



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:10 pm BST

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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

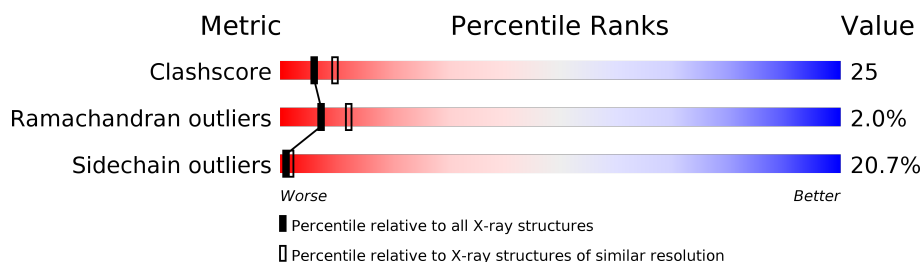
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 respectively. 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 $\leq 5\%$

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 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
			2789	1772	471	534	12			

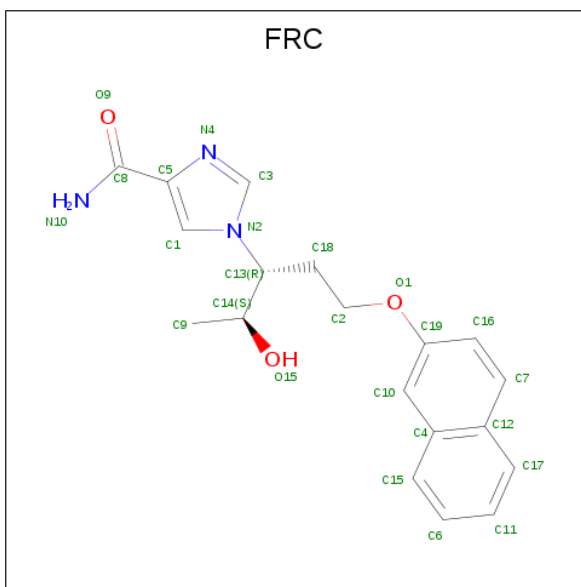
There are 15 discrepancies between the modelled and reference sequences:

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 MIAZONE-4-CARBOXAMIDE (three-letter code: FRC) (formula: C₁₉H₂₁N₃O₃).



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

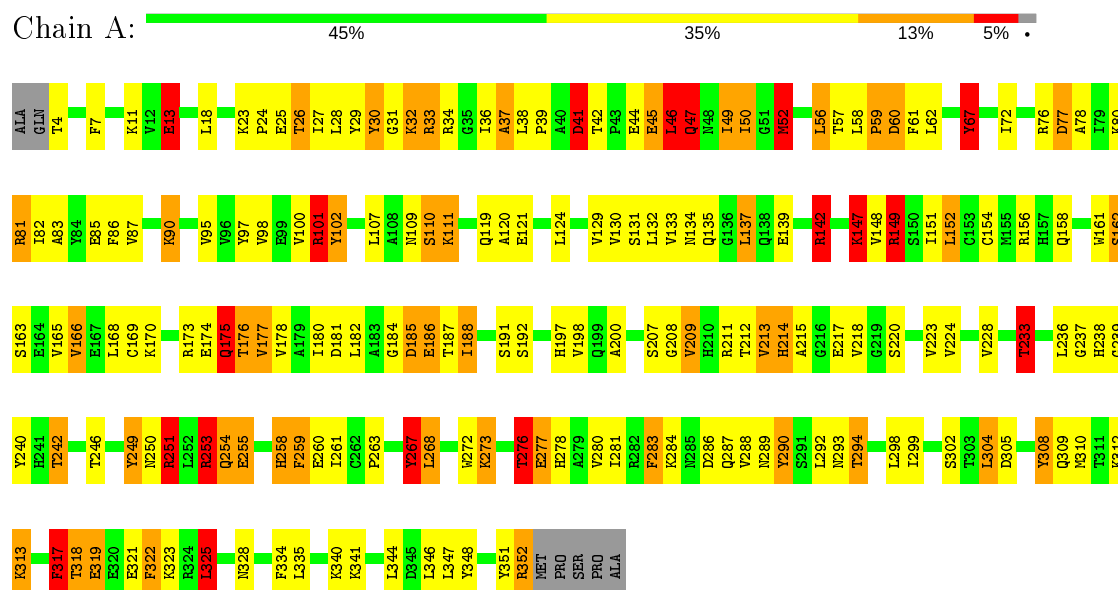
- Molecule 4 is water.

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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	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
$\langle I/\sigma(I) \rangle$ ¹	15.58 (at 2.00Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.244 , 0.276 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3001	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

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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

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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 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	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

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 25.

All (138) 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: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:39:PRO:HG3	1:A:67:TYR:CE2	2.35	0.61
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.83	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:109:ASN:HB3	1:A:119:GLN:OE1	2.03	0.59
1:A:261:ILE:HD12	1:A:290:TYR:HB2	1.84	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
1:A:152:LEU:HD22	1:A:177:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:PRO:HB2	1:A:310:MET:SD	2.52	0.50
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.46	0.50
1:A:170:LYS:HD2	1:A:207:SER:OG	2.12	0.50
1:A:107:LEU:HB2	1:A:129:VAL:HG11	1.94	0.49
1:A:305:ASP:O	1:A:309:GLN:HG2	2.12	0.49
1:A:318:THR:HG22	1:A:321:GLU:H	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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: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:322:PHE:HA	1:A:325:LEU:CD1	2.42	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: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:308:TYR:CD2	1:A:322:PHE:CE2	3.05	0.45
1:A:102:TYR:CE2	1:A:133:VAL:HG11	2.51	0.45
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.45	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:169:CYS:O	1:A:173:ARG:HB3	2.19	0.42
1:A:162:SER:HB3	1:A:200:ALA:HB2	2.00	0.42
1:A:304:LEU:HD22	1:A:308:TYR:CE1	2.54	0.42
1:A:52:MET:HE3	1:A:299:ILE:HG23	2.01	0.42
1:A:26:THR:HB	1:A:81:ARG:NH2	2.34	0.42
1:A:209:VAL:HG21	4:A:1174:HOH:O	2.20	0.42
1:A:253:ARG:HG2	4:A:1003:HOH:O	2.18	0.42
1:A:188:ILE:HG12	1:A:191:SER:HB3	2.01	0.42
1:A:182:LEU:HB3	1:A:213:VAL:HG13	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.83	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.93	0.41
1:A:312:LYS:HG2	1:A:313:LYS:HZ3	1.85	0.41
1:A:47:GLN:HE21	1:A:47:GLN:HB2	1.44	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:287:GLN:HA	1:A:287:GLN:OE1	2.20	0.40
1:A:7:PHE:CD1	1:A:319:GLU:HG3	2.56	0.40
1:A:224:VAL:O	1:A:228:VAL:HG23	2.22	0.40
1:A:284:LYS:HE3	1:A:284:LYS:HB3	1.91	0.40
1:A:87:VAL:HG13	1:A:148:VAL:HG21	2.02	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 [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%)	306 (88%)	34 (10%)	7 (2%)	7 12

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

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Mol	Chain	Res	Type
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%)	1 2

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

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Mol	Chain	Res	Type
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
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	23,27,27	1.79	3 (13%)	25,37,37	1.40	3 (12%)

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	-	-	1/10/18/18	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FRC	C1-N2	5.81	1.46	1.38
3	A	1001	FRC	C5-N4	3.52	1.48	1.37
3	A	1001	FRC	C10-C19	2.72	1.41	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FRC	O9-C8-C5	3.66	122.67	119.61
3	A	1001	FRC	O15-C14-C9	2.98	118.58	109.74
3	A	1001	FRC	C5-C1-N2	-2.32	105.48	107.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

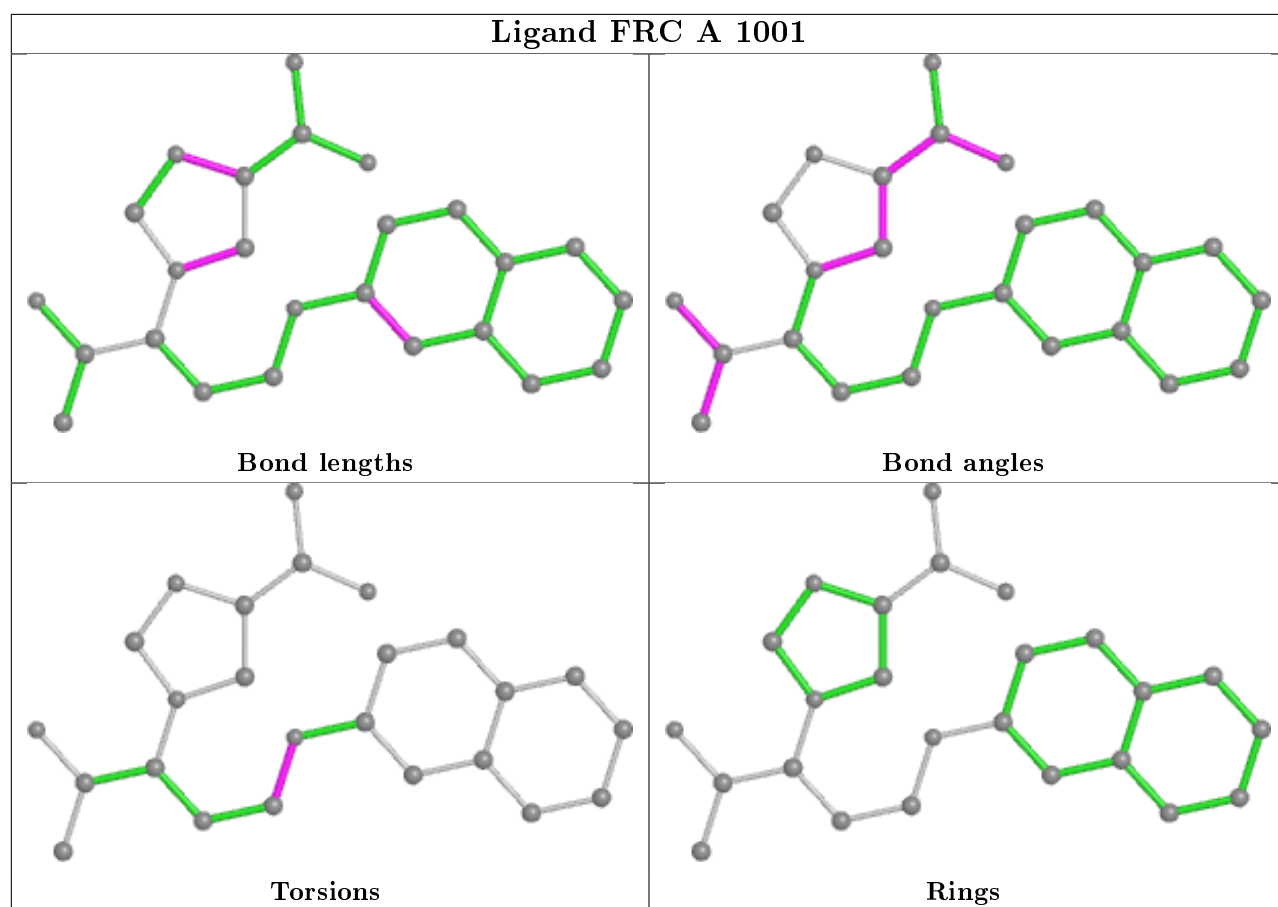
Mol	Chain	Res	Type	Atoms
3	A	1001	FRC	C18-C2-O1-C19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FRC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

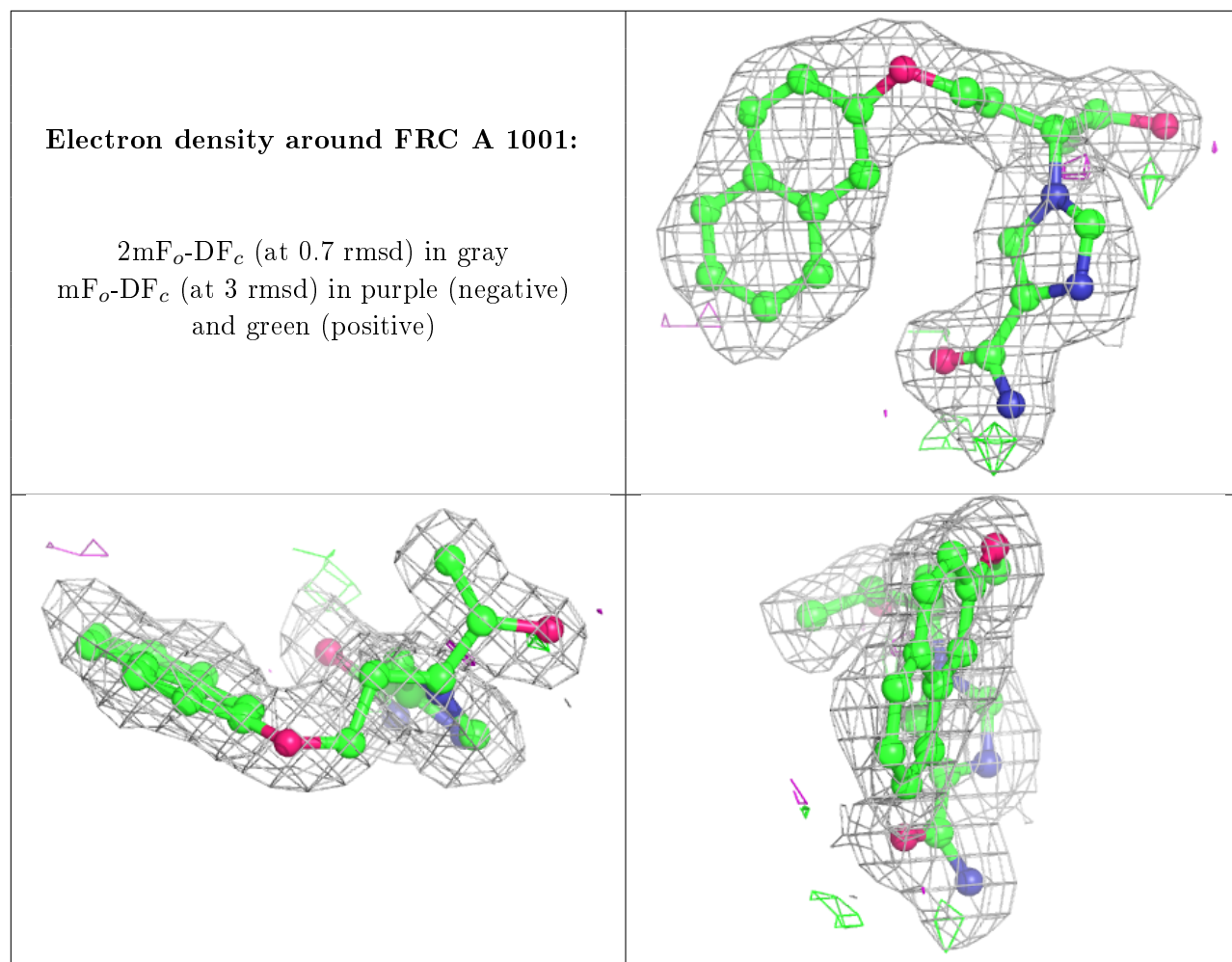
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.