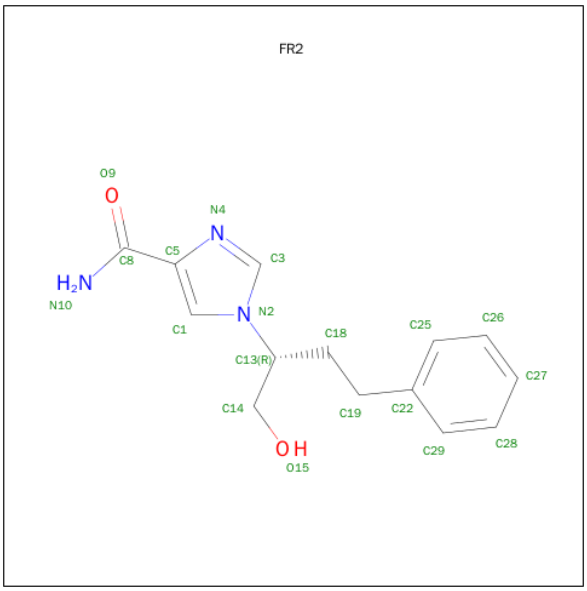
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	ASN	SEE REMARK 999	UNP P56658
A	32	LYS	ARG	SEE REMARK 999	UNP P56658
A	33	ARG	LYS	SEE REMARK 999	UNP P56658
A	57	THR	SER	SEE REMARK 999	UNP P56658
A	60	ASP	GLU	SEE REMARK 999	UNP P56658
A	77	ASP	GLU	SEE REMARK 999	UNP P56658
A	79	ILE	VAL	SEE REMARK 999	UNP P56658
A	199	GLN	LYS	SEE REMARK 999	UNP P56658
A	246	THR	ALA	SEE REMARK 999	UNP P56658
A	261	ILE	VAL	SEE REMARK 999	UNP P56658
A	279	ALA	PRO	SEE REMARK 999	UNP P56658
A	281	ILE	VAL	SEE REMARK 999	UNP P56658
A	313	LYS	ASN	SEE REMARK 999	UNP P56658
A	314	ASP	GLU	SEE REMARK 999	UNP P56658
A	352	ARG	GLY	SEE REMARK 999	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 1-((1R)-1-(HYDROXYMETHYL)-3-PHENYLPROPYL)-1H-IMIDAZOLE-4-CARBOXAMIDE (three-letter code: FR2) (formula: $C_{14}H_{17}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	480	Total	O	0	0
			480	480		

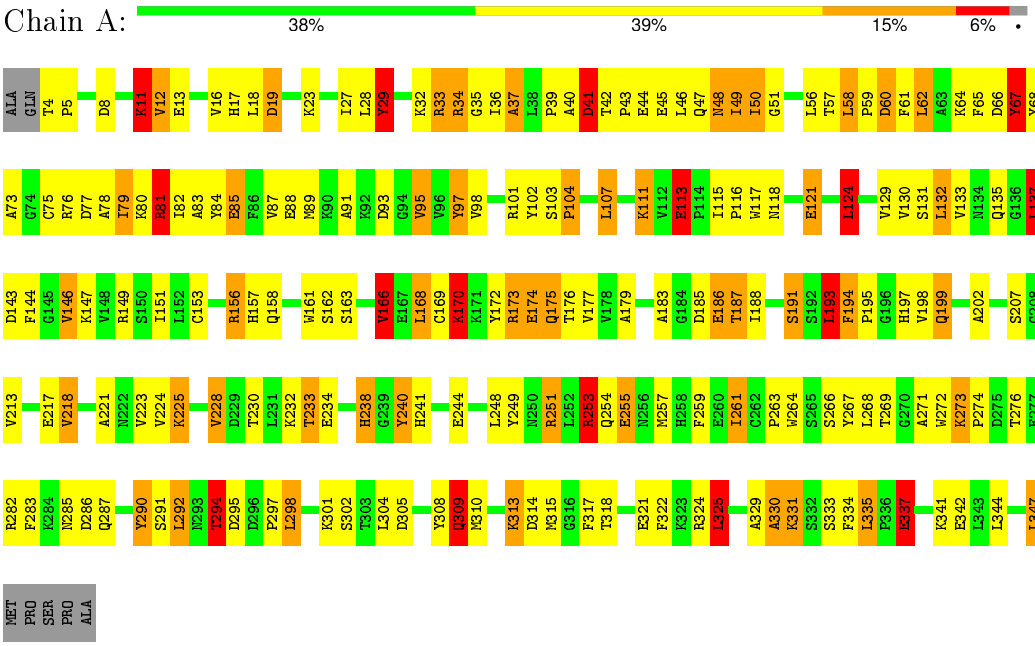
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: Adenosine Deaminase

Chain A:



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 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.63Å 77.63Å 135.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.206 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3288	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FR2, ZN

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	1.76	34/2852 (1.2%)	2.38	152/3866 (3.9%)

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	2	13

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ARG	CZ-NH2	-8.52	1.22	1.33
1	A	211	ARG	CD-NE	-8.13	1.32	1.46
1	A	103	SER	CA-CB	7.78	1.64	1.52
1	A	324	ARG	NE-CZ	7.45	1.42	1.33
1	A	198	VAL	CB-CG2	7.30	1.68	1.52
1	A	183	ALA	CA-CB	7.26	1.67	1.52
1	A	213	VAL	CA-CB	7.10	1.69	1.54
1	A	330	ALA	CA-CB	7.01	1.67	1.52
1	A	191	SER	CA-CB	7.01	1.63	1.52
1	A	240	TYR	CE2-CZ	6.98	1.47	1.38
1	A	139	GLU	CG-CD	6.86	1.62	1.51
1	A	173	ARG	NE-CZ	6.79	1.41	1.33
1	A	337	GLU	CG-CD	6.36	1.61	1.51
1	A	202	ALA	CA-CB	6.10	1.65	1.52
1	A	81	ARG	NE-CZ	6.10	1.41	1.33
1	A	210	HIS	CG-CD2	6.10	1.46	1.35
1	A	333	SER	CB-OG	6.09	1.50	1.42
1	A	342	GLU	CD-OE1	-5.88	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	SER	CA-CB	5.88	1.61	1.52
1	A	139	GLU	CB-CG	5.77	1.63	1.52
1	A	103	SER	CB-OG	5.57	1.49	1.42
1	A	195	PRO	N-CD	-5.56	1.40	1.47
1	A	17	HIS	CA-CB	5.41	1.65	1.53
1	A	186	GLU	CG-CD	5.40	1.60	1.51
1	A	97	TYR	CB-CG	5.33	1.59	1.51
1	A	104	PRO	N-CA	-5.29	1.38	1.47
1	A	334	PHE	CE1-CZ	5.24	1.47	1.37
1	A	249	TYR	CG-CD2	5.24	1.46	1.39
1	A	102	TYR	CG-CD2	5.22	1.46	1.39
1	A	271	ALA	CA-CB	5.13	1.63	1.52
1	A	131	SER	CB-OG	-5.06	1.35	1.42
1	A	334	PHE	CG-CD1	5.06	1.46	1.38
1	A	213	VAL	CB-CG1	5.05	1.63	1.52
1	A	228	VAL	CB-CG2	5.04	1.63	1.52

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	ARG	NE-CZ-NH1	37.03	138.81	120.30
1	A	146	VAL	CA-CB-CG2	-24.09	74.76	110.90
1	A	149	ARG	CD-NE-CZ	16.24	146.34	123.60
1	A	209	VAL	CA-CB-CG2	14.61	132.81	110.90
1	A	211	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	A	325	LEU	CB-CG-CD2	12.20	131.74	111.00
1	A	149	ARG	NH1-CZ-NH2	-12.12	106.06	119.40
1	A	146	VAL	CG1-CB-CG2	-12.10	91.53	110.90
1	A	149	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	A	81	ARG	NE-CZ-NH2	11.29	125.95	120.30
1	A	251	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	A	89	MET	CA-CB-CG	10.35	130.89	113.30
1	A	254	GLN	CA-CB-CG	-10.27	90.81	113.40
1	A	37	ALA	N-CA-CB	10.00	124.10	110.10
1	A	325	LEU	CA-CB-CG	9.59	137.36	115.30
1	A	170	LYS	CD-CE-NZ	-9.46	89.93	111.70
1	A	221	ALA	CB-CA-C	-9.34	96.09	110.10
1	A	76	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	A	67	TYR	CB-CG-CD1	-8.39	115.96	121.00
1	A	211	ARG	CB-CG-CD	-8.38	89.82	111.60
1	A	166	VAL	CG1-CB-CG2	8.23	124.07	110.90
1	A	185	ASP	CB-CG-OD2	8.12	125.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	TYR	CB-CG-CD1	-8.00	116.20	121.00
1	A	253	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	324	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	A	240	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	A	269	THR	CA-CB-CG2	7.45	122.83	112.40
1	A	177	VAL	CG1-CB-CG2	7.44	122.80	110.90
1	A	308	TYR	CG-CD2-CE2	-7.44	115.35	121.30
1	A	111	LYS	CA-CB-CG	7.41	129.71	113.40
1	A	233	THR	CA-CB-OG1	7.34	124.41	109.00
1	A	351	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	A	139	GLU	CB-CA-C	7.23	124.86	110.40
1	A	161	TRP	CH2-CZ2-CE2	7.22	124.62	117.40
1	A	156	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	347	LEU	CB-CG-CD1	7.16	123.17	111.00
1	A	97	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	A	107	LEU	CB-CG-CD1	7.05	122.99	111.00
1	A	251	ARG	CD-NE-CZ	-7.04	113.74	123.60
1	A	228	VAL	CA-CB-CG2	-6.98	100.43	110.90
1	A	309	GLN	CA-CB-CG	6.97	128.73	113.40
1	A	77	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	37	ALA	CB-CA-C	-6.82	99.87	110.10
1	A	81	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	218	VAL	CA-CB-CG1	6.67	120.90	110.90
1	A	286	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	223	VAL	CA-CB-CG1	6.65	120.88	110.90
1	A	29	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	16	VAL	CG1-CB-CG2	6.58	121.42	110.90
1	A	233	THR	N-CA-CB	6.52	122.68	110.30
1	A	308	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	A	308	TYR	CD1-CG-CD2	6.49	125.04	117.90
1	A	34	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	58	LEU	CD1-CG-CD2	-6.46	91.13	110.50
1	A	233	THR	CB-CA-C	-6.43	94.24	111.60
1	A	158	GLN	CA-CB-CG	6.40	127.48	113.40
1	A	198	VAL	CG1-CB-CG2	-6.40	100.66	110.90
1	A	218	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	A	131	SER	N-CA-CB	6.30	119.94	110.50
1	A	98	VAL	CG1-CB-CG2	-6.29	100.83	110.90
1	A	269	THR	C-N-CA	-6.27	109.13	122.30
1	A	193	LEU	CB-CG-CD2	6.23	121.60	111.00
1	A	84	TYR	CZ-CE2-CD2	-6.22	114.20	119.80
1	A	129	VAL	CG1-CB-CG2	6.21	120.83	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MET	CG-SD-CE	6.19	110.11	100.20
1	A	142	ARG	CB-CG-CD	6.19	127.69	111.60
1	A	309	GLN	CB-CG-CD	6.19	127.69	111.60
1	A	158	GLN	CB-CA-C	-6.18	98.04	110.40
1	A	335	LEU	CB-CA-C	-6.12	98.58	110.20
1	A	249	TYR	CZ-CE2-CD2	-6.09	114.32	119.80
1	A	209	VAL	CA-CB-CG1	6.06	119.99	110.90
1	A	348	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	317	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	294	THR	CA-CB-CG2	6.04	120.85	112.40
1	A	225	LYS	CB-CA-C	-6.00	98.41	110.40
1	A	67	TYR	CG-CD1-CE1	-5.91	116.57	121.30
1	A	253	ARG	CG-CD-NE	5.89	124.16	111.80
1	A	113	GLU	CA-CB-CG	5.84	126.25	113.40
1	A	281	ILE	CA-CB-CG1	5.84	122.10	111.00
1	A	175	GLN	C-N-CA	5.83	136.28	121.70
1	A	304	LEU	N-CA-C	5.83	126.73	111.00
1	A	254	GLN	CB-CG-CD	-5.82	96.47	111.60
1	A	84	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	A	335	LEU	CB-CG-CD1	5.78	120.82	111.00
1	A	325	LEU	CB-CA-C	5.77	121.17	110.20
1	A	211	ARG	NH1-CZ-NH2	5.77	125.75	119.40
1	A	324	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	224	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	A	187	THR	OG1-CB-CG2	-5.73	96.83	110.00
1	A	33	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	223	VAL	CG1-CB-CG2	5.69	120.01	110.90
1	A	113	GLU	N-CA-CB	-5.69	100.36	110.60
1	A	132	LEU	CB-CG-CD2	5.68	120.66	111.00
1	A	143	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	41	ASP	N-CA-C	5.65	126.26	111.00
1	A	12	VAL	CA-CB-CG1	5.62	119.33	110.90
1	A	130	VAL	CA-CB-CG2	-5.61	102.48	110.90
1	A	124	LEU	CB-CG-CD2	5.60	120.52	111.00
1	A	137	LEU	CB-CG-CD1	5.58	120.49	111.00
1	A	19	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	89	MET	CB-CA-C	5.54	121.47	110.40
1	A	194	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	193	LEU	CB-CG-CD1	5.53	120.39	111.00
1	A	56	LEU	C-N-CA	-5.51	107.91	121.70
1	A	35	GLY	C-N-CA	-5.46	108.05	121.70
1	A	95	VAL	CA-CB-CG1	5.46	119.09	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	LEU	N-CA-CB	5.44	121.28	110.40
1	A	290	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	308	TYR	CD1-CE1-CZ	-5.37	114.97	119.80
1	A	176	THR	N-CA-CB	-5.36	100.12	110.30
1	A	168	LEU	CB-CG-CD1	5.35	120.09	111.00
1	A	157	HIS	CA-CB-CG	-5.33	104.53	113.60
1	A	177	VAL	CA-CB-CG1	5.33	118.89	110.90
1	A	121	GLU	C-N-CA	-5.28	111.22	122.30
1	A	294	THR	OG1-CB-CG2	5.27	122.12	110.00
1	A	62	LEU	CB-CG-CD2	5.26	119.95	111.00
1	A	87	VAL	CA-CB-CG2	5.26	118.80	110.90
1	A	286	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	217	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	308	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	351	TYR	C-N-CA	-5.22	108.65	121.70
1	A	139	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	A	173	ARG	C-N-CA	5.21	134.74	121.70
1	A	48	ASN	N-CA-CB	5.20	119.97	110.60
1	A	281	ILE	CA-CB-CG2	5.20	121.30	110.90
1	A	166	VAL	CA-CB-CG2	5.19	118.69	110.90
1	A	11	LYS	CD-CE-NZ	5.19	123.64	111.70
1	A	60	ASP	CA-CB-CG	5.18	124.79	113.40
1	A	298	LEU	CD1-CG-CD2	-5.18	94.97	110.50
1	A	79	ILE	CA-CB-CG1	-5.15	101.21	111.00
1	A	101	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	89	MET	N-CA-CB	-5.15	101.33	110.60
1	A	290	TYR	CD1-CG-CD2	5.15	123.56	117.90
1	A	156	ARG	CA-CB-CG	-5.14	102.09	113.40
1	A	282	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	60	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	51	GLY	N-CA-C	5.12	125.91	113.10
1	A	161	TRP	CZ3-CH2-CZ2	-5.11	115.47	121.60
1	A	146	VAL	CA-CB-CG1	5.09	118.54	110.90
1	A	37	ALA	CA-C-N	-5.07	106.04	117.20
1	A	76	ARG	N-CA-C	5.07	124.68	111.00
1	A	77	ASP	CA-CB-CG	5.06	124.54	113.40
1	A	352	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	16	VAL	CA-CB-CG2	-5.06	103.32	110.90
1	A	331	LYS	CB-CG-CD	-5.05	98.46	111.60
1	A	56	LEU	CB-CA-C	-5.05	100.60	110.20
1	A	8	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	253	ARG	CB-CG-CD	5.02	124.66	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	285	ASN	CB-CA-C	-5.02	100.37	110.40
1	A	172	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	12	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	49	ILE	CA-CB-CG2	5.01	120.91	110.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	THR	CB
1	A	294	THR	CB

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	153	CYS	Peptide
1	A	173	ARG	Sidechain,Peptide
1	A	194	PHE	Sidechain
1	A	211	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	29	TYR	Sidechain
1	A	351	TYR	Sidechain
1	A	352	ARG	Sidechain
1	A	61	PHE	Sidechain
1	A	67	TYR	Sidechain
1	A	81	ARG	Sidechain

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	2788	0	2742	152	0
2	A	1	0	0	0	0
3	A	19	0	17	2	0
4	A	480	0	0	62	0
All	All	3288	0	2759	152	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 27.

All (152) 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:12:VAL:HB	4:A:1133:HOH:O	1.64	0.97
1:A:57:THR:HB	1:A:59:PRO:HD2	1.47	0.97
1:A:278:HIS:HD2	1:A:280:VAL:H	1.18	0.91
1:A:187:THR:HG22	4:A:1355:HOH:O	1.77	0.83
1:A:325:LEU:HG	4:A:1356:HOH:O	1.81	0.78
1:A:115:ILE:HB	4:A:1293:HOH:O	1.83	0.78
1:A:263:PRO:HD3	4:A:1371:HOH:O	1.82	0.77
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.66	0.77
1:A:322:PHE:HA	1:A:325:LEU:HD22	1.65	0.77
1:A:218:VAL:HB	4:A:1329:HOH:O	1.84	0.76
1:A:68:TYR:HD1	4:A:1340:HOH:O	1.68	0.76
1:A:72:ILE:HG22	1:A:78:ALA:HB1	1.69	0.73
1:A:264:TRP:HA	4:A:1394:HOH:O	1.88	0.73
1:A:264:TRP:HE3	4:A:1394:HOH:O	1.72	0.73
1:A:337:GLU:HG3	1:A:341:LYS:HE3	1.70	0.72
1:A:292:LEU:HA	4:A:1371:HOH:O	1.89	0.71
1:A:27:ILE:HD13	1:A:68:TYR:HB2	1.71	0.71
1:A:11:LYS:HE3	4:A:1441:HOH:O	1.91	0.71
1:A:310:MET:SD	4:A:1394:HOH:O	2.48	0.70
1:A:267:TYR:HB2	1:A:272:TRP:HE3	1.55	0.70
1:A:50:ILE:HG21	1:A:68:TYR:HD2	1.57	0.69
1:A:298:LEU:HD12	4:A:1085:HOH:O	1.93	0.69
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.27	0.68
1:A:278:HIS:CD2	1:A:280:VAL:H	2.08	0.68
1:A:267:TYR:HB2	1:A:272:TRP:CE3	2.29	0.67
1:A:138:GLN:O	1:A:142:ARG:HG2	1.95	0.66
1:A:72:ILE:HD13	4:A:1326:HOH:O	1.95	0.65
1:A:266:SER:OG	1:A:278:HIS:HE1	1.78	0.65
1:A:115:ILE:HG21	4:A:1260:HOH:O	1.96	0.65
1:A:325:LEU:HD23	4:A:1356:HOH:O	1.98	0.63
1:A:73:ALA:HB2	4:A:1393:HOH:O	1.98	0.63
1:A:169:CYS:SG	4:A:1342:HOH:O	2.56	0.62
1:A:58:LEU:HD23	1:A:58:LEU:C	2.21	0.61
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.82	0.61
1:A:23:LYS:HD2	1:A:85:GLU:CG	2.30	0.61
1:A:23:LYS:HG3	4:A:1363:HOH:O	2.01	0.60
1:A:66:ASP:HA	4:A:1183:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:HB2	1:A:117:TRP:CD1	2.36	0.60
1:A:107:LEU:HD13	4:A:1393:HOH:O	2.01	0.60
1:A:264:TRP:CE3	4:A:1394:HOH:O	2.52	0.60
1:A:241:HIS:HD2	1:A:244:GLU:OE2	1.83	0.60
1:A:121:GLU:HA	4:A:1260:HOH:O	2.02	0.59
1:A:337:GLU:HG3	1:A:341:LYS:CE	2.31	0.59
1:A:132:LEU:HD22	4:A:1325:HOH:O	2.02	0.59
1:A:309:GLN:HE21	1:A:313:LYS:HD3	1.67	0.59
1:A:287:GLN:HG2	4:A:1330:HOH:O	2.02	0.58
1:A:79:ILE:HD12	1:A:124:LEU:HD11	1.85	0.58
1:A:337:GLU:O	1:A:341:LYS:HG2	2.04	0.58
1:A:322:PHE:HA	1:A:325:LEU:CD2	2.34	0.57
1:A:276:THR:HB	4:A:1234:HOH:O	2.02	0.57
1:A:47:GLN:OE1	1:A:301:LYS:HG2	2.05	0.57
1:A:211:ARG:NH2	1:A:232:LYS:O	2.37	0.57
1:A:273:LYS:HG2	4:A:1156:HOH:O	2.04	0.56
1:A:118:ASN:HB3	4:A:1190:HOH:O	2.05	0.56
1:A:50:ILE:HG21	1:A:68:TYR:CD2	2.40	0.56
1:A:347:LEU:HG	4:A:1018:HOH:O	2.05	0.56
1:A:331:LYS:HG3	1:A:344:LEU:HD21	1.87	0.56
1:A:72:ILE:HG22	1:A:78:ALA:CB	2.36	0.56
1:A:13:GLU:OE1	1:A:294:THR:HB	2.05	0.55
1:A:248:LEU:HD12	4:A:1207:HOH:O	2.06	0.55
1:A:166:VAL:O	1:A:170:LYS:HG3	2.06	0.55
1:A:264:TRP:HZ2	4:A:1092:HOH:O	1.88	0.55
1:A:318:THR:HB	4:A:1449:HOH:O	2.08	0.54
1:A:209:VAL:HG13	4:A:1342:HOH:O	2.07	0.54
1:A:72:ILE:HG23	4:A:1326:HOH:O	2.07	0.54
1:A:11:LYS:HD3	4:A:1178:HOH:O	2.06	0.54
1:A:107:LEU:HG	4:A:1341:HOH:O	2.08	0.54
1:A:162:SER:OG	1:A:197:HIS:HD2	1.90	0.54
1:A:72:ILE:CG2	1:A:78:ALA:HB1	2.38	0.53
1:A:62:LEU:HD13	4:A:1401:HOH:O	2.08	0.53
1:A:188:ILE:HB	1:A:191:SER:HB3	1.90	0.53
1:A:147:LYS:HE3	4:A:1217:HOH:O	2.09	0.53
1:A:179:ALA:C	4:A:1342:HOH:O	2.47	0.53
1:A:142:ARG:HB3	4:A:1016:HOH:O	2.07	0.53
1:A:261:ILE:HD11	1:A:283:PHE:CE2	2.44	0.52
1:A:18:LEU:HG	4:A:1203:HOH:O	2.09	0.52
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.92	0.51
1:A:80:LYS:HE3	1:A:135:GLN:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HD3	4:A:1183:HOH:O	2.10	0.51
1:A:5:PRO:HD3	4:A:1479:HOH:O	2.10	0.51
1:A:34:ARG:NH1	1:A:75:CYS:HB2	2.26	0.50
1:A:175:GLN:HB2	4:A:1024:HOH:O	2.10	0.50
1:A:104:PRO:HD2	4:A:1164:HOH:O	2.11	0.50
1:A:322:PHE:O	1:A:325:LEU:HD22	2.12	0.50
1:A:281:ILE:C	1:A:281:ILE:HD12	2.32	0.50
1:A:78:ALA:O	1:A:82:ILE:HG23	2.11	0.49
1:A:29:TYR:OH	1:A:33:ARG:NH1	2.47	0.48
1:A:348:TYR:HB3	1:A:352:ARG:NH2	2.28	0.48
1:A:199:GLN:HG2	4:A:1230:HOH:O	2.11	0.48
1:A:33:ARG:HG3	4:A:1424:HOH:O	2.13	0.48
1:A:210:HIS:HD2	1:A:234:GLU:OE2	1.96	0.48
1:A:81:ARG:O	1:A:85:GLU:HB2	2.13	0.48
1:A:273:LYS:H	1:A:273:LYS:HD3	1.78	0.48
1:A:11:LYS:HE2	1:A:93:ASP:O	2.14	0.47
1:A:156:ARG:HD2	1:A:186:GLU:HA	1.96	0.47
1:A:290:TYR:CE2	1:A:325:LEU:HD12	2.49	0.47
1:A:261:ILE:HD11	1:A:283:PHE:HE2	1.79	0.47
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.96	0.47
1:A:321:GLU:HG3	1:A:325:LEU:HD13	1.97	0.47
1:A:65:PHE:CD1	3:A:1001:FR2:H25	2.50	0.46
1:A:193:LEU:HD12	1:A:230:THR:HG21	1.97	0.46
1:A:156:ARG:O	1:A:197:HIS:HE1	1.98	0.46
1:A:12:VAL:CG2	1:A:329:ALA:HB3	2.46	0.45
1:A:91:ALA:HB2	4:A:1122:HOH:O	2.15	0.45
1:A:133:VAL:HG12	1:A:137:LEU:HD22	1.97	0.45
1:A:322:PHE:CA	1:A:325:LEU:HD22	2.43	0.45
1:A:255:GLU:H	1:A:255:GLU:HG2	1.59	0.45
1:A:170:LYS:HD2	1:A:207:SER:CB	2.47	0.45
1:A:19:ASP:HA	4:A:1203:HOH:O	2.17	0.45
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.75	0.45
1:A:113:GLU:HG2	4:A:1104:HOH:O	2.16	0.45
1:A:34:ARG:CZ	1:A:75:CYS:HB2	2.48	0.44
1:A:42:THR:O	1:A:43:PRO:C	2.55	0.44
1:A:313:LYS:HA	1:A:313:LYS:NZ	2.32	0.44
1:A:259:PHE:HB3	1:A:261:ILE:CD1	2.48	0.44
1:A:4:THR:HB	4:A:1480:HOH:O	2.17	0.44
1:A:49:ILE:HG21	1:A:49:ILE:HD13	1.71	0.44
1:A:97:TYR:HA	1:A:147:LYS:O	2.18	0.43
1:A:57:THR:HG23	4:A:1298:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TYR:CD2	1:A:274:PRO:HG3	2.53	0.43
1:A:305:ASP:O	1:A:309:GLN:HB2	2.17	0.43
1:A:253:ARG:HG2	4:A:1213:HOH:O	2.18	0.43
1:A:88:GLU:HG3	1:A:144:PHE:CE2	2.54	0.43
1:A:23:LYS:HD2	1:A:85:GLU:HG2	1.99	0.43
1:A:40:ALA:HB2	1:A:49:ILE:HD12	2.01	0.43
1:A:23:LYS:HD2	1:A:85:GLU:HG3	2.01	0.43
1:A:46:LEU:O	1:A:47:GLN:C	2.56	0.43
1:A:72:ILE:HD13	1:A:72:ILE:HG23	1.70	0.42
1:A:151:ILE:HG13	4:A:1400:HOH:O	2.19	0.42
1:A:218:VAL:CB	4:A:1329:HOH:O	2.56	0.42
1:A:45:GLU:HG3	4:A:1432:HOH:O	2.19	0.42
1:A:50:ILE:HG22	1:A:64:LYS:HG2	2.01	0.42
1:A:281:ILE:HD12	1:A:281:ILE:O	2.19	0.42
1:A:211:ARG:NH2	1:A:211:ARG:HB2	2.34	0.42
1:A:162:SER:OG	1:A:197:HIS:CD2	2.72	0.42
1:A:330:ALA:HB2	4:A:1018:HOH:O	2.20	0.42
1:A:62:LEU:HD22	3:A:1001:FR2:C26	2.50	0.42
1:A:40:ALA:O	1:A:41:ASP:OD1	2.38	0.42
1:A:209:VAL:CG1	4:A:1342:HOH:O	2.66	0.42
1:A:261:ILE:HB	1:A:291:SER:O	2.20	0.42
1:A:253:ARG:HH11	1:A:253:ARG:CG	2.33	0.41
1:A:238:HIS:HB3	1:A:240:TYR:CE2	2.55	0.41
1:A:39:PRO:HA	4:A:1051:HOH:O	2.19	0.41
1:A:309:GLN:NE2	1:A:313:LYS:HD3	2.35	0.41
1:A:228:VAL:HG22	4:A:1151:HOH:O	2.19	0.41
1:A:40:ALA:HB1	1:A:45:GLU:HB3	2.01	0.41
1:A:12:VAL:HG21	1:A:329:ALA:HB3	2.02	0.41
1:A:67:TYR:HD2	4:A:1292:HOH:O	2.02	0.41
1:A:267:TYR:HD2	1:A:274:PRO:HG3	1.85	0.41
1:A:95:VAL:O	1:A:146:VAL:HG21	2.20	0.41
1:A:322:PHE:HD2	1:A:325:LEU:HD21	1.86	0.40
1:A:276:THR:HG23	4:A:1232:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	323 (93%)	19 (6%)	5 (1%)	14 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	174	GLU
1	A	315	MET
1	A	238	HIS
1	A	295	ASP

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%)	264 (87%)	40 (13%)	5 2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	28	LEU
1	A	32	LYS
1	A	36	ILE
1	A	41	ASP
1	A	44	GLU

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Mol	Chain	Res	Type
1	A	48	ASN
1	A	50	ILE
1	A	60	ASP
1	A	72	ILE
1	A	85	GLU
1	A	111	LYS
1	A	113	GLU
1	A	124	LEU
1	A	137	LEU
1	A	142	ARG
1	A	163	SER
1	A	166	VAL
1	A	168	LEU
1	A	170	LYS
1	A	174	GLU
1	A	193	LEU
1	A	199	GLN
1	A	211	ARG
1	A	225	LYS
1	A	233	THR
1	A	253	ARG
1	A	255	GLU
1	A	261	ILE
1	A	273	LYS
1	A	281	ILE
1	A	292	LEU
1	A	294	THR
1	A	309	GLN
1	A	313	LYS
1	A	314	ASP
1	A	325	LEU
1	A	335	LEU
1	A	337	GLU
1	A	352	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	138	GLN
1	A	197	HIS
1	A	210	HIS

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Mol	Chain	Res	Type
1	A	241	HIS
1	A	250	ASN
1	A	278	HIS
1	A	287	GLN
1	A	309	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	FR2	A	1001	-	17,20,20	1.75	4 (23%)	16,26,26	1.60	5 (31%)

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	FR2	A	1001	-	-	0/7/15/15	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR2	C3-N4	-3.37	1.28	1.35
3	A	1001	FR2	C5-C8	-2.61	1.46	1.51
3	A	1001	FR2	C5-N4	2.19	1.44	1.37
3	A	1001	FR2	C1-N2	4.65	1.44	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	FR2	O15-C14-C13	-3.12	98.82	113.27
3	A	1001	FR2	O9-C8-N10	-2.65	118.86	122.59
3	A	1001	FR2	C27-C28-C29	-2.18	116.99	120.19
3	A	1001	FR2	O9-C8-C5	2.60	122.07	119.67
3	A	1001	FR2	C5-C8-N10	2.72	118.87	116.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR2	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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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