



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 PM UTC

PDB ID : 1QXL / pdb_00001qxl
Title : Crystal structure of Adenosine deaminase complexed with FR235380
Authors : Kinoshita, T.
Deposited on : 2003-09-08
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

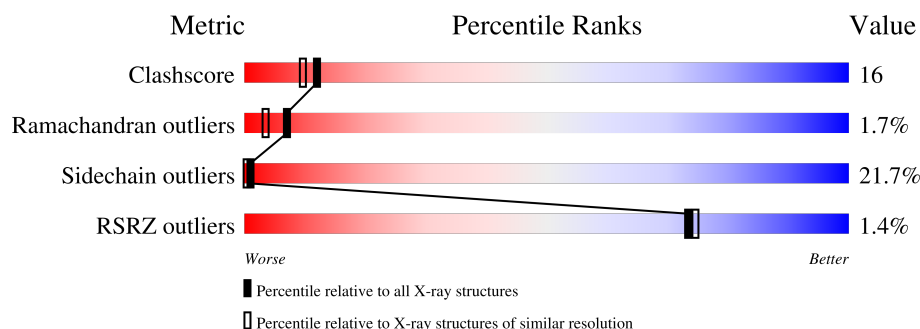
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 of 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 $\leq 5\%$. 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

There are 4 unique types of molecules in this entry. The entry contains 2982 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	1773	470	533	12			

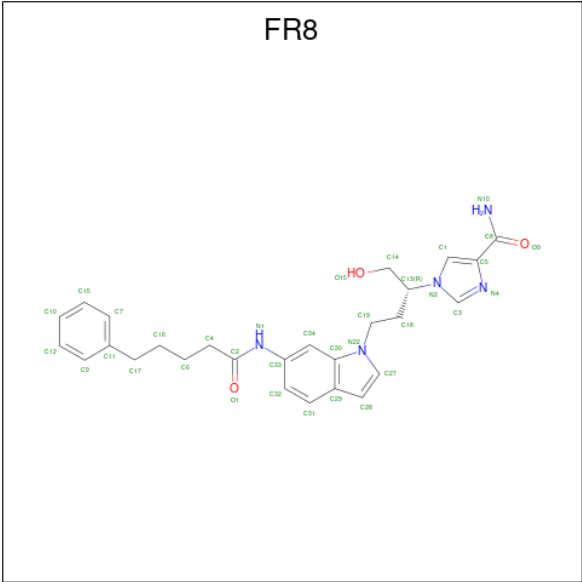
There are 16 discrepancies between the modelled and reference sequences:

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	47	LEU	GLN	conflict	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 (CCD ID: 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-{6-[(5-PHENYLPENTANOYL)AMINO]-1H-INDOL-1-YL}PROPYL)-1H-IMIDAZOLE-4-CARBOXAMIDE (CCD ID: FR8) (formula: C₂₇H₃₁N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	27	5	3		

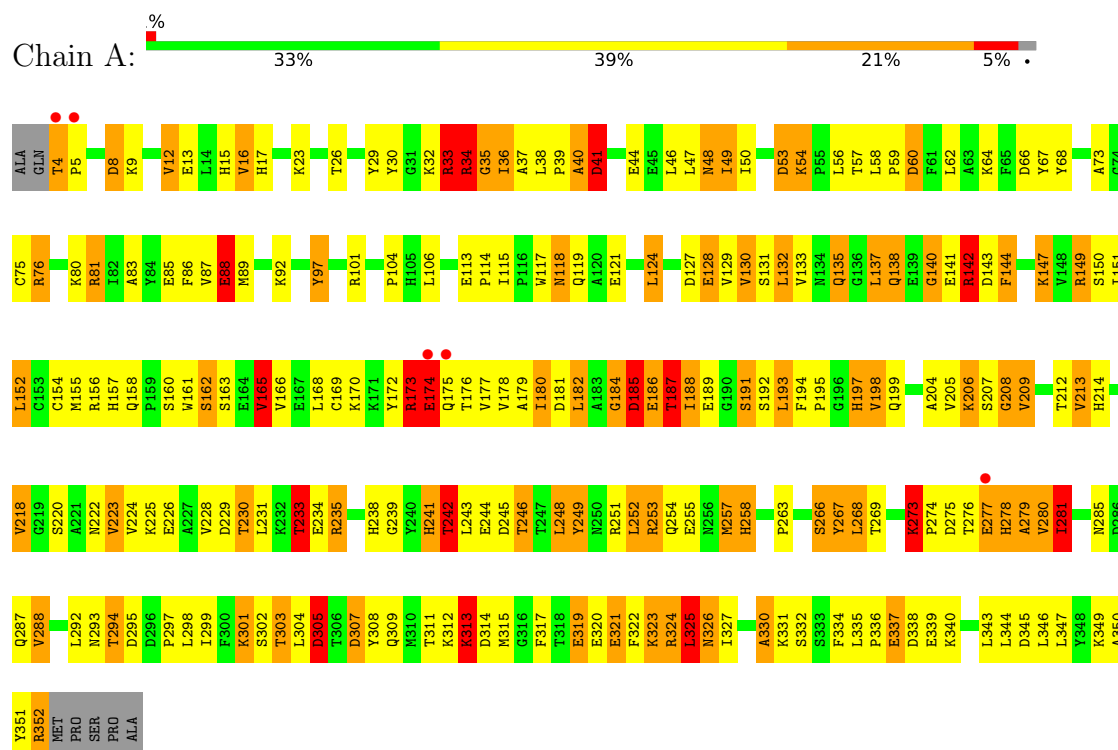
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	158	Total	O	0	0
			158	158		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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	78.37Å 78.37Å 137.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.25 – 2.25 51.25 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (51.25-2.25) 97.3 (51.25-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.25Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.232 , 0.253 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2982	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: FR8, 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	1.46	18/2852 (0.6%)	2.61	235/3866 (6.1%)

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	13

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ASP	N-CA	8.57	1.57	1.46
1	A	294	THR	CB-OG1	7.31	1.55	1.43
1	A	214	HIS	CG-ND1	-6.99	1.30	1.38
1	A	218	VAL	CA-C	6.95	1.59	1.52
1	A	197	HIS	CE1-NE2	6.37	1.39	1.32
1	A	253	ARG	NE-CZ	6.30	1.40	1.33
1	A	258	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	189	GLU	CD-OE2	6.13	1.37	1.25
1	A	278	HIS	CG-ND1	-6.01	1.31	1.38
1	A	173	ARG	CA-C	5.94	1.60	1.52
1	A	157	HIS	ND1-CE1	5.71	1.38	1.32
1	A	279	ALA	CA-C	5.58	1.60	1.52
1	A	17	HIS	CE1-NE2	5.42	1.38	1.32
1	A	157	HIS	CG-CD2	5.30	1.41	1.35
1	A	40	ALA	N-CA	5.27	1.52	1.46
1	A	299	ILE	CA-C	-5.27	1.46	1.52
1	A	15	HIS	CG-ND1	-5.12	1.32	1.38
1	A	12	VAL	CA-CB	-5.04	1.48	1.54

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	18.49	131.09	112.60
1	A	223	VAL	N-CA-C	10.86	121.70	110.62
1	A	235	ARG	NE-CZ-NH1	-10.49	111.01	121.50
1	A	88	GLU	N-CA-C	10.47	123.75	111.71
1	A	229	ASP	CA-C-N	-9.82	105.46	122.36
1	A	229	ASP	C-N-CA	-9.82	105.46	122.36
1	A	185	ASP	N-CA-CB	9.72	126.92	110.49
1	A	198	VAL	N-CA-C	9.60	119.63	110.42
1	A	266	SER	N-CA-C	9.59	121.73	111.28
1	A	313	LYS	CA-C-N	-9.52	105.15	122.38
1	A	313	LYS	C-N-CA	-9.52	105.15	122.38
1	A	157	HIS	CA-C-N	-9.15	112.78	122.85
1	A	157	HIS	C-N-CA	-9.15	112.78	122.85
1	A	337	GLU	CA-C-N	-9.11	108.06	120.44
1	A	337	GLU	C-N-CA	-9.11	108.06	120.44
1	A	299	ILE	N-CA-C	9.05	119.86	110.72
1	A	253	ARG	CA-CB-CG	8.76	131.63	114.10
1	A	175	GLN	CA-C-N	8.75	137.44	121.70
1	A	175	GLN	C-N-CA	8.75	137.44	121.70
1	A	277	GLU	CA-C-N	-8.63	108.87	120.95
1	A	277	GLU	C-N-CA	-8.63	108.87	120.95
1	A	29	TYR	N-CA-C	8.62	121.76	111.33
1	A	53	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	235	ARG	NE-CZ-NH2	8.46	126.81	119.20
1	A	174	GLU	N-CA-C	8.27	128.42	110.80
1	A	213	VAL	CA-C-N	-8.26	109.68	121.50
1	A	213	VAL	C-N-CA	-8.26	109.68	121.50
1	A	293	ASN	CA-C-N	-8.25	109.14	122.26
1	A	293	ASN	C-N-CA	-8.25	109.14	122.26
1	A	132	LEU	N-CA-C	8.10	119.89	111.14
1	A	87	VAL	CA-C-N	-8.10	108.62	120.28
1	A	87	VAL	C-N-CA	-8.10	108.62	120.28
1	A	150	SER	N-CA-C	8.07	122.16	109.81
1	A	273	LYS	CB-CA-C	8.06	119.22	109.31
1	A	301	LYS	CA-C-N	-7.95	109.72	122.53
1	A	301	LYS	C-N-CA	-7.95	109.72	122.53
1	A	138	GLN	CA-C-N	-7.88	107.36	121.14
1	A	138	GLN	C-N-CA	-7.88	107.36	121.14
1	A	304	LEU	CB-CA-C	-7.80	97.43	110.68
1	A	16	VAL	CB-CA-C	-7.76	98.56	111.29
1	A	173	ARG	N-CA-CB	-7.76	96.75	109.56
1	A	218	VAL	CA-C-O	7.72	125.48	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	SER	N-CA-C	7.68	120.54	111.71
1	A	66	ASP	CA-CB-CG	-7.64	104.96	112.60
1	A	68	TYR	N-CA-C	7.62	121.84	112.23
1	A	235	ARG	CB-CG-CD	-7.53	93.98	111.30
1	A	173	ARG	N-CA-C	7.51	120.87	110.35
1	A	46	LEU	N-CA-C	7.50	119.10	111.07
1	A	189	GLU	OE1-CD-OE2	7.48	140.86	122.90
1	A	249	TYR	N-CA-C	7.48	120.09	111.11
1	A	325	LEU	N-CA-CB	-7.45	98.73	110.28
1	A	32	LYS	CA-C-N	-7.45	107.42	122.31
1	A	32	LYS	C-N-CA	-7.45	107.42	122.31
1	A	8	ASP	CA-CB-CG	-7.40	105.20	112.60
1	A	311	THR	N-CA-C	7.23	120.21	111.82
1	A	314	ASP	CA-CB-CG	-7.22	105.38	112.60
1	A	127	ASP	CA-C-N	-7.21	108.69	120.72
1	A	127	ASP	C-N-CA	-7.21	108.69	120.72
1	A	307	ASP	CA-C-O	7.19	128.18	120.55
1	A	254	GLN	CA-C-O	7.05	128.08	119.97
1	A	131	SER	N-CA-C	7.00	119.51	111.11
1	A	33	ARG	CA-C-N	-6.98	110.34	121.44
1	A	33	ARG	C-N-CA	-6.98	110.34	121.44
1	A	218	VAL	N-CA-CB	-6.97	102.00	112.67
1	A	92	LYS	N-CA-C	6.97	120.88	112.38
1	A	86	PHE	CA-CB-CG	-6.96	106.84	113.80
1	A	248	LEU	CA-C-N	-6.95	111.15	120.54
1	A	248	LEU	C-N-CA	-6.95	111.15	120.54
1	A	204	ALA	N-CA-C	6.94	119.44	111.11
1	A	182	LEU	CD1-CG-CD2	6.90	125.99	110.80
1	A	218	VAL	CB-CA-C	6.89	117.52	110.70
1	A	187	THR	CA-CB-CG2	6.85	122.15	110.50
1	A	62	LEU	N-CA-C	6.83	119.74	111.82
1	A	233	THR	CB-CA-C	-6.82	97.42	109.62
1	A	281	ILE	N-CA-C	6.70	118.31	111.00
1	A	41	ASP	N-CA-C	6.67	122.61	112.54
1	A	245	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	130	VAL	N-CA-C	6.65	119.36	111.05
1	A	208	GLY	CA-C-N	-6.64	113.81	122.37
1	A	208	GLY	C-N-CA	-6.64	113.81	122.37
1	A	280	VAL	N-CA-C	6.57	119.26	111.05
1	A	213	VAL	N-CA-C	6.57	117.58	108.12
1	A	184	GLY	CA-C-N	-6.56	109.02	121.54
1	A	184	GLY	C-N-CA	-6.56	109.02	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	SER	CA-C-N	-6.55	109.68	121.14
1	A	163	SER	C-N-CA	-6.55	109.68	121.14
1	A	304	LEU	N-CA-C	6.54	119.25	111.33
1	A	34	ARG	CA-C-N	-6.53	115.67	123.44
1	A	34	ARG	C-N-CA	-6.53	115.67	123.44
1	A	257	MET	CG-SD-CE	-6.50	86.61	100.90
1	A	155	MET	N-CA-C	6.46	119.26	108.73
1	A	172	TYR	N-CA-C	6.43	120.06	112.72
1	A	169	CYS	N-CA-C	6.42	118.81	111.11
1	A	269	THR	N-CA-C	6.42	120.37	112.54
1	A	173	ARG	CG-CD-NE	-6.38	97.96	112.00
1	A	143	ASP	N-CA-C	6.36	121.24	112.90
1	A	234	GLU	CA-C-N	-6.36	112.18	122.36
1	A	234	GLU	C-N-CA	-6.36	112.18	122.36
1	A	64	LYS	CA-CB-CG	-6.29	101.51	114.10
1	A	64	LYS	CG-CD-CE	-6.29	96.83	111.30
1	A	281	ILE	CB-CG1-CD1	-6.25	100.68	113.80
1	A	294	THR	OG1-CB-CG2	6.24	121.79	109.30
1	A	279	ALA	N-CA-CB	-6.24	99.94	110.49
1	A	119	GLN	CB-CG-CD	-6.23	102.00	112.60
1	A	57	THR	N-CA-C	6.22	118.56	110.53
1	A	175	GLN	N-CA-CB	-6.21	100.00	110.49
1	A	175	GLN	O-C-N	-6.18	114.37	122.59
1	A	60	ASP	N-CA-CB	6.18	119.73	110.22
1	A	76	ARG	N-CA-C	6.17	118.79	111.33
1	A	175	GLN	N-CA-C	6.12	123.85	110.80
1	A	332	SER	CB-CA-C	-6.12	99.86	110.09
1	A	254	GLN	CB-CG-CD	-6.09	102.24	112.60
1	A	330	ALA	N-CA-C	6.08	117.99	111.36
1	A	16	VAL	CG1-CB-CG2	6.05	124.11	110.80
1	A	54	LYS	CA-C-N	-6.05	113.71	119.76
1	A	54	LYS	C-N-CA	-6.05	113.71	119.76
1	A	245	ASP	CA-C-N	-6.03	110.43	120.68
1	A	245	ASP	C-N-CA	-6.03	110.43	120.68
1	A	121	GLU	N-CA-C	6.03	118.45	109.59
1	A	295	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	49	ILE	CA-C-N	-5.99	111.18	121.97
1	A	49	ILE	C-N-CA	-5.99	111.18	121.97
1	A	287	GLN	CA-C-N	-5.99	110.88	120.34
1	A	287	GLN	C-N-CA	-5.99	110.88	120.34
1	A	127	ASP	N-CA-C	5.97	117.79	111.28
1	A	149	ARG	CA-C-N	-5.96	112.35	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	C-N-CA	-5.96	112.35	123.03
1	A	35	GLY	CA-C-N	-5.96	110.53	120.30
1	A	35	GLY	C-N-CA	-5.96	110.53	120.30
1	A	246	THR	N-CA-C	5.93	119.70	112.23
1	A	162	SER	CA-C-N	-5.89	111.36	120.31
1	A	162	SER	C-N-CA	-5.89	111.36	120.31
1	A	165	VAL	N-CA-C	5.88	116.35	110.23
1	A	140	GLY	CA-C-N	-5.88	112.79	120.44
1	A	140	GLY	C-N-CA	-5.88	112.79	120.44
1	A	149	ARG	CD-NE-CZ	-5.84	116.22	124.40
1	A	209	VAL	N-CA-C	5.84	117.00	108.58
1	A	181	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	189	GLU	CA-C-N	-5.79	112.30	122.09
1	A	189	GLU	C-N-CA	-5.79	112.30	122.09
1	A	326	ASN	CB-CG-ND2	-5.74	107.79	116.40
1	A	321	GLU	N-CA-C	5.71	117.18	111.07
1	A	194	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	225	LYS	N-CA-C	5.68	118.21	111.33
1	A	129	VAL	CA-C-N	-5.68	111.49	120.47
1	A	129	VAL	C-N-CA	-5.68	111.49	120.47
1	A	319	GLU	CA-C-N	-5.68	112.23	120.29
1	A	319	GLU	C-N-CA	-5.68	112.23	120.29
1	A	287	GLN	CG-CD-NE2	-5.67	107.89	116.40
1	A	59	PRO	CA-C-N	-5.67	112.12	120.28
1	A	59	PRO	C-N-CA	-5.67	112.12	120.28
1	A	285	ASN	N-CA-C	5.66	118.22	111.71
1	A	53	ASP	N-CA-CB	5.66	118.97	110.65
1	A	33	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	A	338	ASP	N-CA-C	5.65	117.25	111.14
1	A	48	ASN	N-CA-C	5.65	118.21	111.71
1	A	198	VAL	CA-CB-CG1	5.64	120.00	110.40
1	A	40	ALA	CB-CA-C	-5.63	99.21	110.42
1	A	278	HIS	CA-CB-CG	-5.63	108.17	113.80
1	A	48	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	325	LEU	CB-CA-C	5.59	121.41	110.67
1	A	165	VAL	CA-CB-CG2	5.58	119.89	110.40
1	A	278	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	A	242	THR	CA-CB-OG1	5.56	117.94	109.60
1	A	324	ARG	N-CA-C	5.54	118.08	111.71
1	A	241	HIS	N-CA-C	5.53	119.65	113.01
1	A	323	LYS	CA-C-N	-5.51	112.35	120.28
1	A	323	LYS	C-N-CA	-5.51	112.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	CG-CD-NE	5.50	124.11	112.00
1	A	205	VAL	CG1-CB-CG2	-5.50	98.70	110.80
1	A	278	HIS	CG-CD2-NE2	5.50	112.69	107.20
1	A	242	THR	N-CA-C	5.49	119.08	112.38
1	A	331	LYS	CA-C-O	5.49	126.30	120.10
1	A	178	VAL	N-CA-C	5.49	119.41	113.43
1	A	230	THR	CA-C-O	5.44	125.38	119.24
1	A	73	ALA	CA-C-N	-5.43	111.03	121.78
1	A	73	ALA	C-N-CA	-5.43	111.03	121.78
1	A	268	LEU	N-CA-C	5.42	117.19	111.28
1	A	302	SER	N-CA-C	5.41	116.49	108.86
1	A	192	SER	N-CA-CB	5.39	119.34	110.39
1	A	33	ARG	N-CA-C	5.38	119.55	113.15
1	A	178	VAL	CA-C-O	5.35	124.04	118.96
1	A	80	LYS	N-CA-C	5.35	117.11	111.28
1	A	160	SER	N-CA-C	5.35	117.86	111.71
1	A	230	THR	N-CA-C	5.35	120.46	113.88
1	A	198	VAL	CA-CB-CG2	5.33	119.47	110.40
1	A	117	TRP	N-CA-C	5.33	119.06	112.24
1	A	241	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	307	ASP	N-CA-C	5.33	117.09	111.28
1	A	323	LYS	CA-C-O	5.31	126.05	120.42
1	A	186	GLU	CA-C-N	5.31	129.70	120.68
1	A	186	GLU	C-N-CA	5.31	129.70	120.68
1	A	49	ILE	CA-CB-CG1	5.29	119.40	110.40
1	A	193	LEU	CA-C-N	-5.29	113.45	120.65
1	A	193	LEU	C-N-CA	-5.29	113.45	120.65
1	A	235	ARG	CA-CB-CG	5.27	124.64	114.10
1	A	303	THR	N-CA-CB	-5.27	102.52	111.69
1	A	83	ALA	N-CA-C	5.25	116.70	110.97
1	A	251	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	198	VAL	N-CA-CB	5.24	116.68	110.55
1	A	280	VAL	CA-C-N	-5.23	112.17	120.55
1	A	280	VAL	C-N-CA	-5.23	112.17	120.55
1	A	62	LEU	CA-C-O	5.23	125.99	119.97
1	A	278	HIS	CA-C-N	-5.23	111.55	121.54
1	A	278	HIS	C-N-CA	-5.23	111.55	121.54
1	A	206	LYS	CA-C-N	-5.19	114.91	122.86
1	A	206	LYS	C-N-CA	-5.19	114.91	122.86
1	A	189	GLU	CG-CD-OE1	-5.19	106.45	118.40
1	A	241	HIS	CA-C-N	-5.19	112.29	120.60
1	A	241	HIS	C-N-CA	-5.19	112.29	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	214	HIS	CA-CB-CG	5.18	118.98	113.80
1	A	280	VAL	CA-CB-CG1	5.18	119.20	110.40
1	A	165	VAL	N-CA-CB	5.17	116.05	110.62
1	A	339	GLU	CA-C-O	5.17	125.74	119.49
1	A	233	THR	CA-CB-OG1	5.16	117.34	109.60
1	A	288	VAL	CB-CA-C	5.15	117.21	111.45
1	A	331	LYS	N-CA-C	5.14	117.62	111.71
1	A	144	PHE	CA-C-N	-5.14	111.96	121.93
1	A	144	PHE	C-N-CA	-5.14	111.96	121.93
1	A	320	GLU	N-CA-C	5.14	116.96	111.36
1	A	218	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	128	GLU	N-CA-C	5.13	118.80	112.54
1	A	142	ARG	CB-CA-C	5.11	120.12	109.95
1	A	312	LYS	CA-C-O	5.09	125.56	119.60
1	A	205	VAL	N-CA-CB	5.08	116.15	110.51
1	A	252	LEU	N-CA-C	5.08	116.82	111.28
1	A	228	VAL	N-CA-C	5.08	115.31	110.53
1	A	352	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	135	GLN	CB-CG-CD	-5.04	104.04	112.60
1	A	106	LEU	N-CA-C	5.03	119.05	113.01
1	A	36	ILE	CA-C-O	5.03	125.90	120.47
1	A	220	SER	N-CA-C	5.03	116.60	110.41
1	A	97	TYR	CA-C-N	-5.00	114.73	122.69
1	A	97	TYR	C-N-CA	-5.00	114.73	122.69

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	235	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	308	TYR	Sidechain
1	A	33	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	351	TYR	Sidechain
1	A	352	ARG	Sidechain
1	A	4	THR	Peptide
1	A	41	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	2746	88	0
2	A	1	0	0	0	0
3	A	35	0	31	0	0
4	A	158	0	0	6	0
All	All	2982	0	2777	88	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 16.

All (88) 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:239:GLY:O	1:A:242:THR:HG23	1.85	0.77
1:A:345:ASP:HB3	1:A:349:LYS:HZ2	1.49	0.76
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.66	0.75
1:A:185:ASP:OD1	1:A:187:THR:HB	1.87	0.75
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.21	0.75
1:A:278:HIS:CD2	1:A:280:VAL:H	2.05	0.73
1:A:113:GLU:HA	1:A:114:PRO:C	2.16	0.70
1:A:281:ILE:HG22	1:A:317:PHE:HE1	1.59	0.67
1:A:88:GLU:HB3	1:A:144:PHE:CE2	2.31	0.66
1:A:281:ILE:H	1:A:281:ILE:HD13	1.62	0.63
1:A:162:SER:HA	1:A:165:VAL:HG13	1.79	0.63
1:A:156:ARG:O	1:A:197:HIS:HE1	1.81	0.63
1:A:278:HIS:HD2	1:A:280:VAL:HG12	1.62	0.62
1:A:224:VAL:HG21	1:A:242:THR:HG22	1.81	0.61
1:A:132:LEU:HD13	4:A:1068:HOH:O	2.00	0.59
1:A:322:PHE:HA	1:A:325:LEU:HD13	1.84	0.59
1:A:350:ALA:HB3	4:A:1102:HOH:O	2.01	0.59
1:A:345:ASP:HB3	1:A:349:LYS:NZ	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:HD1	1:A:147:LYS:HG2	1.68	0.58
1:A:138:GLN:HB3	1:A:142:ARG:HH22	1.68	0.58
1:A:133:VAL:O	1:A:137:LEU:HB2	2.04	0.58
1:A:343:LEU:O	1:A:347:LEU:HD22	2.04	0.58
1:A:278:HIS:HD2	1:A:280:VAL:H	1.48	0.57
1:A:101:ARG:HA	1:A:151:ILE:O	2.05	0.56
1:A:281:ILE:HG21	1:A:315:MET:HB3	1.88	0.55
1:A:38:LEU:H	1:A:38:LEU:HD22	1.72	0.54
1:A:133:VAL:HG12	1:A:137:LEU:HD22	1.90	0.53
1:A:104:PRO:HG3	1:A:152:LEU:HG	1.89	0.53
1:A:12:VAL:H	1:A:326:ASN:ND2	2.07	0.53
1:A:152:LEU:HD22	1:A:177:VAL:HG11	1.91	0.52
1:A:44:GLU:O	1:A:48:ASN:ND2	2.42	0.52
1:A:97:TYR:HD1	1:A:147:LYS:CG	2.21	0.52
1:A:257:MET:HE3	1:A:258:HIS:N	2.24	0.52
1:A:154:CYS:SG	1:A:180:ILE:HD11	2.50	0.52
1:A:13:GLU:HA	4:A:1125:HOH:O	2.11	0.51
1:A:280:VAL:HG22	1:A:317:PHE:HZ	1.76	0.51
1:A:162:SER:OG	1:A:197:HIS:HD2	1.94	0.51
1:A:124:LEU:CD2	1:A:128:GLU:HG3	2.42	0.50
1:A:174:GLU:O	1:A:176:THR:HA	2.11	0.50
1:A:321:GLU:O	1:A:325:LEU:HB3	2.13	0.49
1:A:5:PRO:HA	1:A:305:ASP:OD1	2.13	0.48
1:A:273:LYS:HD3	1:A:274:PRO:HD2	1.95	0.48
1:A:128:GLU:O	1:A:132:LEU:HD12	2.14	0.48
1:A:208:GLY:HA2	4:A:1043:HOH:O	2.14	0.47
1:A:179:ALA:HB2	1:A:334:PHE:CD2	2.50	0.47
1:A:267:TYR:C	1:A:267:TYR:CD2	2.93	0.47
1:A:281:ILE:CG2	1:A:315:MET:HB3	2.46	0.46
1:A:188:ILE:HG13	1:A:191:SER:HB3	1.98	0.46
1:A:241:HIS:O	1:A:244:GLU:HG2	2.17	0.45
1:A:263:PRO:HD2	1:A:307:ASP:OD2	2.16	0.45
1:A:309:GLN:HE21	1:A:313:LYS:NZ	2.14	0.45
1:A:281:ILE:HG22	1:A:317:PHE:CE1	2.46	0.45
1:A:88:GLU:HB3	1:A:144:PHE:CD2	2.52	0.45
1:A:252:LEU:HD22	1:A:257:MET:HG3	1.98	0.45
1:A:124:LEU:HD23	1:A:128:GLU:HG3	1.99	0.44
1:A:97:TYR:CD1	1:A:147:LYS:HG2	2.51	0.44
1:A:97:TYR:HA	1:A:147:LYS:O	2.17	0.44
1:A:76:ARG:HA	4:A:1068:HOH:O	2.18	0.44
1:A:140:GLY:O	1:A:141:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLN:CB	1:A:142:ARG:HH22	2.30	0.43
1:A:158:GLN:HG2	1:A:161:TRP:CD2	2.53	0.43
1:A:330:ALA:O	1:A:340:LYS:HD3	2.18	0.43
1:A:170:LYS:O	1:A:173:ARG:HB2	2.19	0.43
1:A:30:TYR:O	1:A:34:ARG:HG3	2.19	0.42
1:A:44:GLU:H	1:A:44:GLU:HG3	1.53	0.42
1:A:50:ILE:HG22	1:A:67:TYR:HD1	1.83	0.42
1:A:81:ARG:O	1:A:85:GLU:HG3	2.19	0.42
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.42	0.42
1:A:158:GLN:HG2	1:A:161:TRP:CE2	2.55	0.42
1:A:248:LEU:O	1:A:249:TYR:C	2.62	0.42
1:A:337:GLU:HG3	4:A:1113:HOH:O	2.20	0.42
1:A:50:ILE:HD13	1:A:50:ILE:HG21	1.60	0.42
1:A:23:LYS:HD2	1:A:89:MET:SD	2.60	0.42
1:A:9:LYS:HD3	1:A:9:LYS:HA	1.51	0.41
1:A:35:GLY:O	1:A:36:ILE:C	2.63	0.41
1:A:113:GLU:HA	1:A:114:PRO:O	2.19	0.41
1:A:278:HIS:O	1:A:279:ALA:C	2.63	0.41
1:A:212:THR:HA	1:A:233:THR:HG22	2.01	0.41
1:A:273:LYS:HA	1:A:274:PRO:HD3	1.92	0.41
1:A:184:GLY:O	1:A:185:ASP:CB	2.65	0.41
1:A:222:ASN:O	1:A:226:GLU:HG3	2.21	0.41
1:A:294:THR:HG23	1:A:297:PRO:HD3	2.03	0.41
1:A:323:LYS:O	1:A:327:ILE:HG12	2.20	0.41
1:A:170:LYS:HD2	1:A:207:SER:OG	2.20	0.40
1:A:273:LYS:O	1:A:275:ASP:N	2.53	0.40
1:A:336:PRO:O	1:A:337:GLU:C	2.62	0.40
1:A:38:LEU:HB3	1:A:39:PRO:HD2	2.03	0.40
1:A:266:SER:OG	1:A:278:HIS:HE1	2.05	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%)	18 (5%)	6 (2%)	7 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	174	GLU
1	A	185	ASP
1	A	37	ALA
1	A	40	ALA
1	A	238	HIS

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%)	238 (78%)	66 (22%)	1 0

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	16	VAL
1	A	26	THR
1	A	33	ARG
1	A	41	ASP
1	A	47	LEU
1	A	49	ILE
1	A	53	ASP
1	A	54	LYS
1	A	56	LEU
1	A	58	LEU
1	A	60	ASP
1	A	75	CYS
1	A	88	GLU

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Mol	Chain	Res	Type
1	A	115	ILE
1	A	118	ASN
1	A	124	LEU
1	A	130	VAL
1	A	135	GLN
1	A	137	LEU
1	A	147	LYS
1	A	152	LEU
1	A	165	VAL
1	A	166	VAL
1	A	168	LEU
1	A	174	GLU
1	A	180	ILE
1	A	182	LEU
1	A	186	GLU
1	A	187	THR
1	A	188	ILE
1	A	193	LEU
1	A	195	PRO
1	A	198	VAL
1	A	199	GLN
1	A	206	LYS
1	A	209	VAL
1	A	218	VAL
1	A	223	VAL
1	A	230	THR
1	A	231	LEU
1	A	233	THR
1	A	242	THR
1	A	243	LEU
1	A	246	THR
1	A	253	ARG
1	A	255	GLU
1	A	268	LEU
1	A	273	LYS
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	288	VAL
1	A	292	LEU
1	A	298	LEU
1	A	301	LYS

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Mol	Chain	Res	Type
1	A	303	THR
1	A	305	ASP
1	A	313	LYS
1	A	319	GLU
1	A	324	ARG
1	A	325	LEU
1	A	335	LEU
1	A	344	LEU
1	A	346	LEU

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	134	ASN
1	A	175	GLN
1	A	197	HIS
1	A	278	HIS
1	A	285	ASN
1	A	289	ASN
1	A	309	GLN
1	A	326	ASN

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 oligosaccharides 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	FR8	A	1001	-	38,38,38	1.48	8 (21%)	46,51,51	1.28	4 (8%)

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	FR8	A	1001	-	-	5/26/26/26	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR8	C1-N2	3.89	1.46	1.37
3	A	1001	FR8	C33-N1	-3.19	1.35	1.41
3	A	1001	FR8	C5-N4	3.10	1.47	1.39
3	A	1001	FR8	C1-C5	-2.98	1.33	1.37
3	A	1001	FR8	C31-C29	-2.47	1.36	1.41
3	A	1001	FR8	C13-N2	-2.18	1.45	1.48
3	A	1001	FR8	C34-C30	-2.12	1.36	1.39
3	A	1001	FR8	C32-C33	2.01	1.42	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR8	C18-C19-N22	-3.43	107.24	112.55
3	A	1001	FR8	C34-C30-C29	-2.97	119.83	122.29
3	A	1001	FR8	C1-N2-C3	2.59	108.08	106.37
3	A	1001	FR8	C5-C8-N10	2.02	118.32	116.28

There are no chirality outliers.

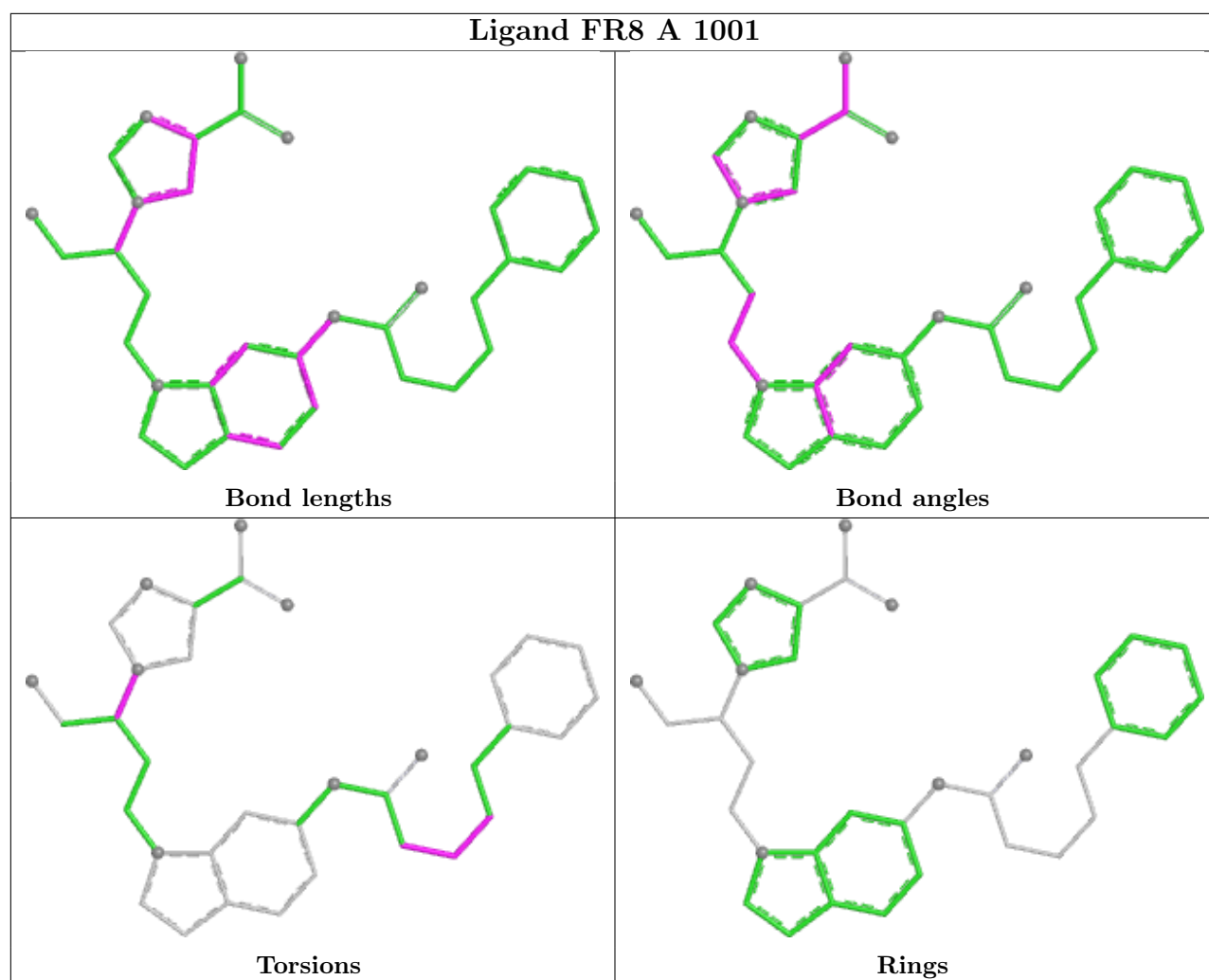
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FR8	C2-C4-C6-C16
3	A	1001	FR8	C17-C16-C6-C4
3	A	1001	FR8	C14-C13-N2-C1
3	A	1001	FR8	C18-C13-N2-C3
3	A	1001	FR8	C18-C13-N2-C1

There are no ring outliers.

No monomer is involved in short contacts.

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 [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%)	-0.14	5 (1%) 73 74	13, 28, 50, 63	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	GLN	2.6
1	A	5	PRO	2.3
1	A	174	GLU	2.2
1	A	277	GLU	2.1
1	A	4	THR	2.0

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](#)

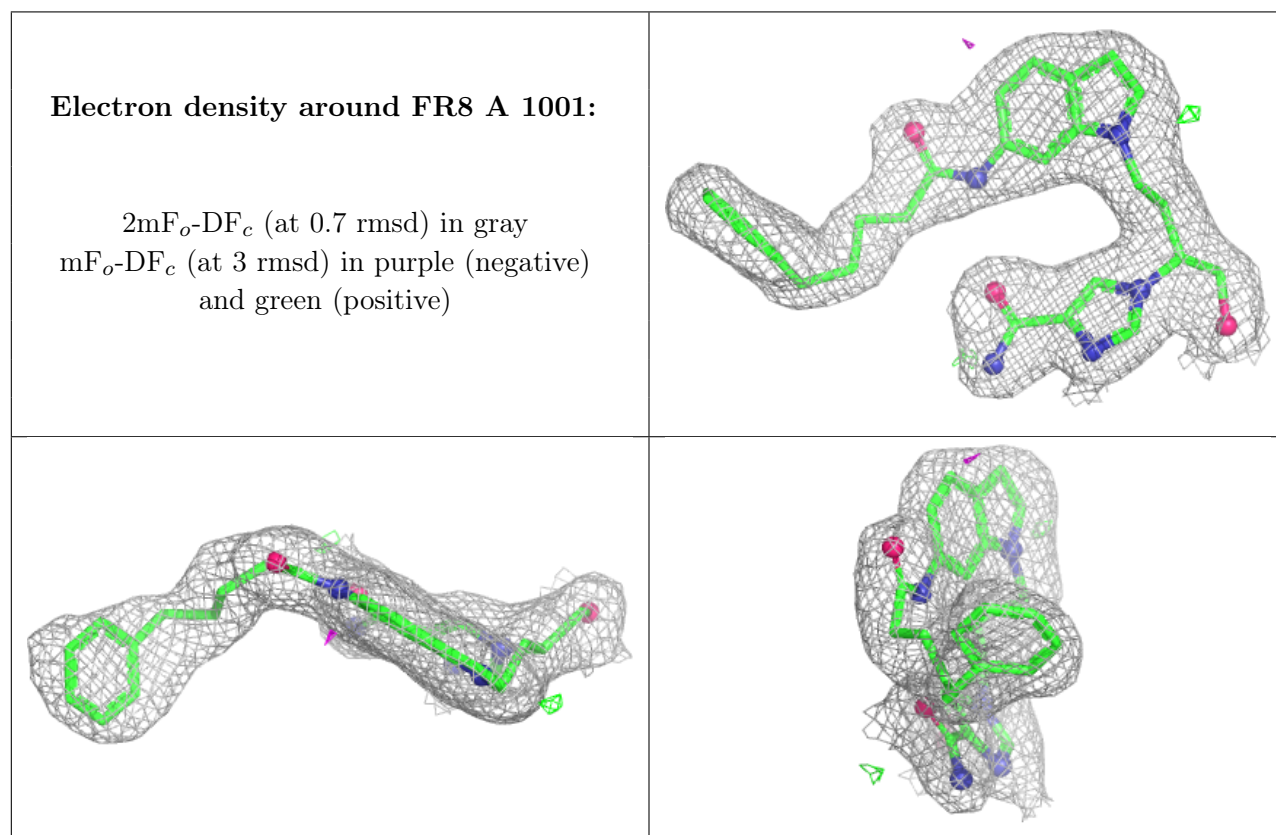
There are no oligosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
3	FR8	A	1001	35/35	0.95	0.07	17,23,39,40	0
2	ZN	A	400	1/1	1.00	0.02	23,23,23,23	0

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](#)

There are no such residues in this entry.