



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:08 AM UTC

PDB ID : 2E1W / pdb_00002e1w
Title : Crystal structure of adenosine deaminase complexed with potent inhibitors
Authors : Kinoshita, T.
Deposited on : 2006-10-30
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 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

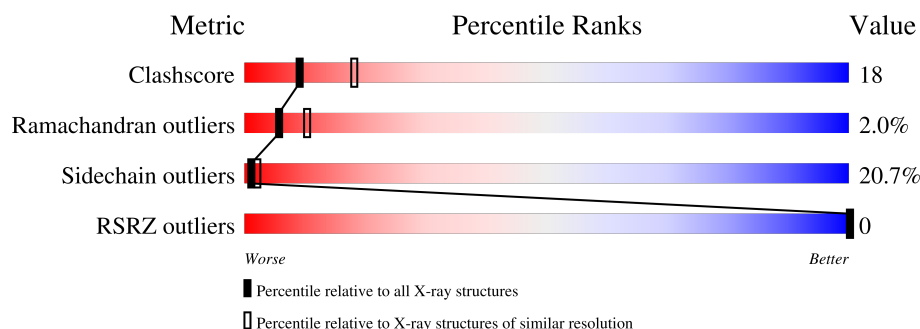
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	35% 37% 20% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2935 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			

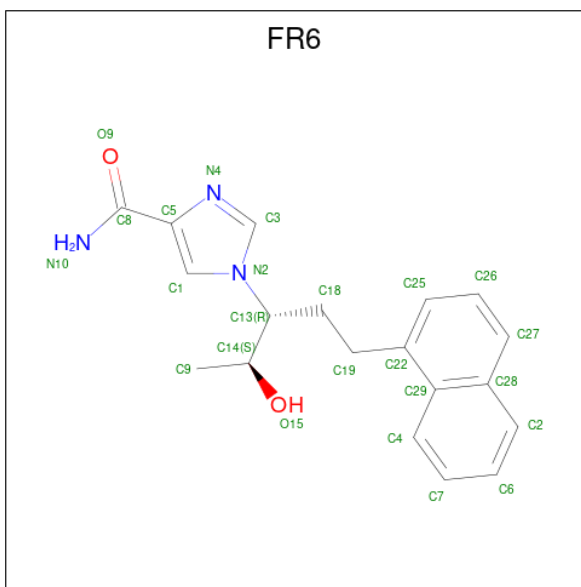
There are 15 discrepancies between the modelled and reference sequences:

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 (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,2S)-2-HYDROXY-1-[2-(1-NAPHTHYL)ETHYL]PROPYL}-1H-IMIDAZOLE-4-CARBOXAMIDE (CCD ID: FR6) (formula: C₁₉H₂₁N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	19	3	2		

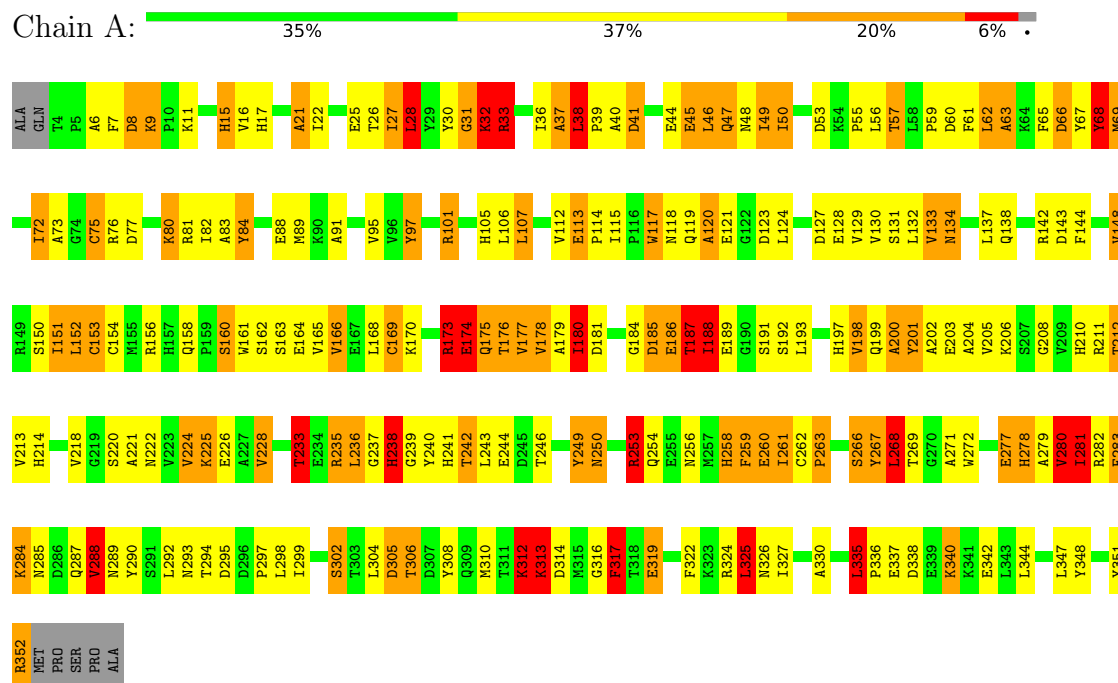
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		

3 Residue-property plots

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	78.41Å 78.41Å 137.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.50 29.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.79-2.50) 75.4 (29.79-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.51Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.218 , 0.246 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2935	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: FR6, 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	1.17	3/2853 (0.1%)	2.46	224/3867 (5.8%)

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	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	HIS	CE1-NE2	7.09	1.39	1.32
1	A	15	HIS	CG-ND1	-6.18	1.31	1.38
1	A	238	HIS	CE1-NE2	5.55	1.38	1.32

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASP	N-CA-CB	-11.97	91.17	110.21
1	A	184	GLY	N-CA-C	-10.48	88.33	113.18
1	A	278	HIS	CA-CB-CG	-9.81	103.99	113.80
1	A	283	PHE	CA-C-N	-9.81	107.69	120.44
1	A	283	PHE	C-N-CA	-9.81	107.69	120.44
1	A	165	VAL	N-CA-C	9.79	119.80	110.30
1	A	169	CYS	CA-CB-SG	-9.37	92.86	114.40
1	A	7	PHE	CA-C-N	-9.09	109.59	122.41
1	A	7	PHE	C-N-CA	-9.09	109.59	122.41
1	A	198	VAL	N-CA-C	9.01	119.82	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	TYR	N-CA-C	8.91	122.15	111.82
1	A	317	PHE	CA-CB-CG	8.88	122.68	113.80
1	A	269	THR	N-CA-C	8.88	121.04	111.36
1	A	277	GLU	CA-C-N	-8.79	108.65	120.95
1	A	277	GLU	C-N-CA	-8.79	108.65	120.95
1	A	28	LEU	N-CA-C	8.65	120.71	111.28
1	A	283	PHE	N-CA-C	8.63	120.46	111.14
1	A	233	THR	N-CA-C	8.58	121.39	110.24
1	A	164	GLU	N-CA-C	8.45	122.85	112.54
1	A	317	PHE	N-CA-CB	8.31	122.92	110.29
1	A	220	SER	N-CA-C	8.28	120.46	110.19
1	A	27	ILE	CA-C-N	-8.24	109.23	120.28
1	A	27	ILE	C-N-CA	-8.24	109.23	120.28
1	A	285	ASN	N-CA-C	8.10	121.13	111.33
1	A	32	LYS	N-CA-C	8.05	119.84	111.14
1	A	16	VAL	CA-C-N	-8.05	111.44	122.30
1	A	16	VAL	C-N-CA	-8.05	111.44	122.30
1	A	281	ILE	N-CA-C	8.02	118.07	110.53
1	A	95	VAL	N-CA-C	8.00	120.38	108.54
1	A	236	LEU	CA-C-N	-7.99	113.79	120.98
1	A	236	LEU	C-N-CA	-7.99	113.79	120.98
1	A	179	ALA	N-CA-C	7.97	120.83	108.96
1	A	313	LYS	CA-C-N	-7.94	107.68	121.66
1	A	313	LYS	C-N-CA	-7.94	107.68	121.66
1	A	120	ALA	CA-C-N	-7.89	110.41	122.09
1	A	120	ALA	C-N-CA	-7.89	110.41	122.09
1	A	246	THR	N-CA-C	7.86	122.63	112.89
1	A	322	PHE	N-CA-C	7.73	120.60	111.71
1	A	37	ALA	N-CA-C	7.71	119.89	110.41
1	A	48	ASN	CA-C-N	-7.70	109.39	121.02
1	A	48	ASN	C-N-CA	-7.70	109.39	121.02
1	A	175	GLN	CA-C-N	7.70	135.56	121.70
1	A	175	GLN	C-N-CA	7.70	135.56	121.70
1	A	287	GLN	N-CA-C	7.67	121.97	111.39
1	A	337	GLU	N-CA-C	7.62	120.47	111.71
1	A	316	GLY	CA-C-N	-7.61	108.76	121.39
1	A	316	GLY	C-N-CA	-7.61	108.76	121.39
1	A	63	ALA	N-CA-C	7.46	120.28	111.71
1	A	228	VAL	N-CA-C	7.45	117.42	110.42
1	A	33	ARG	NE-CZ-NH2	7.34	125.81	119.20
1	A	82	ILE	N-CA-C	7.31	118.11	110.72
1	A	290	TYR	N-CA-C	7.29	120.44	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	SER	N-CA-C	7.28	121.92	112.89
1	A	162	SER	N-CA-C	7.28	119.29	111.36
1	A	169	CYS	N-CA-C	7.25	118.83	111.07
1	A	284	LYS	N-CA-C	7.24	118.82	111.07
1	A	174	GLU	CA-C-N	7.17	134.01	122.32
1	A	174	GLU	C-N-CA	7.17	134.01	122.32
1	A	338	ASP	N-CA-C	7.06	119.58	111.11
1	A	326	ASN	N-CA-C	7.05	119.05	111.36
1	A	121	GLU	N-CA-C	7.03	121.77	109.96
1	A	15	HIS	CE1-NE2-CD2	-7.03	101.97	109.00
1	A	177	VAL	CA-C-N	-6.95	114.42	122.14
1	A	177	VAL	C-N-CA	-6.95	114.42	122.14
1	A	48	ASN	N-CA-C	6.93	119.86	111.82
1	A	15	HIS	CA-C-N	-6.91	113.53	123.06
1	A	15	HIS	C-N-CA	-6.91	113.53	123.06
1	A	325	LEU	N-CA-C	6.90	118.80	111.28
1	A	177	VAL	N-CA-C	6.84	118.44	108.58
1	A	191	SER	N-CA-C	6.79	119.70	111.82
1	A	75	CYS	N-CA-C	6.73	118.84	109.15
1	A	130	VAL	CA-C-O	-6.69	114.89	121.58
1	A	97	TYR	CA-C-N	-6.68	113.84	123.06
1	A	97	TYR	C-N-CA	-6.68	113.84	123.06
1	A	250	ASN	N-CA-C	6.64	118.52	111.28
1	A	133	VAL	CA-C-N	-6.62	109.43	120.68
1	A	133	VAL	C-N-CA	-6.62	109.43	120.68
1	A	69	MET	N-CA-C	6.61	122.64	113.45
1	A	254	GLN	CB-CG-CD	-6.59	101.39	112.60
1	A	138	GLN	N-CA-C	6.59	118.26	111.14
1	A	327	ILE	N-CA-C	6.59	116.72	110.53
1	A	342	GLU	N-CA-C	6.56	118.51	111.36
1	A	76	ARG	N-CA-C	6.51	122.05	111.37
1	A	72	ILE	N-CA-C	6.50	117.58	112.12
1	A	279	ALA	N-CA-C	6.48	119.17	111.33
1	A	6	ALA	N-CA-C	6.41	119.25	111.82
1	A	148	VAL	N-CA-C	6.39	117.12	108.17
1	A	32	LYS	CA-C-N	-6.39	109.11	120.99
1	A	32	LYS	C-N-CA	-6.39	109.11	120.99
1	A	8	ASP	N-CA-C	6.38	119.79	108.24
1	A	163	SER	CA-C-N	-6.35	110.12	120.72
1	A	163	SER	C-N-CA	-6.35	110.12	120.72
1	A	299	ILE	CA-C-N	-6.33	111.68	122.56
1	A	299	ILE	C-N-CA	-6.33	111.68	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	A	134	ASN	N-CA-C	6.32	120.19	112.23
1	A	117	TRP	N-CA-C	6.30	120.21	111.90
1	A	197	HIS	CA-C-N	-6.26	111.53	120.42
1	A	197	HIS	C-N-CA	-6.26	111.53	120.42
1	A	84	TYR	N-CA-C	6.26	118.66	111.02
1	A	326	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	200	ALA	N-CA-C	6.22	118.61	111.02
1	A	314	ASP	CA-C-N	-6.17	112.81	122.49
1	A	314	ASP	C-N-CA	-6.17	112.81	122.49
1	A	41	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	302	SER	N-CA-C	6.15	118.30	109.14
1	A	269	THR	CA-C-N	-6.13	116.80	123.30
1	A	269	THR	C-N-CA	-6.13	116.80	123.30
1	A	204	ALA	N-CA-C	6.12	117.61	111.07
1	A	129	VAL	N-CA-C	6.12	116.29	110.42
1	A	319	GLU	N-CA-C	6.08	118.71	111.71
1	A	144	PHE	N-CA-C	6.07	121.43	113.30
1	A	38	LEU	CB-CA-C	6.07	122.12	110.17
1	A	45	GLU	CA-C-O	6.06	126.08	119.24
1	A	180	ILE	N-CA-C	6.04	117.71	108.71
1	A	105	HIS	N-CA-C	6.04	117.86	111.28
1	A	249	TYR	N-CA-C	6.03	118.38	111.02
1	A	208	GLY	CA-C-N	-6.02	112.86	122.50
1	A	208	GLY	C-N-CA	-6.02	112.86	122.50
1	A	254	GLN	CA-C-N	-6.02	113.56	122.83
1	A	254	GLN	C-N-CA	-6.02	113.56	122.83
1	A	260	GLU	N-CA-C	5.99	118.95	108.52
1	A	88	GLU	N-CA-C	5.98	118.57	111.33
1	A	82	ILE	CA-C-N	-5.93	112.73	120.44
1	A	82	ILE	C-N-CA	-5.93	112.73	120.44
1	A	335	LEU	CA-C-N	-5.93	113.86	119.85
1	A	335	LEU	C-N-CA	-5.93	113.86	119.85
1	A	150	SER	N-CA-C	5.89	118.81	109.50
1	A	340	LYS	N-CA-C	5.85	117.33	111.07
1	A	351	TYR	N-CA-C	5.84	120.11	113.15
1	A	214	HIS	CB-CA-C	-5.83	101.81	110.67
1	A	186	GLU	N-CA-C	5.82	121.40	113.37
1	A	160	SER	N-CA-C	5.81	118.36	111.33
1	A	176	THR	CA-C-N	-5.80	114.89	122.37
1	A	176	THR	C-N-CA	-5.80	114.89	122.37
1	A	127	ASP	N-CA-C	5.79	117.26	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	LYS	N-CA-C	5.79	118.33	111.33
1	A	62	LEU	CA-C-O	5.78	126.87	120.63
1	A	189	GLU	N-CA-C	5.77	118.85	110.42
1	A	33	ARG	N-CA-C	5.75	119.77	112.87
1	A	26	THR	N-CA-C	5.73	117.53	111.28
1	A	76	ARG	CA-C-N	-5.72	110.49	121.94
1	A	76	ARG	C-N-CA	-5.72	110.49	121.94
1	A	268	LEU	N-CA-C	5.71	118.28	111.71
1	A	224	VAL	N-CA-C	5.70	115.78	110.42
1	A	258	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	31	GLY	CA-C-N	-5.65	112.76	120.44
1	A	31	GLY	C-N-CA	-5.65	112.76	120.44
1	A	256	ASN	CA-C-N	-5.64	112.86	120.82
1	A	256	ASN	C-N-CA	-5.64	112.86	120.82
1	A	175	GLN	CA-CB-CG	5.63	125.37	114.10
1	A	272	TRP	N-CA-C	5.63	117.70	108.52
1	A	9	LYS	CA-C-N	-5.62	113.91	119.92
1	A	9	LYS	C-N-CA	-5.62	113.91	119.92
1	A	76	ARG	CB-CA-C	-5.61	101.53	110.84
1	A	325	LEU	CB-CA-C	5.59	120.08	110.79
1	A	306	THR	N-CA-C	5.57	117.36	111.28
1	A	304	LEU	N-CA-C	5.56	117.34	111.28
1	A	305	ASP	N-CA-C	5.55	118.09	111.71
1	A	175	GLN	N-CA-C	5.54	118.66	108.58
1	A	127	ASP	CA-C-N	-5.49	110.88	121.58
1	A	127	ASP	C-N-CA	-5.49	110.88	121.58
1	A	153	CYS	N-CA-C	5.48	117.67	108.73
1	A	271	ALA	CA-C-N	-5.44	115.43	123.05
1	A	271	ALA	C-N-CA	-5.44	115.43	123.05
1	A	258	HIS	N-CA-C	5.44	117.57	109.25
1	A	106	LEU	N-CA-C	5.43	119.53	113.01
1	A	77	ASP	N-CA-C	5.43	119.77	113.20
1	A	15	HIS	CG-CD2-NE2	5.42	112.62	107.20
1	A	337	GLU	CA-C-N	-5.39	113.26	120.54
1	A	337	GLU	C-N-CA	-5.39	113.26	120.54
1	A	73	ALA	CA-C-N	-5.39	110.84	121.41
1	A	73	ALA	C-N-CA	-5.39	110.84	121.41
1	A	288	VAL	CA-CB-CG2	5.38	119.55	110.40
1	A	280	VAL	N-CA-C	5.34	120.45	109.34
1	A	30	TYR	N-CA-C	5.34	118.25	111.69
1	A	91	ALA	N-CA-C	5.33	117.50	111.11
1	A	259	PHE	N-CA-C	5.30	117.88	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLN	CA-C-N	-5.29	112.95	122.15
1	A	119	GLN	C-N-CA	-5.29	112.95	122.15
1	A	187	THR	CA-C-O	5.28	124.62	118.97
1	A	305	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	156	ARG	N-CA-C	5.26	117.70	111.33
1	A	317	PHE	N-CA-C	5.26	118.26	110.48
1	A	202	ALA	N-CA-C	5.24	117.07	111.36
1	A	221	ALA	N-CA-C	5.24	119.16	112.34
1	A	263	PRO	CB-CA-C	5.24	120.21	111.56
1	A	285	ASN	CA-C-N	-5.23	113.56	122.56
1	A	285	ASN	C-N-CA	-5.23	113.56	122.56
1	A	299	ILE	N-CA-C	5.22	116.69	111.00
1	A	88	GLU	CB-CG-CD	-5.21	103.74	112.60
1	A	143	ASP	N-CA-C	5.21	117.86	111.82
1	A	26	THR	CA-C-N	-5.20	114.01	120.56
1	A	26	THR	C-N-CA	-5.20	114.01	120.56
1	A	178	VAL	N-CA-C	5.20	118.72	113.47
1	A	21	ALA	CA-C-O	5.19	127.59	121.78
1	A	118	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	206	LYS	CA-C-O	5.18	125.92	120.42
1	A	272	TRP	CD2-CE2-CZ2	-5.18	117.22	122.40
1	A	66	ASP	N-CA-C	5.16	117.58	111.33
1	A	312	LYS	CA-C-N	-5.16	112.99	121.92
1	A	312	LYS	C-N-CA	-5.16	112.99	121.92
1	A	142	ARG	CA-CB-CG	-5.14	103.81	114.10
1	A	226	GLU	N-CA-C	5.14	117.55	111.33
1	A	33	ARG	CD-NE-CZ	5.13	131.59	124.40
1	A	123	ASP	N-CA-C	5.11	119.21	112.92
1	A	336	PRO	CA-C-N	-5.10	112.94	120.28
1	A	336	PRO	C-N-CA	-5.10	112.94	120.28
1	A	48	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	261	ILE	N-CA-C	5.08	116.12	109.21
1	A	212	THR	CA-C-N	-5.07	116.06	123.06
1	A	212	THR	C-N-CA	-5.07	116.06	123.06
1	A	235	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	174	GLU	N-CA-C	5.07	121.59	110.80
1	A	225	LYS	N-CA-C	5.05	119.70	111.37
1	A	278	HIS	CA-C-N	-5.04	113.47	120.38
1	A	278	HIS	C-N-CA	-5.04	113.47	120.38
1	A	188	ILE	CA-CB-CG1	5.04	118.97	110.40
1	A	53	ASP	CA-C-O	5.04	125.12	119.18
1	A	151	ILE	CA-C-N	-5.04	115.15	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	C-N-CA	-5.04	115.15	122.65
1	A	8	ASP	N-CA-CB	5.02	117.88	110.49
1	A	253	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	226	GLU	CA-C-O	5.01	126.04	120.63

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain
1	A	201	TYR	Sidechain
1	A	267	TYR	Sidechain
1	A	282	ARG	Sidechain
1	A	324	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	348	TYR	Sidechain
1	A	36	ILE	Peptide
1	A	37	ALA	Peptide
1	A	67	TYR	Sidechain
1	A	68	TYR	Sidechain
1	A	84	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	102	0
2	A	1	0	0	0	0
3	A	24	0	21	0	0
4	A	121	0	0	22	0
All	All	2935	0	2764	102	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 18.

All (102) 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:154:CYS:SG	1:A:180:ILE:HD11	2.23	0.78
1:A:152:LEU:HD23	1:A:169:CYS:SG	2.25	0.77
1:A:263:PRO:HB2	1:A:310:MET:HE1	1.64	0.77
1:A:83:ALA:HB1	1:A:137:LEU:HG	1.68	0.74
1:A:261:ILE:O	1:A:293:ASN:HB2	1.88	0.74
1:A:180:ILE:HG12	1:A:181:ASP:N	2.09	0.68
1:A:131:SER:HA	1:A:134:ASN:OD1	1.94	0.67
1:A:80:LYS:HA	4:A:441:HOH:O	1.93	0.67
1:A:249:TYR:CE2	1:A:283:PHE:HE1	2.14	0.65
1:A:166:VAL:HG11	1:A:203:GLU:HB3	1.78	0.64
1:A:174:GLU:O	1:A:176:THR:HA	1.99	0.62
1:A:180:ILE:HD13	1:A:201:TYR:CE1	2.34	0.62
1:A:180:ILE:HD13	1:A:201:TYR:CZ	2.34	0.62
1:A:38:LEU:HB2	1:A:39:PRO:HD3	1.82	0.60
1:A:278:HIS:O	1:A:281:ILE:HG13	2.01	0.60
1:A:302:SER:HB2	1:A:306:THR:OG1	2.01	0.60
1:A:133:VAL:HA	4:A:441:HOH:O	2.00	0.60
1:A:312:LYS:HE2	1:A:313:LYS:HZ1	1.67	0.60
1:A:352:ARG:HG2	1:A:352:ARG:HH21	1.66	0.60
1:A:158:GLN:HG2	1:A:161:TRP:CE2	2.37	0.59
1:A:15:HIS:O	1:A:15:HIS:CD2	2.56	0.59
1:A:101:ARG:HB3	1:A:151:ILE:HB	1.84	0.59
1:A:292:LEU:HD13	1:A:325:LEU:HD11	1.83	0.59
1:A:56:LEU:HD13	1:A:60:ASP:HB3	1.85	0.59
1:A:237:GLY:HA2	1:A:260:GLU:HB2	1.85	0.59
1:A:281:ILE:HG22	1:A:284:LYS:HE3	1.84	0.59
1:A:241:HIS:O	1:A:244:GLU:HG2	2.03	0.58
1:A:310:MET:HG3	4:A:500:HOH:O	2.03	0.58
1:A:312:LYS:HE2	1:A:313:LYS:NZ	2.19	0.58
1:A:260:GLU:HA	4:A:516:HOH:O	2.02	0.58
1:A:50:ILE:HG22	4:A:413:HOH:O	2.03	0.58
1:A:15:HIS:O	1:A:15:HIS:HD2	1.86	0.57
1:A:185:ASP:OD1	1:A:187:THR:HB	2.05	0.56
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.70	0.56
1:A:166:VAL:HB	4:A:448:HOH:O	2.07	0.54
1:A:235:ARG:HD2	1:A:260:GLU:OE1	2.08	0.53
1:A:15:HIS:HA	1:A:101:ARG:NH2	2.23	0.52
1:A:46:LEU:HD13	4:A:509:HOH:O	2.07	0.52
1:A:63:ALA:HB1	4:A:453:HOH:O	2.09	0.51
1:A:313:LYS:NZ	1:A:313:LYS:HB3	2.26	0.51
1:A:83:ALA:HB2	1:A:133:VAL:HG13	1.93	0.51
1:A:152:LEU:CD2	1:A:169:CYS:SG	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:CE2	1:A:283:PHE:CE1	2.98	0.50
1:A:101:ARG:HB2	1:A:153:CYS:SG	2.52	0.50
1:A:31:GLY:HA3	1:A:38:LEU:HD22	1.94	0.50
1:A:178:VAL:O	1:A:210:HIS:HB2	2.12	0.49
1:A:308:TYR:O	1:A:312:LYS:HB2	2.12	0.49
1:A:259:PHE:HB2	4:A:427:HOH:O	2.12	0.48
1:A:117:TRP:HA	4:A:481:HOH:O	2.13	0.48
1:A:181:ASP:HA	1:A:212:THR:O	2.14	0.48
1:A:260:GLU:HG3	4:A:516:HOH:O	2.13	0.48
1:A:166:VAL:HG21	1:A:200:ALA:HA	1.95	0.48
1:A:39:PRO:HG2	1:A:49:ILE:HD11	1.96	0.47
1:A:46:LEU:HD12	4:A:440:HOH:O	2.13	0.47
1:A:293:ASN:HB3	4:A:420:HOH:O	2.13	0.47
1:A:235:ARG:HD3	1:A:258:HIS:CD2	2.50	0.47
1:A:173:ARG:O	1:A:175:GLN:N	2.48	0.47
1:A:55:PRO:HA	1:A:268:LEU:O	2.14	0.46
1:A:239:GLY:O	1:A:242:THR:HG23	2.16	0.46
1:A:249:TYR:HE2	1:A:283:PHE:CE1	2.32	0.46
1:A:224:VAL:HG21	1:A:242:THR:HG22	1.98	0.45
1:A:63:ALA:O	1:A:66:ASP:HB2	2.16	0.45
1:A:39:PRO:HB3	4:A:464:HOH:O	2.16	0.45
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.52	0.45
1:A:9:LYS:HB3	1:A:9:LYS:HE3	1.85	0.45
1:A:188:ILE:HG21	1:A:188:ILE:HD13	1.75	0.44
1:A:61:PHE:CE2	1:A:65:PHE:HE1	2.36	0.44
1:A:180:ILE:HD12	4:A:472:HOH:O	2.17	0.44
1:A:213:VAL:N	1:A:233:THR:HG21	2.32	0.44
1:A:250:ASN:O	1:A:253:ARG:HG3	2.17	0.44
1:A:44:GLU:H	1:A:44:GLU:CD	2.26	0.44
1:A:69:MET:HE1	1:A:107:LEU:HD12	2.00	0.43
1:A:258:HIS:HA	1:A:289:ASN:O	2.18	0.43
1:A:113:GLU:HA	1:A:114:PRO:HA	1.76	0.43
1:A:317:PHE:HB2	4:A:468:HOH:O	2.18	0.43
1:A:22:ILE:HD13	1:A:72:ILE:HD13	2.00	0.43
1:A:117:TRP:HZ3	4:A:482:HOH:O	2.02	0.42
1:A:313:LYS:HB3	1:A:313:LYS:HZ2	1.83	0.42
1:A:330:ALA:O	1:A:340:LYS:HD2	2.19	0.42
1:A:33:ARG:HH21	1:A:33:ARG:HB3	1.83	0.42
1:A:238:HIS:HB3	1:A:240:TYR:CZ	2.55	0.42
1:A:27:ILE:HG21	1:A:68:TYR:HB2	2.02	0.42
1:A:158:GLN:HG2	1:A:161:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HH21	1:A:33:ARG:CB	2.33	0.41
1:A:128:GLU:O	1:A:132:LEU:HD12	2.20	0.41
1:A:288:VAL:HG22	4:A:478:HOH:O	2.20	0.41
1:A:312:LYS:HB3	1:A:313:LYS:NZ	2.36	0.41
1:A:97:TYR:OH	1:A:335:LEU:HD13	2.20	0.41
1:A:201:TYR:HD2	1:A:211:ARG:HD2	1.85	0.41
1:A:21:ALA:HB2	1:A:297:PRO:HD2	2.02	0.41
1:A:236:LEU:O	1:A:260:GLU:HB2	2.20	0.41
1:A:120:ALA:HB1	4:A:423:HOH:O	2.20	0.41
1:A:21:ALA:HB3	4:A:497:HOH:O	2.20	0.41
1:A:178:VAL:HG22	4:A:495:HOH:O	2.21	0.41
1:A:33:ARG:HB3	1:A:33:ARG:NH2	2.36	0.41
1:A:57:THR:OG1	1:A:59:PRO:HD2	2.21	0.41
1:A:228:VAL:HG22	4:A:475:HOH:O	2.20	0.41
1:A:262:CYS:SG	1:A:295:ASP:HB2	2.62	0.40
1:A:278:HIS:HD2	1:A:280:VAL:HG12	1.86	0.40
1:A:28:LEU:O	1:A:32:LYS:HG2	2.22	0.40
1:A:27:ILE:HD13	1:A:68:TYR:CB	2.51	0.40
1:A:238:HIS:HB3	1:A:240:TYR:CE2	2.56	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%)	305 (88%)	35 (10%)	7 (2%)	6 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
1	A	174	GLU

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	186	GLU
1	A	238	HIS
1	A	38	LEU
1	A	173	ARG

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	8	ASP
1	A	11	LYS
1	A	25	GLU
1	A	28	LEU
1	A	32	LYS
1	A	33	ARG
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	57	THR
1	A	62	LEU
1	A	75	CYS
1	A	80	LYS
1	A	89	MET
1	A	101	ARG
1	A	107	LEU
1	A	113	GLU
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	148	VAL
1	A	152	LEU
1	A	160	SER
1	A	166	VAL
1	A	168	LEU
1	A	174	GLU
1	A	177	VAL
1	A	180	ILE
1	A	187	THR
1	A	188	ILE
1	A	192	SER
1	A	193	LEU
1	A	198	VAL
1	A	199	GLN
1	A	205	VAL
1	A	218	VAL
1	A	222	ASN
1	A	225	LYS
1	A	233	THR
1	A	242	THR
1	A	243	LEU
1	A	253	ARG
1	A	266	SER
1	A	267	TYR
1	A	268	LEU
1	A	277	GLU
1	A	280	VAL
1	A	281	ILE
1	A	288	VAL
1	A	294	THR
1	A	298	LEU
1	A	305	ASP
1	A	312	LYS
1	A	313	LYS
1	A	317	PHE
1	A	319	GLU
1	A	325	LEU
1	A	335	LEU
1	A	344	LEU
1	A	347	LEU
1	A	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	118	ASN
1	A	175	GLN
1	A	197	HIS
1	A	241	HIS
1	A	256	ASN
1	A	285	ASN
1	A	309	GLN

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	FR6	A	1	-	25,26,26	1.57	4 (16%)	29,36,36	1.36	4 (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	FR6	A	1	-	-	4/17/17/17	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	FR6	C1-N2	4.23	1.47	1.37
3	A	1	FR6	C5-N4	3.43	1.48	1.39
3	A	1	FR6	C7-C4	2.10	1.41	1.36
3	A	1	FR6	C1-C5	-2.00	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	FR6	O9-C8-C5	4.65	124.72	120.25
3	A	1	FR6	C2-C28-C27	-2.36	117.63	123.01
3	A	1	FR6	C1-N2-C3	2.23	107.84	106.37
3	A	1	FR6	O9-C8-N10	-2.03	118.34	122.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

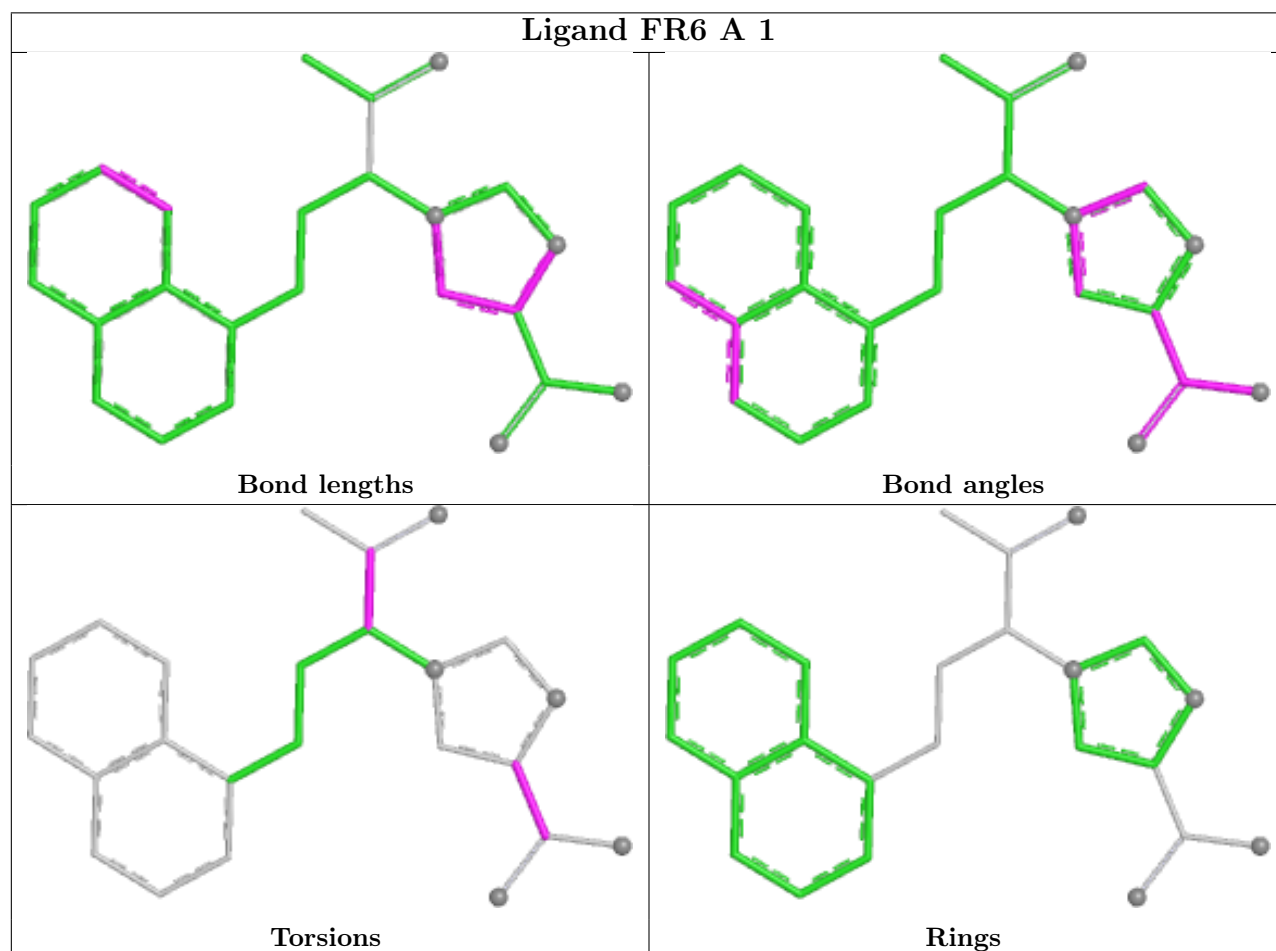
Mol	Chain	Res	Type	Atoms
3	A	1	FR6	N2-C13-C14-C9
3	A	1	FR6	N4-C5-C8-O9
3	A	1	FR6	N4-C5-C8-N10
3	A	1	FR6	C1-C5-C8-N10

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%)	-0.19	0 100 100	7, 20, 35, 44	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

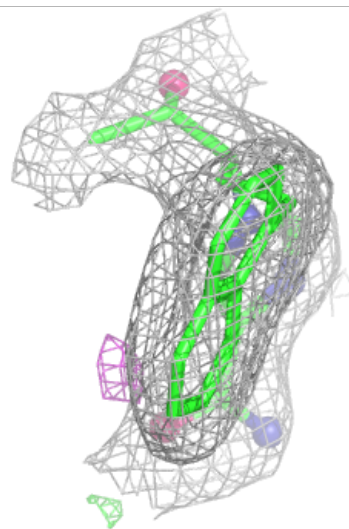
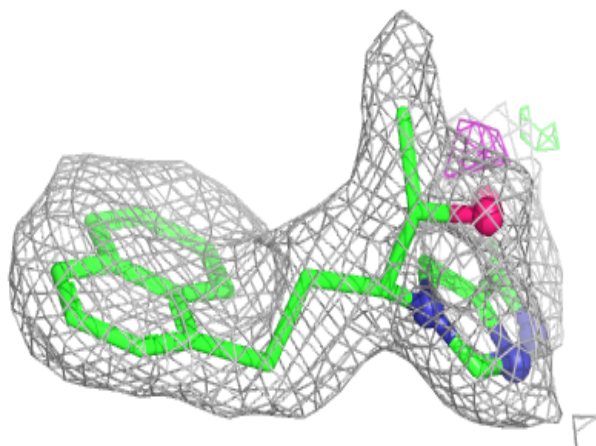
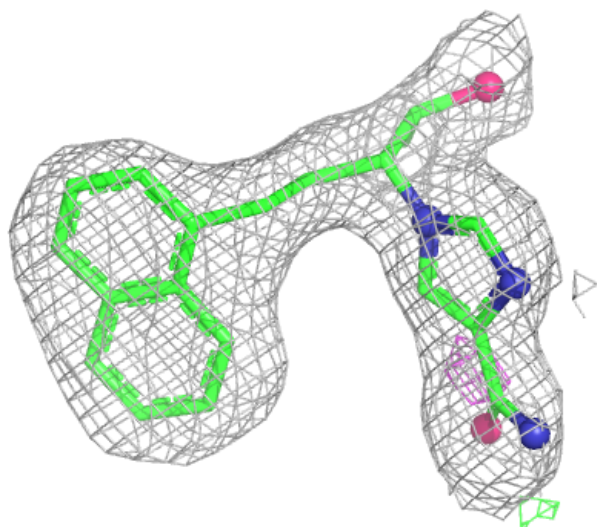
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	FR6	A	1	24/24	0.91	0.10	10,16,20,21	0
2	ZN	A	400	1/1	0.97	0.03	16,16,16,16	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.

Electron density around FR6 A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.