



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 PM UTC

PDB ID : 1KRM / pdb_00001krm
Title : Crystal structure of bovine adenosine deaminase complexed with 6-hydroxyl-1,6-dihydropurine riboside
Authors : Kinoshita, T.
Deposited on : 2002-01-10
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

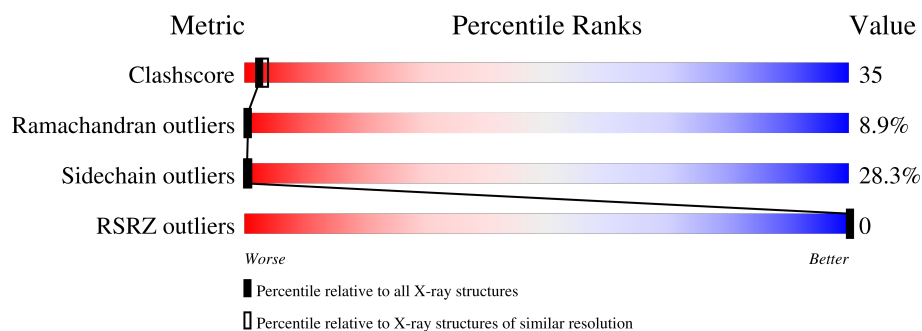
1 Overall quality at a glance

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	15% 34% 35% 15% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3298 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
			Total	C	N	O	S			
1	A	349	2788	1773	470	533	12	0	0	0

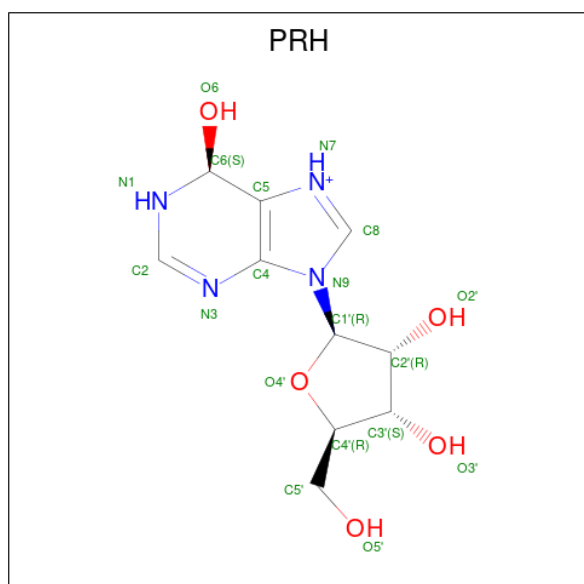
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	GLN	conflict	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 6-HYDROXY-1,6-DIHYDRO PURINE NUCLEOSIDE (CCD ID: PRH) (formula: C₁₀H₁₅N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	4	5		

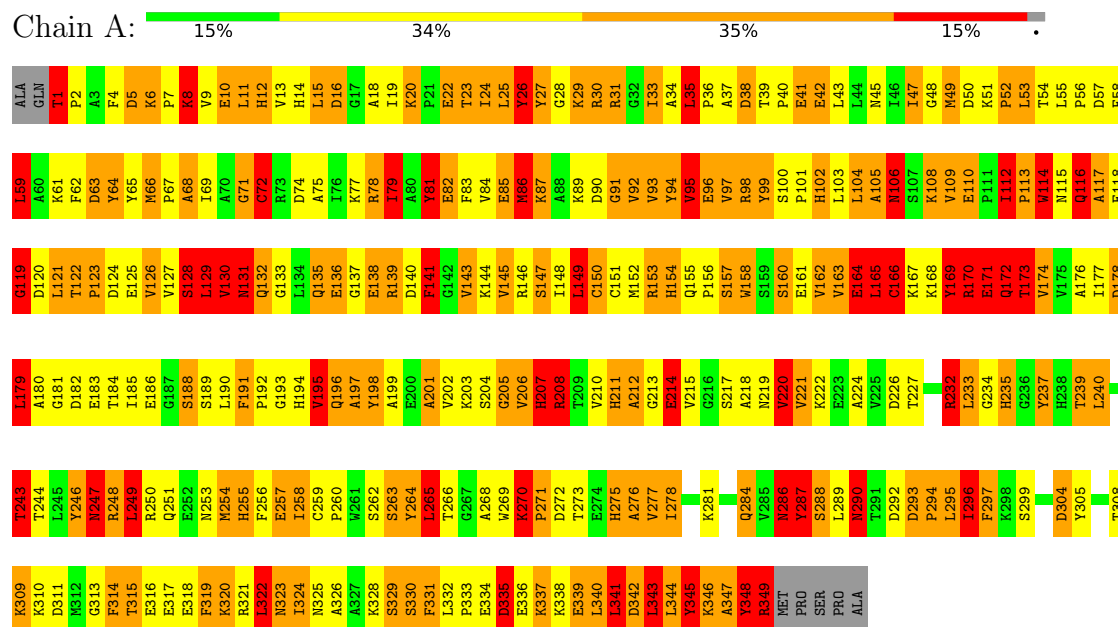
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	490	Total	O	0	0
			490	490		

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	80.03Å 80.03Å 141.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	75.4 (8.00-2.50) 71.9 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.94Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.198 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 98.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3298	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: PRH, 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	1.44	14/2852 (0.5%)	2.84	344/3866 (8.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	VAL	CA-CB	-7.19	1.45	1.54
1	A	112	ILE	CA-C	6.45	1.59	1.52
1	A	211	HIS	CE1-NE2	6.14	1.38	1.32
1	A	255	HIS	CG-ND1	-5.74	1.31	1.38
1	A	12	HIS	CG-CD2	5.68	1.42	1.35
1	A	221	VAL	CA-CB	-5.67	1.47	1.54
1	A	102	HIS	CG-ND1	-5.58	1.32	1.38
1	A	244	THR	N-CA	5.57	1.53	1.46
1	A	154	HIS	ND1-CE1	5.46	1.38	1.32
1	A	177	ILE	CA-CB	-5.34	1.48	1.54
1	A	208	ARG	CA-C	-5.31	1.46	1.52
1	A	207	HIS	CE1-NE2	5.24	1.37	1.32
1	A	12	HIS	CE1-NE2	5.12	1.37	1.32
1	A	39	THR	CA-C	-5.10	1.47	1.53

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CA-CB-CG	13.08	125.68	112.60
1	A	270	LYS	CB-CA-C	11.80	125.08	108.68
1	A	119	GLY	CA-C-N	-11.70	104.53	120.44
1	A	119	GLY	C-N-CA	-11.70	104.53	120.44
1	A	72	CYS	N-CA-C	11.62	135.56	110.80
1	A	117	ALA	N-CA-C	11.44	126.45	109.07
1	A	272	ASP	CA-CB-CG	-11.08	101.52	112.60
1	A	121	LEU	N-CA-C	10.52	125.06	109.59
1	A	95	VAL	N-CA-C	10.45	123.53	108.48
1	A	45	ASN	CA-CB-CG	-10.39	102.21	112.60
1	A	50	ASP	N-CA-C	10.31	126.82	114.04
1	A	92	VAL	N-CA-C	10.31	123.10	108.36
1	A	106	ASN	CA-CB-CG	-10.30	102.30	112.60
1	A	91	GLY	CA-C-N	-10.21	110.06	122.93
1	A	91	GLY	C-N-CA	-10.21	110.06	122.93
1	A	78	ARG	CD-NE-CZ	-10.15	110.19	124.40
1	A	323	ASN	CA-CB-CG	-9.99	102.61	112.60
1	A	272	ASP	N-CA-C	9.96	125.00	113.15
1	A	321	ARG	CA-C-N	-9.89	107.03	120.28
1	A	321	ARG	C-N-CA	-9.89	107.03	120.28
1	A	49	MET	CA-C-N	-9.82	105.04	122.42
1	A	49	MET	C-N-CA	-9.82	105.04	122.42
1	A	324	ILE	N-CA-C	9.50	119.54	110.42
1	A	227	THR	N-CA-C	9.35	123.19	111.69
1	A	321	ARG	N-CA-C	9.34	122.45	111.71
1	A	221	VAL	N-CA-C	9.20	119.25	110.42
1	A	335	ASP	CA-CB-CG	9.04	121.64	112.60
1	A	290	ASN	CA-C-N	-8.95	106.86	122.79
1	A	290	ASN	C-N-CA	-8.95	106.86	122.79
1	A	219	ASN	CA-CB-CG	-8.85	103.75	112.60
1	A	95	VAL	CA-C-N	-8.81	111.05	122.77
1	A	95	VAL	C-N-CA	-8.81	111.05	122.77
1	A	276	ALA	N-CA-C	8.81	120.89	111.28
1	A	40	PRO	CA-C-N	-8.76	107.85	120.29
1	A	40	PRO	C-N-CA	-8.76	107.85	120.29
1	A	308	THR	N-CA-C	8.66	124.24	112.90
1	A	204	SER	N-CA-C	8.61	123.44	111.56
1	A	72	CYS	CA-CB-SG	-8.53	94.77	114.40
1	A	13	VAL	CA-C-N	-8.51	111.13	123.05
1	A	13	VAL	C-N-CA	-8.51	111.13	123.05
1	A	41	GLU	N-CA-C	8.41	120.53	111.36
1	A	145	VAL	N-CA-C	8.40	120.03	107.51
1	A	184	THR	CA-C-N	-8.36	110.14	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	THR	C-N-CA	-8.36	110.14	122.01
1	A	235	HIS	CA-CB-CG	8.27	122.07	113.80
1	A	69	ILE	CA-C-N	-8.18	108.89	121.66
1	A	69	ILE	C-N-CA	-8.18	108.89	121.66
1	A	131	ASN	CA-C-N	-8.15	109.54	120.54
1	A	131	ASN	C-N-CA	-8.15	109.54	120.54
1	A	105	ALA	O-C-N	-8.13	114.59	123.04
1	A	348	TYR	N-CA-C	8.11	123.24	112.13
1	A	182	ASP	CB-CA-C	-8.04	94.42	110.42
1	A	102	HIS	CA-CB-CG	-8.04	105.76	113.80
1	A	128	SER	N-CA-C	7.95	122.08	112.38
1	A	266	THR	CB-CA-C	-7.88	97.71	110.79
1	A	214	GLU	CA-C-N	-7.82	112.56	122.26
1	A	214	GLU	C-N-CA	-7.82	112.56	122.26
1	A	143	VAL	CA-C-N	-7.80	111.77	122.30
1	A	143	VAL	C-N-CA	-7.80	111.77	122.30
1	A	133	GLY	N-CA-C	7.79	123.04	114.40
1	A	265	LEU	N-CA-C	7.78	121.26	111.69
1	A	169	TYR	CA-C-N	-7.77	112.08	122.42
1	A	169	TYR	C-N-CA	-7.77	112.08	122.42
1	A	145	VAL	CA-C-N	-7.76	110.37	122.87
1	A	145	VAL	C-N-CA	-7.76	110.37	122.87
1	A	31	ARG	CA-C-N	-7.76	115.08	123.30
1	A	31	ARG	C-N-CA	-7.76	115.08	123.30
1	A	8	LYS	N-CA-C	7.73	127.27	110.80
1	A	197	ALA	CA-C-N	-7.73	109.80	120.38
1	A	197	ALA	C-N-CA	-7.73	109.80	120.38
1	A	275	HIS	CA-C-N	-7.66	110.02	120.28
1	A	275	HIS	C-N-CA	-7.66	110.02	120.28
1	A	150	CYS	CB-CA-C	-7.63	98.36	110.79
1	A	177	ILE	N-CA-C	7.61	119.56	108.53
1	A	94	TYR	CA-C-N	-7.55	112.65	123.06
1	A	94	TYR	C-N-CA	-7.55	112.65	123.06
1	A	335	ASP	N-CA-CB	-7.54	97.75	110.49
1	A	174	VAL	N-CA-C	7.43	118.57	108.17
1	A	158	TRP	CB-CA-C	-7.41	96.44	110.67
1	A	179	LEU	N-CA-C	7.39	120.57	108.52
1	A	188	SER	CB-CA-C	-7.37	99.02	110.81
1	A	232	ARG	CA-C-N	-7.35	112.38	122.30
1	A	232	ARG	C-N-CA	-7.35	112.38	122.30
1	A	249	LEU	N-CA-CB	7.33	121.17	110.26
1	A	292	ASP	CA-C-N	-7.26	115.04	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ASP	C-N-CA	-7.26	115.04	122.74
1	A	337	LYS	CA-C-N	-7.25	111.01	120.44
1	A	337	LYS	C-N-CA	-7.25	111.01	120.44
1	A	218	ALA	CA-C-O	7.20	128.21	119.49
1	A	171	GLU	N-CA-C	7.18	126.10	110.80
1	A	271	PRO	CA-C-N	-7.18	107.95	122.31
1	A	271	PRO	C-N-CA	-7.18	107.95	122.31
1	A	178	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	323	ASN	CA-C-N	-7.16	111.53	120.56
1	A	323	ASN	C-N-CA	-7.16	111.53	120.56
1	A	272	ASP	CA-C-N	-7.16	110.56	121.86
1	A	272	ASP	C-N-CA	-7.16	110.56	121.86
1	A	113	PRO	N-CA-C	7.13	122.40	111.57
1	A	170	ARG	N-CA-C	7.11	119.86	108.41
1	A	114	TRP	N-CA-C	7.08	125.88	110.80
1	A	299	SER	N-CA-C	7.06	117.91	108.38
1	A	8	LYS	CB-CA-C	-7.04	96.42	110.42
1	A	125	GLU	N-CA-C	7.01	119.96	111.40
1	A	207	HIS	CA-C-N	-7.00	110.73	122.29
1	A	207	HIS	C-N-CA	-7.00	110.73	122.29
1	A	339	GLU	N-CA-C	7.00	121.57	112.89
1	A	93	VAL	CB-CA-C	-6.97	100.97	112.26
1	A	314	PHE	N-CA-C	6.94	120.17	108.02
1	A	254	MET	CA-C-N	-6.94	111.65	121.99
1	A	254	MET	C-N-CA	-6.94	111.65	121.99
1	A	198	TYR	CA-C-N	-6.93	109.47	121.66
1	A	198	TYR	C-N-CA	-6.93	109.47	121.66
1	A	158	TRP	N-CA-C	6.86	119.77	111.82
1	A	308	THR	CA-C-N	-6.84	109.62	121.66
1	A	308	THR	C-N-CA	-6.84	109.62	121.66
1	A	186	GLU	CA-C-N	-6.83	112.48	122.46
1	A	186	GLU	C-N-CA	-6.83	112.48	122.46
1	A	79	ILE	CA-CB-CG1	6.79	121.95	110.40
1	A	183	GLU	CA-C-O	6.79	127.97	120.63
1	A	201	ALA	N-CA-C	6.79	118.37	110.97
1	A	304	ASP	N-CA-C	6.74	119.24	111.02
1	A	50	ASP	CA-C-N	-6.72	110.95	120.49
1	A	50	ASP	C-N-CA	-6.72	110.95	120.49
1	A	309	LYS	CA-C-N	-6.72	109.64	122.53
1	A	309	LYS	C-N-CA	-6.72	109.64	122.53
1	A	170	ARG	CA-C-N	6.69	134.32	121.54
1	A	170	ARG	C-N-CA	6.69	134.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	GLU	N-CA-C	6.68	119.17	111.02
1	A	172	GLN	CA-C-N	6.66	130.54	119.35
1	A	172	GLN	C-N-CA	6.66	130.54	119.35
1	A	103	LEU	N-CA-C	6.61	120.44	112.38
1	A	97	VAL	CB-CA-C	-6.60	101.84	111.68
1	A	248	ARG	CA-C-N	-6.60	107.58	121.64
1	A	248	ARG	C-N-CA	-6.60	107.58	121.64
1	A	102	HIS	N-CA-C	6.58	119.01	111.11
1	A	284	GLN	CA-CB-CG	6.57	127.24	114.10
1	A	105	ALA	CA-C-N	6.57	133.52	121.70
1	A	105	ALA	C-N-CA	6.57	133.52	121.70
1	A	154	HIS	N-CA-C	6.56	121.11	113.18
1	A	193	GLY	N-CA-C	6.54	120.56	112.64
1	A	152	MET	N-CA-CB	-6.54	100.11	110.77
1	A	38	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	336	GLU	N-CA-C	6.48	120.05	111.75
1	A	47	ILE	CA-C-N	-6.42	112.36	121.54
1	A	47	ILE	C-N-CA	-6.42	112.36	121.54
1	A	166	CYS	CB-CA-C	-6.42	100.08	110.74
1	A	112	ILE	N-CA-C	6.42	122.74	108.88
1	A	22	GLU	CA-C-N	-6.41	110.56	120.31
1	A	22	GLU	C-N-CA	-6.41	110.56	120.31
1	A	237	TYR	N-CA-C	6.41	118.84	111.02
1	A	112	ILE	CA-C-N	-6.39	114.05	120.31
1	A	112	ILE	C-N-CA	-6.39	114.05	120.31
1	A	147	SER	CA-C-N	6.39	131.87	122.99
1	A	147	SER	C-N-CA	6.39	131.87	122.99
1	A	215	VAL	N-CA-C	6.38	117.59	111.91
1	A	135	GLN	CA-CB-CG	-6.38	101.33	114.10
1	A	89	LYS	CA-C-N	-6.36	109.40	120.97
1	A	89	LYS	C-N-CA	-6.36	109.40	120.97
1	A	27	TYR	N-CA-C	6.35	119.01	111.71
1	A	42	GLU	CA-C-N	-6.34	111.98	120.79
1	A	42	GLU	C-N-CA	-6.34	111.98	120.79
1	A	277	VAL	CA-C-N	-6.34	109.90	120.30
1	A	277	VAL	C-N-CA	-6.34	109.90	120.30
1	A	74	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	181	GLY	CA-C-O	-6.33	115.87	122.01
1	A	329	SER	N-CA-C	6.32	120.73	112.89
1	A	124	ASP	CA-CB-CG	-6.30	106.30	112.60
1	A	116	GLN	CA-C-N	-6.28	110.89	121.75
1	A	116	GLN	C-N-CA	-6.28	110.89	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	N-CA-C	6.24	124.09	110.80
1	A	122	THR	N-CA-C	6.24	119.32	110.40
1	A	188	SER	N-CA-C	6.22	118.58	111.11
1	A	93	VAL	N-CA-C	6.22	118.86	111.09
1	A	293	ASP	CB-CA-C	-6.20	100.92	111.15
1	A	296	ILE	CA-CB-CG1	6.15	120.86	110.40
1	A	99	TYR	N-CA-C	6.13	116.65	108.38
1	A	288	SER	N-CA-C	6.13	119.51	108.48
1	A	218	ALA	CA-C-N	-6.12	112.08	120.28
1	A	218	ALA	C-N-CA	-6.12	112.08	120.28
1	A	290	ASN	N-CA-C	6.12	117.84	108.42
1	A	322	LEU	N-CA-C	6.12	117.95	111.28
1	A	130	VAL	CA-C-N	-6.11	112.28	120.54
1	A	130	VAL	C-N-CA	-6.11	112.28	120.54
1	A	284	GLN	N-CA-C	6.11	119.85	111.54
1	A	331	PHE	N-CA-C	6.11	119.17	110.68
1	A	330	SER	CB-CA-C	-6.11	98.27	110.42
1	A	20	LYS	N-CA-C	6.05	117.44	109.93
1	A	195	VAL	CA-C-N	-6.05	112.37	120.54
1	A	195	VAL	C-N-CA	-6.05	112.37	120.54
1	A	59	LEU	N-CA-C	6.05	120.27	113.01
1	A	5	ASP	CA-CB-CG	-6.03	106.57	112.60
1	A	247	ASN	CA-C-O	6.01	126.76	119.31
1	A	152	MET	CG-SD-CE	-5.99	87.72	100.90
1	A	263	SER	N-CA-C	5.98	118.28	111.11
1	A	167	LYS	CA-C-N	-5.97	111.59	121.92
1	A	167	LYS	C-N-CA	-5.97	111.59	121.92
1	A	166	CYS	N-CA-CB	5.97	119.51	109.78
1	A	151	CYS	CA-C-N	-5.96	113.57	122.39
1	A	151	CYS	C-N-CA	-5.96	113.57	122.39
1	A	224	ALA	N-CA-C	5.96	118.54	111.33
1	A	348	TYR	CA-C-N	5.95	132.41	121.70
1	A	348	TYR	C-N-CA	5.95	132.41	121.70
1	A	91	GLY	N-CA-C	5.95	127.28	113.18
1	A	174	VAL	CA-C-N	-5.95	111.27	121.97
1	A	174	VAL	C-N-CA	-5.95	111.27	121.97
1	A	164	GLU	CB-CG-CD	-5.94	102.50	112.60
1	A	45	ASN	N-CA-C	5.92	120.35	113.18
1	A	207	HIS	N-CA-C	5.92	123.40	110.80
1	A	12	HIS	CA-C-N	-5.89	113.75	122.23
1	A	12	HIS	C-N-CA	-5.89	113.75	122.23
1	A	168	LYS	CA-C-N	-5.88	111.21	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LYS	C-N-CA	-5.88	111.21	122.61
1	A	96	GLU	CA-C-N	-5.87	111.80	122.43
1	A	96	GLU	C-N-CA	-5.87	111.80	122.43
1	A	109	VAL	N-CA-C	5.87	121.55	109.34
1	A	5	ASP	N-CA-C	5.87	120.04	112.41
1	A	31	ARG	CA-C-O	5.82	126.36	119.56
1	A	207	HIS	CA-C-O	5.80	128.81	120.51
1	A	257	GLU	N-CA-C	5.79	118.86	107.98
1	A	263	SER	CB-CA-C	-5.78	101.57	110.81
1	A	35	LEU	N-CA-CB	-5.78	100.09	110.37
1	A	110	GLU	N-CA-C	5.76	122.54	109.81
1	A	205	GLY	CA-C-O	5.75	125.43	119.27
1	A	192	PRO	CA-C-N	-5.75	113.50	119.99
1	A	192	PRO	C-N-CA	-5.75	113.50	119.99
1	A	94	TYR	N-CA-C	5.74	117.73	107.80
1	A	163	VAL	CA-C-N	-5.74	112.63	120.44
1	A	163	VAL	C-N-CA	-5.74	112.63	120.44
1	A	123	PRO	CA-C-N	-5.74	112.59	120.28
1	A	123	PRO	C-N-CA	-5.74	112.59	120.28
1	A	256	PHE	N-CA-C	5.73	118.01	109.59
1	A	197	ALA	N-CA-C	5.71	117.59	111.36
1	A	320	LYS	CA-CB-CG	-5.71	102.68	114.10
1	A	180	ALA	N-CA-C	5.70	117.85	109.24
1	A	104	LEU	N-CA-C	5.69	119.35	111.55
1	A	292	ASP	CA-CB-CG	5.67	118.28	112.60
1	A	87	LYS	N-CA-C	5.66	119.37	112.23
1	A	206	VAL	N-CA-C	5.66	121.12	109.34
1	A	222	LYS	CA-CB-CG	5.65	125.39	114.10
1	A	162	VAL	N-CA-C	5.63	121.04	109.34
1	A	149	LEU	CA-C-N	-5.62	115.12	123.11
1	A	149	LEU	C-N-CA	-5.62	115.12	123.11
1	A	297	PHE	N-CA-C	5.62	120.25	113.17
1	A	322	LEU	N-CA-CB	5.60	118.36	110.12
1	A	103	LEU	CA-C-O	5.60	126.27	119.49
1	A	211	HIS	CA-CB-CG	5.58	119.38	113.80
1	A	220	VAL	CA-CB-CG2	5.57	119.87	110.40
1	A	315	THR	CA-C-N	-5.56	111.86	120.31
1	A	315	THR	C-N-CA	-5.56	111.86	120.31
1	A	11	LEU	N-CA-C	5.55	120.70	113.88
1	A	141	PHE	CA-C-N	-5.55	112.09	121.85
1	A	141	PHE	C-N-CA	-5.55	112.09	121.85
1	A	239	THR	CA-C-O	5.54	126.25	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LYS	N-CA-C	5.53	120.09	113.23
1	A	48	GLY	N-CA-C	5.53	121.59	112.30
1	A	153	ARG	CA-C-N	-5.50	110.85	121.58
1	A	153	ARG	C-N-CA	-5.50	110.85	121.58
1	A	319	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	102	HIS	CA-C-N	-5.46	111.86	120.60
1	A	102	HIS	C-N-CA	-5.46	111.86	120.60
1	A	118	GLU	CB-CG-CD	-5.46	103.32	112.60
1	A	227	THR	CA-C-O	5.46	126.30	120.24
1	A	7	PRO	N-CA-C	5.45	122.52	112.33
1	A	126	VAL	CA-C-N	-5.44	114.24	120.88
1	A	126	VAL	C-N-CA	-5.44	114.24	120.88
1	A	262	SER	CB-CA-C	-5.44	101.76	110.79
1	A	77	LYS	CA-C-N	-5.44	112.57	120.29
1	A	77	LYS	C-N-CA	-5.44	112.57	120.29
1	A	52	PRO	CA-C-N	-5.44	111.15	121.54
1	A	52	PRO	C-N-CA	-5.44	111.15	121.54
1	A	66	MET	N-CA-C	5.44	121.83	109.81
1	A	106	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	A	116	GLN	CA-CB-CG	5.43	124.96	114.10
1	A	296	ILE	N-CA-C	5.43	118.66	111.17
1	A	321	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	A	106	ASN	CA-C-N	-5.42	113.34	123.05
1	A	106	ASN	C-N-CA	-5.42	113.34	123.05
1	A	338	LYS	N-CA-CB	5.42	117.86	110.01
1	A	98	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	196	GLN	N-CA-C	5.41	117.60	111.11
1	A	179	LEU	N-CA-CB	-5.39	102.08	110.55
1	A	140	ASP	CA-C-N	-5.39	112.88	121.44
1	A	140	ASP	C-N-CA	-5.39	112.88	121.44
1	A	239	THR	CA-CB-CG2	-5.37	101.37	110.50
1	A	347	ALA	CA-C-N	-5.36	114.52	122.56
1	A	347	ALA	C-N-CA	-5.36	114.52	122.56
1	A	342	ASP	N-CA-C	5.35	117.81	111.33
1	A	37	ALA	CA-C-O	-5.33	115.40	120.94
1	A	78	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	118	GLU	CA-C-N	5.32	131.27	121.70
1	A	118	GLU	C-N-CA	5.32	131.27	121.70
1	A	341	LEU	N-CA-C	5.31	118.22	111.69
1	A	18	ALA	CB-CA-C	-5.30	102.16	110.85
1	A	281	LYS	CA-C-N	-5.29	113.67	120.65
1	A	281	LYS	C-N-CA	-5.29	113.67	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	CA-CB-CG	5.28	124.65	114.10
1	A	212	ALA	CA-C-N	-5.26	111.11	121.41
1	A	212	ALA	C-N-CA	-5.26	111.11	121.41
1	A	130	VAL	N-CA-C	5.25	120.27	109.34
1	A	173	THR	CA-C-N	-5.25	116.68	123.19
1	A	173	THR	C-N-CA	-5.25	116.68	123.19
1	A	310	LYS	CB-CA-C	5.25	118.22	109.56
1	A	138	GLU	CB-CG-CD	-5.25	103.68	112.60
1	A	262	SER	N-CA-CB	5.23	117.81	110.12
1	A	77	LYS	CB-CG-CD	-5.21	99.32	111.30
1	A	132	GLN	N-CA-C	5.21	117.36	111.11
1	A	82	GLU	N-CA-C	5.18	119.07	112.34
1	A	74	ASP	CA-C-N	-5.18	112.08	120.72
1	A	74	ASP	C-N-CA	-5.18	112.08	120.72
1	A	323	ASN	N-CA-C	5.17	117.82	111.82
1	A	23	THR	N-CA-CB	5.17	118.29	110.28
1	A	205	GLY	N-CA-C	5.17	120.84	114.69
1	A	173	THR	CB-CA-C	-5.16	99.12	110.99
1	A	211	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
1	A	251	GLN	N-CA-C	5.16	116.98	111.36
1	A	345	TYR	CB-CA-C	-5.15	102.76	110.90
1	A	165	LEU	CA-C-N	-5.14	113.11	120.82
1	A	165	LEU	C-N-CA	-5.14	113.11	120.82
1	A	268	ALA	N-CA-C	5.13	121.73	110.80
1	A	39	THR	CA-C-O	-5.13	115.40	119.71
1	A	102	HIS	CB-CA-C	5.12	119.01	110.81
1	A	330	SER	CA-C-N	-5.12	114.40	122.08
1	A	330	SER	C-N-CA	-5.12	114.40	122.08
1	A	195	VAL	CA-CB-CG2	5.11	119.08	110.40
1	A	118	GLU	CA-C-O	-5.10	115.10	120.92
1	A	258	ILE	CA-CB-CG1	-5.09	101.74	110.40
1	A	247	ASN	CA-C-N	-5.09	112.23	121.14
1	A	247	ASN	C-N-CA	-5.09	112.23	121.14
1	A	309	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	246	TYR	CA-C-N	-5.09	112.24	121.14
1	A	246	TYR	C-N-CA	-5.09	112.24	121.14
1	A	83	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	258	ILE	N-CA-C	5.08	116.55	109.80
1	A	221	VAL	CB-CA-C	-5.07	105.48	111.97
1	A	259	CYS	N-CA-C	5.07	119.03	108.39
1	A	11	LEU	CA-C-O	5.06	124.96	119.24
1	A	63	ASP	CA-C-O	5.04	125.73	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	243	THR	N-CA-C	5.03	121.51	110.80
1	A	86	MET	N-CA-C	5.03	118.18	111.75
1	A	211	HIS	CB-CA-C	-5.03	100.42	110.42
1	A	226	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	27	TYR	CA-CB-CG	-5.01	104.89	113.90
1	A	141	PHE	CA-C-O	5.01	124.45	118.79

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	THR	Peptide
1	A	128	SER	Peptide
1	A	141	PHE	Sidechain
1	A	169	TYR	Sidechain
1	A	172	GLN	Peptide
1	A	191	PHE	Sidechain
1	A	199	ALA	Peptide
1	A	205	GLY	Peptide
1	A	232	ARG	Sidechain
1	A	26	TYR	Sidechain
1	A	287	TYR	Sidechain
1	A	289	LEU	Peptide
1	A	30	ARG	Sidechain
1	A	345	TYR	Sidechain
1	A	348	TYR	Sidechain,Peptide
1	A	349	ARG	Sidechain
1	A	49	MET	Peptide
1	A	64	TYR	Sidechain
1	A	71	GLY	Peptide
1	A	78	ARG	Sidechain
1	A	81	TYR	Sidechain
1	A	90	ASP	Peptide
1	A	99	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	2788	0	2749	196	0
2	A	1	0	0	0	0
3	A	19	0	14	1	0
4	A	490	0	0	15	0
All	All	3298	0	2763	196	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 35.

All (196) 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:221:VAL:HG13	1:A:233:LEU:HD11	1.58	0.85
1:A:316:GLU:HA	1:A:319:PHE:HD1	1.45	0.80
1:A:171:GLU:O	1:A:173:THR:HA	1.84	0.78
1:A:26:TYR:CE1	1:A:30:ARG:HG3	2.21	0.76
1:A:169:TYR:O	1:A:174:VAL:HG22	1.90	0.72
1:A:264:TYR:HB2	1:A:269:TRP:CE3	2.26	0.70
1:A:104:LEU:HB3	1:A:126:VAL:HG11	1.74	0.69
1:A:154:HIS:CD2	1:A:155:GLN:HG2	2.28	0.69
1:A:185:ILE:HB	1:A:188:SER:OG	1.92	0.69
1:A:221:VAL:HG21	1:A:239:THR:HG22	1.75	0.68
1:A:258:ILE:HD12	1:A:287:TYR:HB2	1.77	0.67
1:A:155:GLN:HG3	1:A:158:TRP:CZ2	2.31	0.66
1:A:51:LYS:O	1:A:53:LEU:HD13	1.96	0.65
1:A:258:ILE:HG21	1:A:277:VAL:HB	1.78	0.65
1:A:287:TYR:H	1:A:287:TYR:HD1	1.45	0.64
1:A:264:TYR:HB2	1:A:269:TRP:HE3	1.61	0.64
1:A:81:TYR:CE2	1:A:141:PHE:HE1	2.17	0.63
1:A:22:GLU:H	1:A:22:GLU:CD	2.06	0.62
1:A:28:GLY:HA3	1:A:35:LEU:HD22	1.82	0.62
1:A:138:GLU:OE2	1:A:144:LYS:HG3	1.99	0.61
1:A:19:ILE:HG12	1:A:79:ILE:HG13	1.83	0.60
1:A:344:LEU:HD22	1:A:344:LEU:H	1.66	0.59
1:A:10:GLU:HG2	1:A:95:VAL:HG13	1.84	0.59
1:A:81:TYR:CE2	1:A:141:PHE:CE1	2.90	0.59
1:A:153:ARG:HH12	1:A:189:SER:HB3	1.66	0.59
1:A:114:TRP:HD1	1:A:116:GLN:HE21	1.51	0.59
1:A:113:PRO:C	1:A:115:ASN:HA	2.28	0.59
1:A:52:PRO:HG3	1:A:264:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG12	1:A:176:ALA:HB3	1.86	0.57
1:A:232:ARG:HD3	1:A:257:GLU:OE2	2.04	0.57
1:A:179:LEU:HB3	1:A:210:VAL:HG13	1.87	0.57
1:A:332:LEU:HD13	4:A:850:HOH:O	2.05	0.57
1:A:206:VAL:HG11	4:A:858:HOH:O	2.04	0.57
1:A:105:ALA:HA	1:A:106:ASN:HB2	1.88	0.56
1:A:207:HIS:HD2	1:A:331:PHE:CD1	2.24	0.56
1:A:246:TYR:O	1:A:250:ARG:HG3	2.06	0.56
1:A:206:VAL:HG12	1:A:206:VAL:O	2.06	0.55
1:A:198:TYR:O	1:A:201:ALA:HB3	2.06	0.55
1:A:61:LYS:O	1:A:64:TYR:HB2	2.07	0.55
1:A:136:GLU:O	1:A:139:ARG:HB2	2.08	0.54
1:A:341:LEU:HD23	1:A:345:TYR:CE2	2.42	0.54
1:A:106:ASN:OD1	1:A:119:GLY:HA2	2.06	0.54
1:A:340:LEU:O	1:A:344:LEU:HD22	2.08	0.54
1:A:269:TRP:CZ2	1:A:275:HIS:HB2	2.43	0.54
1:A:275:HIS:ND1	1:A:277:VAL:HG12	2.23	0.54
1:A:20:LYS:HG3	4:A:662:HOH:O	2.08	0.53
1:A:221:VAL:HG12	4:A:887:HOH:O	2.08	0.53
1:A:232:ARG:HG3	1:A:255:HIS:HB3	1.89	0.53
1:A:1:THR:OG1	1:A:2:PRO:HD3	2.08	0.53
1:A:23:THR:O	1:A:27:TYR:HD2	1.92	0.53
1:A:232:ARG:HB2	1:A:255:HIS:HB3	1.91	0.53
1:A:344:LEU:HB3	1:A:348:TYR:CE1	2.44	0.53
1:A:212:ALA:HB3	1:A:233:LEU:HD21	1.91	0.53
1:A:340:LEU:O	1:A:340:LEU:HD22	2.09	0.52
1:A:221:VAL:HG11	1:A:239:THR:HG21	1.91	0.52
1:A:14:HIS:CE1	3:A:401:PRH:C8	2.92	0.52
1:A:185:ILE:HB	1:A:188:SER:HG	1.74	0.52
1:A:35:LEU:HD11	1:A:68:ALA:HB2	1.90	0.52
1:A:25:LEU:HD21	1:A:38:ASP:O	2.10	0.51
1:A:113:PRO:O	1:A:116:GLN:HB3	2.10	0.51
1:A:128:SER:HA	1:A:131:ASN:OD1	2.11	0.51
1:A:81:TYR:HE2	1:A:141:PHE:CE1	2.28	0.51
1:A:104:LEU:O	1:A:126:VAL:HG21	2.10	0.51
1:A:96:GLU:HA	1:A:146:ARG:O	2.10	0.51
1:A:114:TRP:N	1:A:115:ASN:HA	2.26	0.51
1:A:255:HIS:CE1	1:A:288:SER:HB3	2.46	0.51
1:A:286:ASN:OD1	1:A:286:ASN:C	2.54	0.50
1:A:221:VAL:HG21	1:A:239:THR:CG2	2.40	0.50
1:A:129:LEU:O	1:A:130:VAL:C	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HA	4:A:931:HOH:O	2.12	0.49
1:A:82:GLU:O	1:A:85:GLU:HB2	2.12	0.49
1:A:188:SER:HA	1:A:191:PHE:CE1	2.47	0.49
1:A:294:PRO:HG2	4:A:688:HOH:O	2.12	0.49
1:A:31:ARG:NE	1:A:72:CYS:HB2	2.26	0.49
1:A:147:SER:OG	1:A:174:VAL:HG12	2.11	0.49
1:A:19:ILE:HG23	1:A:23:THR:HG22	1.93	0.49
1:A:249:LEU:O	1:A:250:ARG:C	2.55	0.49
1:A:102:HIS:HA	4:A:696:HOH:O	2.12	0.49
1:A:154:HIS:HD2	1:A:155:GLN:HG2	1.76	0.49
1:A:253:ASN:HB3	4:A:1076:HOH:O	2.13	0.48
1:A:42:GLU:O	1:A:43:LEU:C	2.55	0.48
1:A:55:LEU:HG	1:A:59:LEU:HD12	1.95	0.48
1:A:178:ASP:OD2	1:A:179:LEU:N	2.46	0.48
1:A:106:ASN:HB3	1:A:121:LEU:HB2	1.95	0.48
1:A:116:GLN:HG2	1:A:117:ALA:H	1.77	0.48
1:A:58:PHE:CE1	1:A:297:PHE:CZ	3.02	0.48
1:A:92:VAL:HG12	1:A:94:TYR:H	1.79	0.48
1:A:87:LYS:HA	1:A:87:LYS:HD3	1.52	0.48
1:A:170:ARG:HG2	1:A:174:VAL:O	2.13	0.48
1:A:146:ARG:HE	1:A:171:GLU:HG3	1.79	0.48
1:A:108:LYS:O	1:A:109:VAL:C	2.56	0.48
1:A:202:VAL:HG22	1:A:208:ARG:NE	2.29	0.48
1:A:255:HIS:CD2	1:A:257:GLU:HG2	2.49	0.47
1:A:165:LEU:O	1:A:166:CYS:C	2.53	0.47
1:A:270:LYS:HA	1:A:271:PRO:HD3	1.84	0.47
1:A:127:VAL:HG11	1:A:169:TYR:CD2	2.50	0.47
1:A:95:VAL:HB	4:A:867:HOH:O	2.14	0.47
1:A:104:LEU:HD21	4:A:866:HOH:O	2.15	0.47
1:A:35:LEU:HG	1:A:36:PRO:HD2	1.97	0.47
1:A:81:TYR:HE2	1:A:141:PHE:CZ	2.32	0.47
1:A:314:PHE:O	1:A:315:THR:C	2.56	0.46
1:A:258:ILE:HD13	1:A:277:VAL:HG23	1.97	0.46
1:A:247:ASN:N	1:A:247:ASN:OD1	2.48	0.46
1:A:293:ASP:HB2	1:A:297:PHE:CE2	2.51	0.46
1:A:318:GLU:O	1:A:319:PHE:C	2.58	0.46
1:A:158:TRP:O	1:A:161:GLU:HB2	2.16	0.46
1:A:258:ILE:O	1:A:290:ASN:HB2	2.16	0.46
1:A:171:GLU:C	1:A:173:THR:HA	2.40	0.46
1:A:305:TYR:HD2	1:A:319:PHE:CE2	2.34	0.46
1:A:130:VAL:O	1:A:131:ASN:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:HIS:CD2	1:A:331:PHE:CD1	3.04	0.45
1:A:316:GLU:HA	1:A:319:PHE:CD1	2.36	0.45
1:A:11:LEU:HD11	1:A:326:ALA:HB1	1.97	0.45
1:A:105:ALA:HB3	4:A:696:HOH:O	2.17	0.45
1:A:333:PRO:HB2	1:A:335:ASP:HB3	1.99	0.45
1:A:264:TYR:CD1	1:A:265:LEU:HD12	2.52	0.45
1:A:305:TYR:CD2	1:A:319:PHE:CD2	3.05	0.45
1:A:54:THR:O	1:A:55:LEU:C	2.58	0.45
1:A:213:GLY:O	1:A:214:GLU:C	2.60	0.45
1:A:233:LEU:HD12	4:A:901:HOH:O	2.17	0.45
1:A:322:LEU:HD22	1:A:323:ASN:N	2.31	0.45
1:A:166:CYS:O	1:A:170:ARG:HB2	2.17	0.45
1:A:93:VAL:O	1:A:93:VAL:HG12	2.17	0.44
1:A:19:ILE:HG23	1:A:23:THR:CG2	2.47	0.44
1:A:275:HIS:O	1:A:276:ALA:C	2.60	0.44
1:A:315:THR:O	1:A:319:PHE:CD1	2.71	0.44
1:A:166:CYS:HA	1:A:174:VAL:HG21	1.99	0.44
1:A:221:VAL:HG11	1:A:239:THR:CG2	2.47	0.44
1:A:121:LEU:HD22	1:A:126:VAL:HG22	1.98	0.44
1:A:120:ASP:HB2	4:A:1038:HOH:O	2.17	0.44
1:A:149:LEU:HB3	1:A:162:VAL:HG13	2.00	0.44
1:A:239:THR:H	1:A:239:THR:HG23	1.58	0.44
1:A:211:HIS:HA	1:A:234:GLY:O	2.17	0.44
1:A:324:ILE:HD11	1:A:348:TYR:CD1	2.53	0.44
1:A:12:HIS:CE1	1:A:211:HIS:NE2	2.86	0.44
1:A:25:LEU:HD12	1:A:29:LYS:HD3	1.99	0.43
1:A:264:TYR:HD1	1:A:265:LEU:HD12	1.83	0.43
1:A:325:ASN:O	1:A:326:ALA:C	2.60	0.43
1:A:57:ASP:O	1:A:58:PHE:C	2.61	0.43
1:A:198:TYR:N	1:A:198:TYR:CD1	2.86	0.43
1:A:305:TYR:HD2	1:A:319:PHE:CD2	2.37	0.43
1:A:319:PHE:HA	1:A:322:LEU:HD13	1.99	0.43
1:A:275:HIS:CG	1:A:277:VAL:HG12	2.53	0.43
1:A:137:GLY:O	1:A:141:PHE:HD1	2.02	0.43
1:A:264:TYR:HB2	1:A:269:TRP:CZ3	2.53	0.43
1:A:31:ARG:CZ	1:A:72:CYS:H	2.32	0.43
1:A:93:VAL:HG11	1:A:343:LEU:HD12	2.01	0.43
1:A:33:ILE:HG21	1:A:68:ALA:N	2.33	0.43
1:A:195:VAL:O	1:A:196:GLN:C	2.60	0.43
1:A:258:ILE:HD12	1:A:287:TYR:HD2	1.84	0.43
1:A:81:TYR:CD2	1:A:81:TYR:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:O	1:A:247:ASN:OD1	2.36	0.43
1:A:346:LYS:HB2	1:A:346:LYS:HE3	1.54	0.43
1:A:58:PHE:O	1:A:61:LYS:HB2	2.19	0.42
1:A:237:TYR:O	1:A:240:LEU:HG	2.19	0.42
1:A:15:LEU:HD22	4:A:868:HOH:O	2.19	0.42
1:A:92:VAL:O	1:A:143:VAL:HG23	2.19	0.42
1:A:121:LEU:HD22	1:A:126:VAL:CG2	2.49	0.42
1:A:160:SER:O	1:A:163:VAL:HG12	2.19	0.42
1:A:65:TYR:C	1:A:67:PRO:HD2	2.44	0.42
1:A:136:GLU:O	1:A:139:ARG:N	2.52	0.42
1:A:161:GLU:O	1:A:164:GLU:HG3	2.20	0.42
1:A:278:ILE:HG13	1:A:314:PHE:CE1	2.54	0.42
1:A:33:ILE:O	1:A:34:ALA:C	2.60	0.42
1:A:146:ARG:NE	1:A:171:GLU:HG3	2.35	0.42
1:A:75:ALA:O	1:A:79:ILE:HG23	2.18	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HG21	1.85	0.42
1:A:156:PRO:O	1:A:157:SER:C	2.61	0.42
1:A:345:TYR:O	1:A:349:ARG:HB3	2.20	0.42
1:A:71:GLY:CA	1:A:121:LEU:HD12	2.50	0.41
1:A:337:LYS:O	1:A:341:LEU:HB2	2.20	0.41
1:A:324:ILE:HD11	1:A:348:TYR:HD1	1.85	0.41
1:A:112:ILE:HA	1:A:113:PRO:HD3	1.85	0.41
1:A:248:ARG:HH21	1:A:248:ARG:HD3	1.72	0.41
1:A:55:LEU:O	1:A:59:LEU:HD12	2.19	0.41
1:A:26:TYR:O	1:A:30:ARG:HB2	2.21	0.41
1:A:255:HIS:HD2	1:A:257:GLU:HG2	1.85	0.41
1:A:47:ILE:O	1:A:61:LYS:HD2	2.21	0.41
1:A:217:SER:O	1:A:220:VAL:HG23	2.21	0.41
1:A:4:PHE:HB3	1:A:8:LYS:NZ	2.36	0.41
1:A:135:GLN:O	1:A:138:GLU:HB3	2.20	0.41
1:A:146:ARG:HG3	4:A:850:HOH:O	2.20	0.41
1:A:197:ALA:O	1:A:198:TYR:C	2.59	0.41
1:A:143:VAL:O	1:A:143:VAL:HG13	2.21	0.41
1:A:86:MET:HE2	1:A:86:MET:HB3	1.92	0.41
1:A:154:HIS:CD2	1:A:154:HIS:C	2.98	0.41
1:A:156:PRO:HG3	1:A:191:PHE:HD2	1.86	0.40
1:A:98:ARG:HA	1:A:148:ILE:O	2.21	0.40
1:A:55:LEU:O	1:A:56:PRO:C	2.63	0.40
1:A:295:LEU:HG	1:A:296:ILE:N	2.35	0.40
1:A:170:ARG:HB3	1:A:170:ARG:HH11	1.85	0.40
1:A:6:LYS:HB2	1:A:348:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:HB2	1:A:92:VAL:HG22	2.02	0.40
1:A:10:GLU:C	1:A:11:LEU:HG	2.45	0.40
1:A:100:SER:O	1:A:101:PRO:C	2.65	0.40
1:A:255:HIS:ND1	1:A:286:ASN:OD1	2.54	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%)	238 (69%)	78 (22%)	31 (9%)	0 0

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	16	ASP
1	A	33	ILE
1	A	62	PHE
1	A	106	ASN
1	A	129	LEU
1	A	207	HIS
1	A	235	HIS
1	A	313	GLY
1	A	330	SER
1	A	335	ASP
1	A	347	ALA
1	A	24	ILE
1	A	72	CYS
1	A	112	ILE
1	A	114	TRP
1	A	243	THR

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Mol	Chain	Res	Type
1	A	68	ALA
1	A	286	ASN
1	A	343	LEU
1	A	81	TYR
1	A	194	HIS
1	A	260	PRO
1	A	26	TYR
1	A	91	GLY
1	A	119	GLY
1	A	165	LEU
1	A	214	GLU
1	A	130	VAL
1	A	66	MET
1	A	294	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%)	218 (72%)	86 (28%)	0 0

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	5	ASP
1	A	6	LYS
1	A	9	VAL
1	A	10	GLU
1	A	15	LEU
1	A	16	ASP
1	A	25	LEU
1	A	29	LYS
1	A	35	LEU
1	A	41	GLU
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	63	ASP
1	A	72	CYS
1	A	79	ILE
1	A	85	GLU
1	A	86	MET
1	A	95	VAL
1	A	97	VAL
1	A	106	ASN
1	A	108	LYS
1	A	110	GLU
1	A	112	ILE
1	A	116	GLN
1	A	122	THR
1	A	123	PRO
1	A	128	SER
1	A	129	LEU
1	A	131	ASN
1	A	132	GLN
1	A	136	GLU
1	A	139	ARG
1	A	145	VAL
1	A	149	LEU
1	A	150	CYS
1	A	157	SER
1	A	160	SER
1	A	164	GLU
1	A	166	CYS
1	A	170	ARG
1	A	171	GLU
1	A	172	GLN
1	A	173	THR
1	A	179	LEU
1	A	190	LEU
1	A	195	VAL
1	A	203	LYS
1	A	208	ARG
1	A	220	VAL
1	A	232	ARG
1	A	233	LEU
1	A	240	LEU
1	A	243	THR

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	249	LEU
1	A	254	MET
1	A	263	SER
1	A	264	TYR
1	A	265	LEU
1	A	270	LYS
1	A	273	THR
1	A	278	ILE
1	A	284	GLN
1	A	286	ASN
1	A	287	TYR
1	A	290	ASN
1	A	295	LEU
1	A	296	ILE
1	A	304	ASP
1	A	309	LYS
1	A	311	ASP
1	A	317	GLU
1	A	320	LYS
1	A	322	LEU
1	A	328	LYS
1	A	329	SER
1	A	334	GLU
1	A	339	GLU
1	A	340	LEU
1	A	341	LEU
1	A	342	ASP
1	A	343	LEU
1	A	344	LEU
1	A	346	LYS
1	A	349	ARG

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

Mol	Chain	Res	Type
1	A	135	GLN
1	A	154	HIS
1	A	172	GLN
1	A	194	HIS
1	A	207	HIS
1	A	284	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	PRH	A	401	2	18,21,21	2.28	8 (44%)	24,31,31	2.09	9 (37%)

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	PRH	A	401	2	-	0/6/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PRH	C5-N7	-4.94	1.31	1.39
3	A	401	PRH	C2-N1	4.55	1.42	1.34
3	A	401	PRH	C4-N3	3.28	1.42	1.35
3	A	401	PRH	O4'-C4'	-2.81	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PRH	O2'-C2'	2.75	1.49	1.43
3	A	401	PRH	C4-N9	-2.44	1.31	1.38
3	A	401	PRH	O5'-C5'	2.20	1.51	1.42
3	A	401	PRH	C2-N3	2.06	1.34	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	PRH	C2'-C1'-N9	4.12	124.71	113.25
3	A	401	PRH	O2'-C2'-C3'	-3.82	99.56	111.82
3	A	401	PRH	C5-C4-N3	-3.60	121.83	127.24
3	A	401	PRH	O4'-C4'-C3'	-3.59	98.02	105.15
3	A	401	PRH	O3'-C3'-C4'	-2.94	102.65	111.08
3	A	401	PRH	C8-N7-C5	-2.50	102.92	104.99
3	A	401	PRH	C5-C4-N9	2.41	109.94	105.65
3	A	401	PRH	O4'-C1'-C2'	-2.28	101.74	106.62
3	A	401	PRH	O3'-C3'-C2'	2.24	119.00	111.82

There are no chirality outliers.

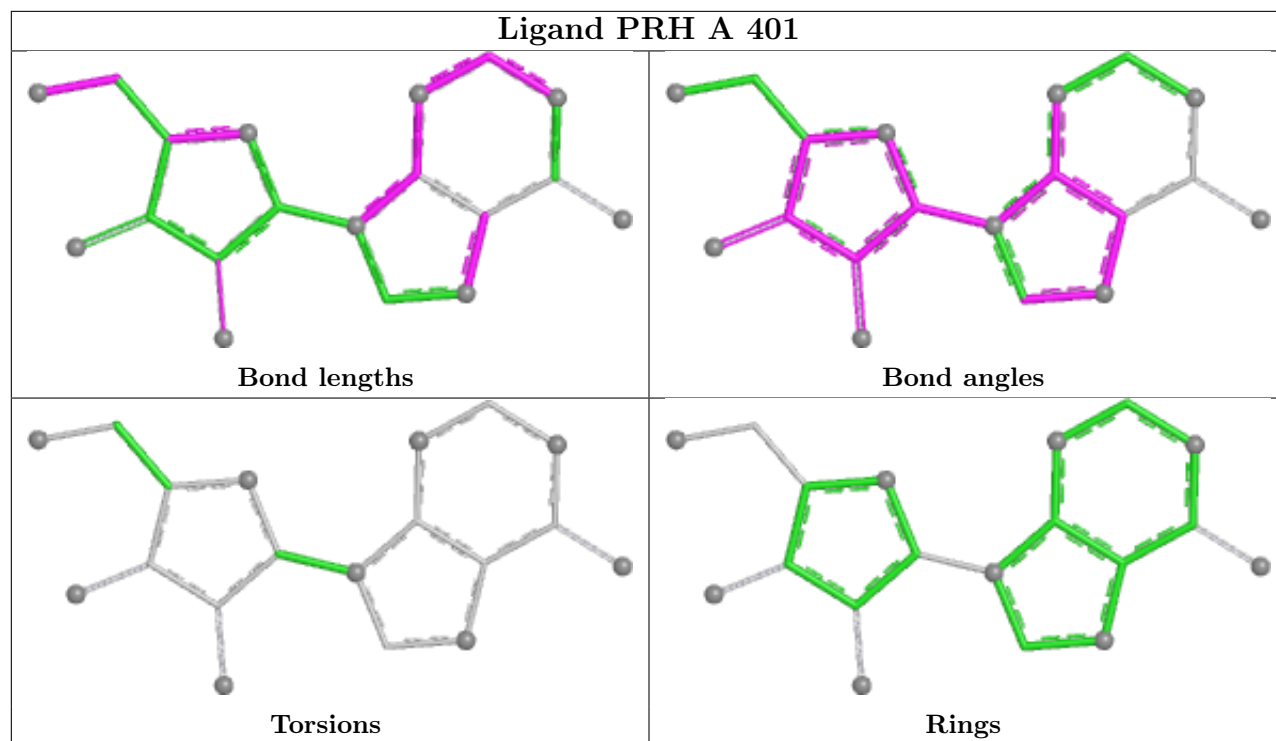
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	PRH	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 [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%)	-0.60	0 100 100	13, 23, 32, 42	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](#)

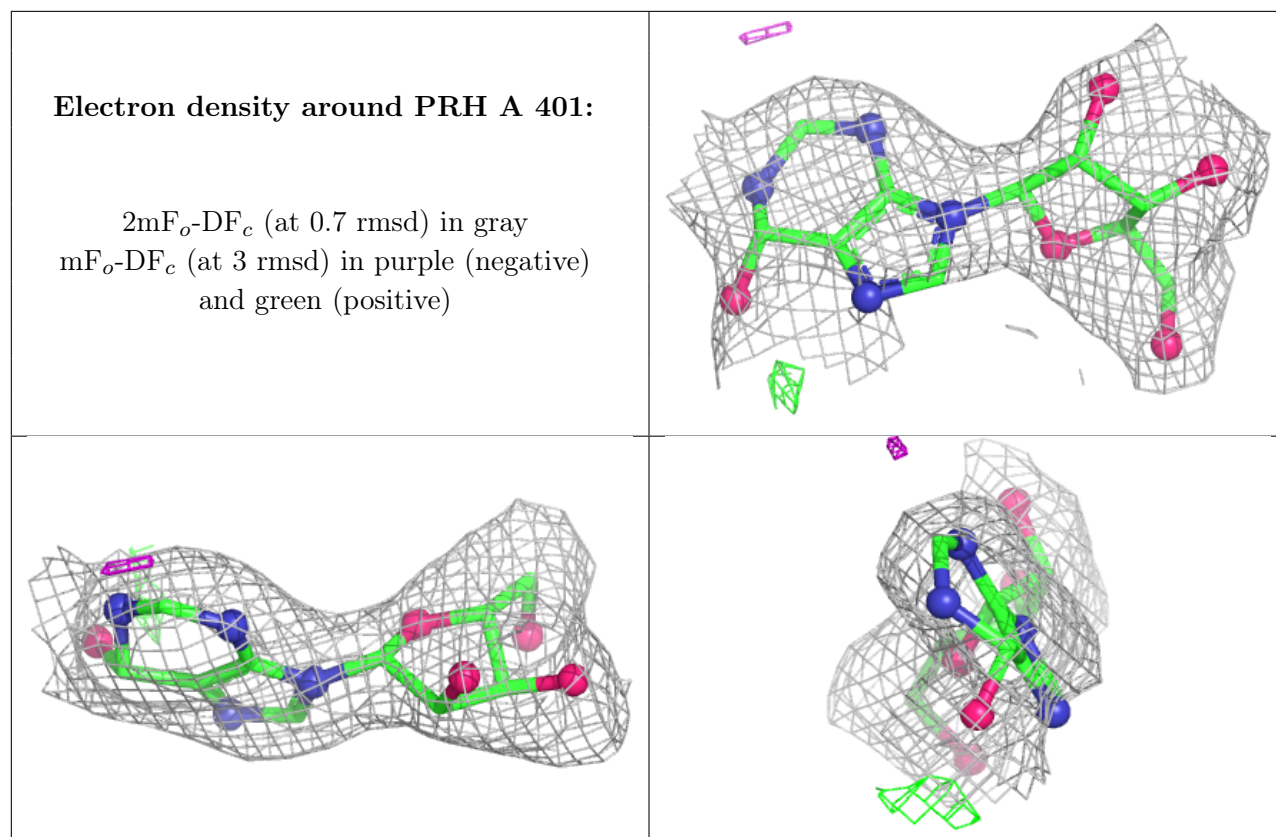
There are no oligosaccharides in this entry.

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	PRH	A	401	19/19	0.94	0.08	19,23,27,27	0
2	ZN	A	501	1/1	0.98	0.05	25,25,25,25	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.