



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:35 AM GMT

PDB ID : 1V7A  
Title : Crystal structures of adenosine deaminase complexed with potent inhibitors  
Authors : Kinoshita, T.  
Deposited on : 2003-12-14  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

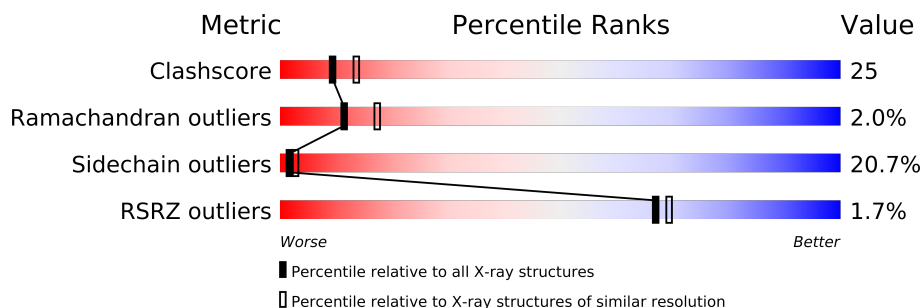
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	356	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3001 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			2789	1772	471	534	12			

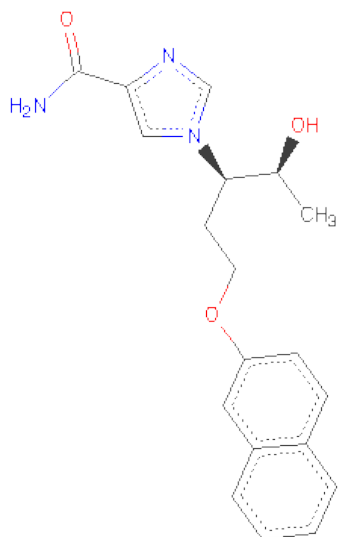
There are 15 discrepancies between the modelled and reference sequences:

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,2S)-2-HYDROXY-1-[2-(2-NAPHTHYLOXY)ETHYL]PROPYL}-1H-1 MIDAZONE-4-CARBOXAMIDE (three-letter code: FRC) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	19	3	3	0	0

- Molecule 4 is water.

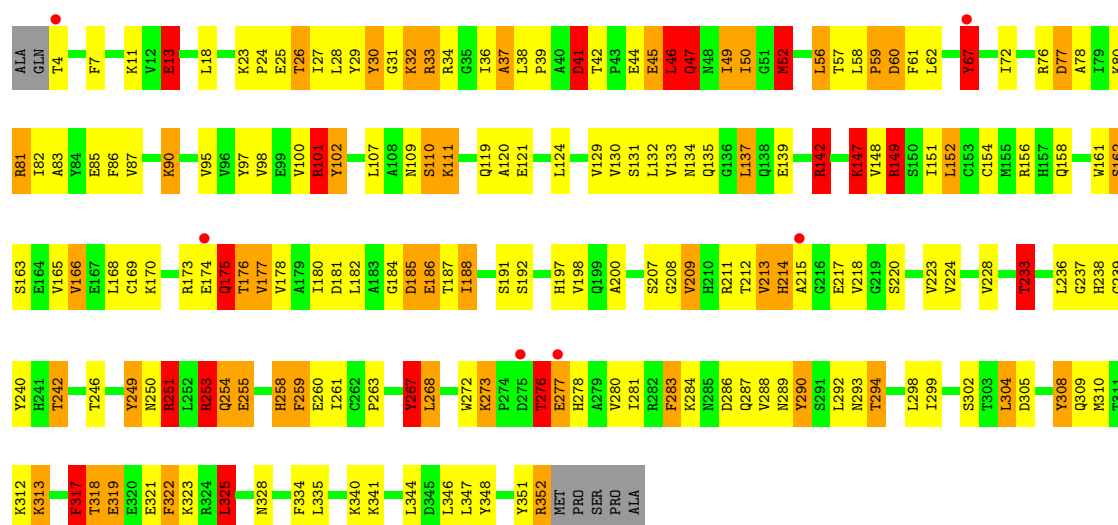
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		

### 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.52Å 77.52Å 136.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 54.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 99.5 (54.81-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15.58 (at 2.00Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.244 , 0.276 0.259 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 17.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28732 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FRC, 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	0.90	0/2853	1.89	62/3867 (1.6%)

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	15

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH1	-14.63	112.98	120.30
1	A	101	ARG	NE-CZ-NH2	13.77	127.18	120.30
1	A	317	PHE	CB-CG-CD2	-12.92	111.75	120.80
1	A	81	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	A	102	TYR	CB-CG-CD1	-9.05	115.57	121.00
1	A	352	ARG	CD-NE-CZ	-8.81	111.26	123.60
1	A	166	VAL	CA-CB-CG1	8.81	124.11	110.90
1	A	30	TYR	CB-CG-CD2	-8.79	115.73	121.00
1	A	33	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	A	253	ARG	NE-CZ-NH2	8.34	124.47	120.30
1	A	317	PHE	CB-CG-CD1	8.20	126.54	120.80
1	A	251	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	249	TYR	CB-CG-CD1	-7.81	116.32	121.00
1	A	33	ARG	CA-CB-CG	-7.69	96.48	113.40
1	A	267	TYR	CB-CG-CD1	-7.49	116.51	121.00
1	A	283	PHE	CB-CG-CD2	-7.33	115.67	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	TYR	CD1-CG-CD2	6.87	125.46	117.90
1	A	142	ARG	CD-NE-CZ	6.81	133.14	123.60
1	A	32	LYS	CA-CB-CG	6.69	128.12	113.40
1	A	147	LYS	CB-CA-C	6.64	123.68	110.40
1	A	325	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	348	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	A	208	GLY	C-N-CA	-6.45	105.57	121.70
1	A	49	ILE	C-N-CA	-6.29	105.97	121.70
1	A	30	TYR	CG-CD2-CE2	-6.26	116.29	121.30
1	A	166	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	A	317	PHE	CA-CB-CG	6.04	128.39	113.90
1	A	214	HIS	N-CA-C	6.01	127.22	111.00
1	A	156	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	240	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	175	GLN	CA-CB-CG	5.97	126.53	113.40
1	A	77	ASP	CA-CB-CG	5.94	126.47	113.40
1	A	283	PHE	CB-CG-CD1	5.86	124.90	120.80
1	A	34	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	209	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	A	276	THR	CA-CB-CG2	5.74	120.43	112.40
1	A	13	GLU	CB-CA-C	5.68	121.77	110.40
1	A	213	VAL	CG1-CB-CG2	-5.62	101.91	110.90
1	A	233	THR	CB-CA-C	-5.61	96.44	111.60
1	A	149	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	308	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	249	TYR	CD1-CG-CD2	5.53	123.98	117.90
1	A	67	TYR	CB-CG-CD1	-5.51	117.70	121.00
1	A	30	TYR	CA-CB-CG	-5.48	102.99	113.40
1	A	340	LYS	CB-CA-C	-5.40	99.59	110.40
1	A	253	ARG	CA-CB-CG	5.40	125.28	113.40
1	A	317	PHE	N-CA-CB	5.36	120.25	110.60
1	A	176	THR	C-N-CA	-5.36	108.31	121.70
1	A	95	VAL	CA-CB-CG1	5.31	118.87	110.90
1	A	120	ALA	C-N-CA	-5.31	108.43	121.70
1	A	47	GLN	CA-CB-CG	-5.29	101.75	113.40
1	A	37	ALA	N-CA-CB	5.28	117.49	110.10
1	A	351	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	46	LEU	CA-CB-CG	-5.23	103.26	115.30
1	A	41	ASP	CA-CB-CG	-5.23	101.89	113.40
1	A	249	TYR	CG-CD2-CE2	-5.21	117.14	121.30
1	A	147	LYS	N-CA-CB	-5.20	101.24	110.60
1	A	56	LEU	CB-CA-C	-5.20	100.33	110.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	TYR	CB-CA-C	-5.17	100.05	110.40
1	A	258	HIS	CA-CB-CG	-5.09	104.95	113.60
1	A	52	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	240	TYR	CD1-CG-CD2	5.03	123.43	117.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	110	SER	Peptide
1	A	121	GLU	Peptide
1	A	149	ARG	Sidechain
1	A	185	ASP	Peptide
1	A	211	ARG	Sidechain
1	A	249	TYR	Sidechain
1	A	251	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	30	TYR	Sidechain
1	A	317	PHE	Peptide
1	A	322	PHE	Sidechain
1	A	352	ARG	Sidechain
1	A	67	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2789	0	2743	138	0
2	A	1	0	0	0	0
3	A	25	0	21	1	0
4	A	186	0	0	28	0
All	All	3001	0	2764	138	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (138) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:SER:HA	1:A:166:VAL:HG22	1.57	0.86
1:A:80:LYS:HA	4:A:1110:HOH:O	1.78	0.81
1:A:23:LYS:HB2	1:A:26:THR:HG23	1.67	0.77
1:A:322:PHE:HA	1:A:325:LEU:HD13	1.67	0.76
1:A:220:SER:O	1:A:223:VAL:HG12	1.85	0.75
1:A:224:VAL:HG21	1:A:242:THR:HG22	1.68	0.74
1:A:139:GLU:HA	1:A:142:ARG:HD2	1.71	0.73
1:A:18:LEU:HD11	1:A:82:ILE:HG13	1.70	0.73
1:A:288:VAL:HG13	1:A:290:TYR:HD1	1.52	0.72
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.77	0.67
1:A:185:ASP:HB2	3:A:1001:FRC:H11	1.77	0.66
1:A:72:ILE:HG21	1:A:82:ILE:HD13	1.78	0.66
1:A:236:LEU:O	1:A:260:GLU:HG3	1.95	0.66
1:A:239:GLY:O	1:A:242:THR:HG23	1.96	0.65
1:A:186:GLU:OE1	1:A:223:VAL:HG11	1.98	0.64
1:A:13:GLU:HG2	1:A:98:VAL:HG23	1.80	0.64
1:A:67:TYR:HB2	4:A:1081:HOH:O	1.99	0.63
1:A:288:VAL:HB	4:A:1147:HOH:O	1.99	0.63
1:A:250:ASN:O	1:A:253:ARG:HD2	1.97	0.63
1:A:290:TYR:HB3	4:A:1096:HOH:O	1.99	0.62
1:A:72:ILE:HG23	1:A:78:ALA:HB1	1.82	0.61
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.83	0.61
1:A:39:PRO:HG3	1:A:67:TYR:CE2	2.35	0.61
1:A:317:PHE:HB2	4:A:1137:HOH:O	2.00	0.60
1:A:97:TYR:HD1	1:A:147:LYS:HG3	1.66	0.60
1:A:13:GLU:HG3	4:A:1089:HOH:O	2.02	0.59
1:A:180:ILE:HB	4:A:1174:HOH:O	2.02	0.59
1:A:261:ILE:HD12	1:A:290:TYR:HB2	1.84	0.59
1:A:109:ASN:HB3	1:A:119:GLN:OE1	2.03	0.59
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.85	0.58
1:A:28:LEU:HD21	1:A:46:LEU:HD13	1.86	0.58
1:A:277:GLU:HB3	4:A:1139:HOH:O	2.02	0.58
1:A:163:SER:CA	1:A:166:VAL:HG22	2.33	0.58
1:A:283:PHE:HB3	1:A:288:VAL:HG11	1.86	0.57
1:A:100:VAL:HG21	4:A:1166:HOH:O	2.04	0.57
1:A:170:LYS:HE2	4:A:1117:HOH:O	2.04	0.57
1:A:292:LEU:HA	4:A:1180:HOH:O	2.05	0.57
1:A:24:PRO:HG2	1:A:47:GLN:NE2	2.20	0.56
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:LEU:HD22	1:A:177:VAL:HG21	1.88	0.56
1:A:278:HIS:HD2	1:A:280:VAL:H	1.52	0.55
1:A:58:LEU:HD23	1:A:62:LEU:HG	1.89	0.55
1:A:161:TRP:O	1:A:165:VAL:HG23	2.07	0.55
1:A:273:LYS:O	1:A:276:THR:HB	2.07	0.54
1:A:46:LEU:HA	4:A:1068:HOH:O	2.06	0.54
1:A:31:GLY:HA2	1:A:36:ILE:HB	1.89	0.54
1:A:263:PRO:HD3	4:A:1180:HOH:O	2.09	0.53
1:A:44:GLU:H	1:A:44:GLU:CD	2.13	0.52
1:A:132:LEU:HD11	4:A:1035:HOH:O	2.08	0.52
1:A:283:PHE:O	1:A:288:VAL:HG12	2.10	0.52
1:A:289:ASN:OD1	1:A:328:ASN:HB3	2.09	0.52
1:A:29:TYR:O	1:A:33:ARG:HB2	2.10	0.52
1:A:280:VAL:HG22	1:A:317:PHE:HZ	1.74	0.52
1:A:97:TYR:HA	1:A:147:LYS:O	2.10	0.51
1:A:50:ILE:HG21	4:A:1081:HOH:O	2.09	0.51
1:A:170:LYS:HD2	1:A:207:SER:CB	2.40	0.51
1:A:28:LEU:O	1:A:32:LYS:HG2	2.11	0.51
1:A:166:VAL:HG12	4:A:1141:HOH:O	2.11	0.50
1:A:81:ARG:HD2	1:A:85:GLU:OE1	2.10	0.50
1:A:217:GLU:HB2	1:A:238:HIS:CG	2.47	0.50
1:A:86:PHE:CE2	1:A:90:LYS:HD3	2.47	0.50
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.46	0.50
1:A:263:PRO:HB2	1:A:310:MET:SD	2.52	0.50
1:A:170:LYS:HD2	1:A:207:SER:OG	2.12	0.50
1:A:318:THR:HG22	1:A:321:GLU:H	1.77	0.49
1:A:305:ASP:O	1:A:309:GLN:HG2	2.12	0.49
1:A:107:LEU:HB2	1:A:129:VAL:HG11	1.94	0.49
1:A:42:THR:HG22	1:A:45:GLU:HB2	1.94	0.49
1:A:27:ILE:HG22	4:A:1178:HOH:O	2.11	0.49
1:A:25:GLU:H	1:A:25:GLU:CD	2.16	0.49
1:A:56:LEU:HB3	1:A:60:ASP:HB3	1.93	0.49
1:A:272:TRP:HB3	4:A:1057:HOH:O	2.12	0.49
1:A:13:GLU:OE1	1:A:294:THR:HB	2.12	0.48
1:A:214:HIS:O	1:A:237:GLY:O	2.32	0.47
1:A:228:VAL:HG22	4:A:1144:HOH:O	2.15	0.47
1:A:162:SER:OG	1:A:197:HIS:HD2	1.98	0.47
1:A:134:ASN:HA	1:A:137:LEU:HD22	1.96	0.47
1:A:224:VAL:HG11	1:A:242:THR:CG2	2.44	0.47
1:A:11:LYS:HD2	1:A:304:LEU:HD13	1.97	0.47
1:A:142:ARG:NH1	1:A:142:ARG:HG3	2.30	0.47
1:A:178:VAL:HG22	4:A:1164:HOH:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:LEU:CD2	1:A:46:LEU:HD13	2.44	0.46
1:A:286:ASP:HB2	4:A:1147:HOH:O	2.15	0.46
1:A:32:LYS:HD3	1:A:41:ASP:OD2	2.15	0.46
1:A:267:TYR:CD2	1:A:267:TYR:C	2.87	0.46
1:A:261:ILE:HD11	1:A:283:PHE:CD2	2.50	0.46
1:A:322:PHE:HA	1:A:325:LEU:CD1	2.42	0.46
1:A:224:VAL:HG11	1:A:242:THR:HG22	1.98	0.46
1:A:258:HIS:HE1	4:A:1167:HOH:O	1.99	0.46
1:A:288:VAL:HG13	1:A:290:TYR:CD1	2.42	0.46
1:A:181:ASP:HA	1:A:212:THR:O	2.16	0.46
1:A:52:MET:HE1	1:A:61:PHE:CD1	2.51	0.46
1:A:57:THR:OG1	1:A:60:ASP:HB2	2.16	0.45
1:A:83:ALA:O	1:A:87:VAL:HG23	2.15	0.45
1:A:166:VAL:HB	4:A:1117:HOH:O	2.15	0.45
1:A:175:GLN:HA	1:A:176:THR:HA	1.35	0.45
1:A:52:MET:HE3	1:A:299:ILE:CG2	2.46	0.45
1:A:308:TYR:CD2	1:A:322:PHE:CE2	3.05	0.45
1:A:253:ARG:HD3	1:A:254:GLN:N	2.32	0.45
1:A:251:ARG:O	1:A:255:GLU:HG2	2.16	0.45
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.45	0.45
1:A:102:TYR:CE2	1:A:133:VAL:HG11	2.51	0.45
1:A:280:VAL:HA	1:A:283:PHE:HB2	2.00	0.44
1:A:344:LEU:HB3	4:A:1173:HOH:O	2.17	0.44
1:A:313:LYS:HA	1:A:313:LYS:NZ	2.32	0.44
1:A:261:ILE:O	1:A:293:ASN:HB2	2.17	0.44
1:A:23:LYS:HB3	1:A:23:LYS:HE2	1.87	0.44
1:A:178:VAL:CG2	1:A:334:PHE:HB2	2.48	0.44
1:A:272:TRP:NE1	1:A:278:HIS:HA	2.34	0.43
1:A:101:ARG:HB3	1:A:151:ILE:HB	2.01	0.43
1:A:304:LEU:HD22	1:A:308:TYR:CE1	2.54	0.42
1:A:162:SER:HB3	1:A:200:ALA:HB2	2.00	0.42
1:A:52:MET:HE3	1:A:299:ILE:HG23	2.01	0.42
1:A:169:CYS:O	1:A:173:ARG:HB3	2.19	0.42
1:A:26:THR:HB	1:A:81:ARG:NH2	2.34	0.42
1:A:253:ARG:HG2	4:A:1003:HOH:O	2.18	0.42
1:A:209:VAL:HG21	4:A:1174:HOH:O	2.20	0.42
1:A:182:LEU:HB3	1:A:213:VAL:HG13	2.02	0.42
1:A:188:ILE:HG12	1:A:191:SER:HB3	2.01	0.42
1:A:341:LYS:HB3	4:A:1136:HOH:O	2.19	0.42
1:A:259:PHE:CD1	1:A:259:PHE:N	2.88	0.42
1:A:278:HIS:CD2	1:A:280:VAL:H	2.36	0.42
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.83	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:GLN:HB2	1:A:47:GLN:HE21	1.44	0.41
1:A:312:LYS:HG2	1:A:313:LYS:HZ3	1.85	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.93	0.41
1:A:45:GLU:OE2	1:A:45:GLU:HA	2.21	0.41
1:A:154:CYS:SG	1:A:180:ILE:HD11	2.61	0.41
1:A:178:VAL:HG23	1:A:334:PHE:HB2	2.03	0.41
1:A:90:LYS:HE2	4:A:1063:HOH:O	2.20	0.41
1:A:7:PHE:CD1	1:A:319:GLU:HG3	2.56	0.40
1:A:287:GLN:OE1	1:A:287:GLN:HA	2.20	0.40
1:A:224:VAL:O	1:A:228:VAL:HG23	2.22	0.40
1:A:87:VAL:HG13	1:A:148:VAL:HG21	2.02	0.40
1:A:284:LYS:HE3	1:A:284:LYS:HB3	1.91	0.40
1:A:158:GLN:HG2	1:A:161:TRP:CD2	2.57	0.40
1:A:42:THR:CG2	1:A:45:GLU:HB2	2.52	0.40
1:A:173:ARG:O	1:A:175:GLN:OE1	2.39	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%)	306 (88%)	34 (10%)	7 (2%)	11 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	175	GLN
1	A	186	GLU
1	A	215	ALA
1	A	184	GLY
1	A	37	ALA
1	A	59	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%)	241 (79%)	63 (21%)	<b>2</b> <b>3</b>

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	13	GLU
1	A	26	THR
1	A	38	LEU
1	A	41	ASP
1	A	45	GLU
1	A	46	LEU
1	A	47	GLN
1	A	49	ILE
1	A	50	ILE
1	A	52	MET
1	A	59	PRO
1	A	60	ASP
1	A	76	ARG
1	A	77	ASP
1	A	90	LYS
1	A	101	ARG
1	A	110	SER
1	A	111	LYS
1	A	124	LEU
1	A	130	VAL
1	A	131	SER
1	A	137	LEU
1	A	142	ARG
1	A	147	LYS
1	A	149	ARG
1	A	152	LEU
1	A	162	SER
1	A	168	LEU
1	A	174	GLU
1	A	175	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	177	VAL
1	A	187	THR
1	A	188	ILE
1	A	192	SER
1	A	198	VAL
1	A	218	VAL
1	A	233	THR
1	A	242	THR
1	A	246	THR
1	A	253	ARG
1	A	254	GLN
1	A	255	GLU
1	A	259	PHE
1	A	267	TYR
1	A	268	LEU
1	A	273	LYS
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	294	THR
1	A	298	LEU
1	A	302	SER
1	A	304	LEU
1	A	313	LYS
1	A	317	PHE
1	A	318	THR
1	A	319	GLU
1	A	323	LYS
1	A	325	LEU
1	A	335	LEU
1	A	346	LEU
1	A	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	48	ASN
1	A	138	GLN
1	A	197	HIS
1	A	254	GLN
1	A	278	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	FRC	A	1001	-	27,27,27	1.93	5 (18%)	36,37,37	1.37	5 (13%)

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	FRC	A	1001	-	-	0/14/18/18	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FRC	C1-N2	5.92	1.46	1.37
3	A	1001	FRC	C5-N4	4.48	1.48	1.39
3	A	1001	FRC	C10-C19	2.74	1.41	1.37
3	A	1001	FRC	C13-N2	-2.71	1.44	1.49

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FRC	O15-C14	2.25	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FRC	O15-C14-C9	3.04	118.58	109.74
3	A	1001	FRC	O9-C8-C5	3.02	122.67	119.65
3	A	1001	FRC	O15-C14-C13	2.84	115.20	108.15
3	A	1001	FRC	C2-C18-C13	-2.48	109.52	113.70
3	A	1001	FRC	C5-C1-N2	-2.39	105.48	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/356 (98%)	0.12	6 (1%) 67 69	2, 7, 22, 30	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	3.8
1	A	174	GLU	2.7
1	A	67	TYR	2.7
1	A	4	THR	2.3
1	A	215	ALA	2.2
1	A	275	ASP	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FRC	A	1001	25/25	0.15	0.17	2,3,6,8	0
2	ZN	A	400	1/1	0.09	-2.23	4,4,4,4	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.