



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:07 AM UTC

PDB ID : 1IEI / pdb_00001iei
Title : CRYSTAL STRUCTURE OF HUMAN ALDOSE REDUCTASE COM-
PLEXED WITH THE INHIBITOR ZENARESTAT.
Authors : Kinoshita, T.; Miyake, H.; Fujii, T.; Takakura, S.; Goto, T.
Deposited on : 2001-04-09
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

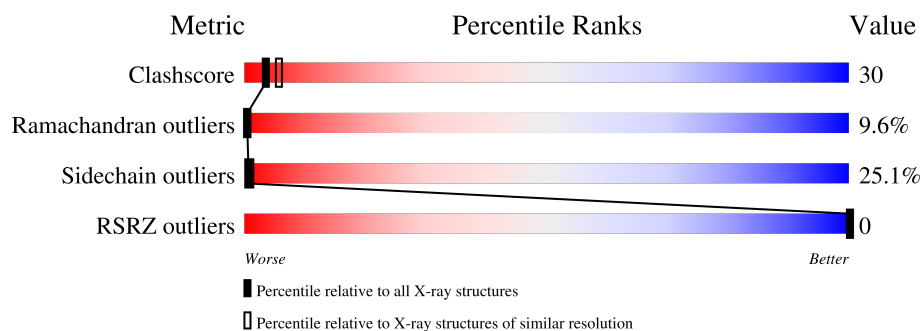
1 Overall quality at a glance

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	316	13% 37% 35% 15%

2 Entry composition [i](#)

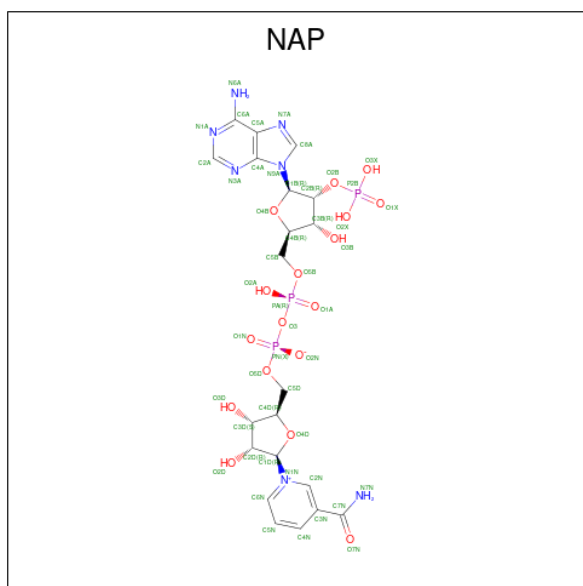
There are 4 unique types of molecules in this entry. The entry contains 2773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDOSE REDUCTASE.

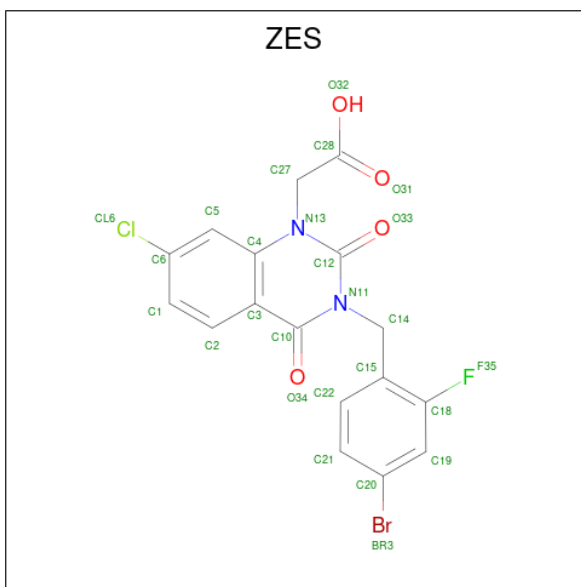
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2513	1615	424	462	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is [3-(4-BROMO-2-FLUORO-BENZYL)-7-CHLORO-2,4-DIOXO-3,4-DIHYDRO-2H-QUINAZOLIN-1-YL]-ACETIC ACID (CCD ID: ZES) (formula: $C_{17}H_{11}BrClFN_2O_4$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			26	1	17	1	1	2	4		

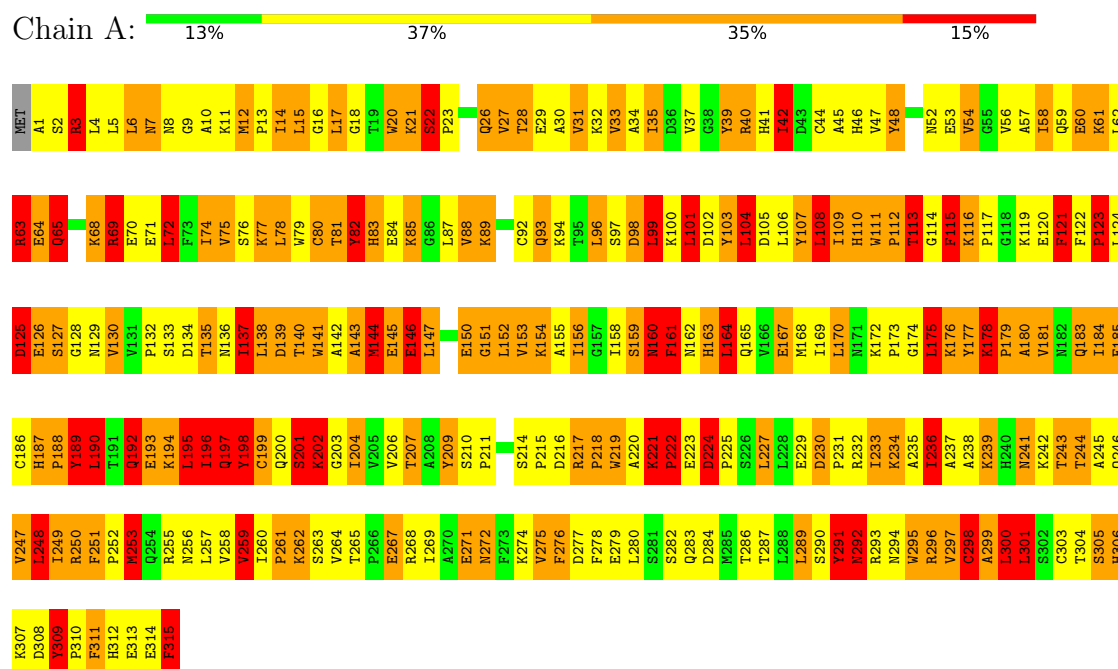
- Molecule 4 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: ALDOSE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.40Å 47.97Å 47.66Å 76.20° 76.70° 67.50°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 56.4 (10.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.82 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.178 , 0.199 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	1.1	Xtriage
Anisotropy	1.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 131.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% 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: ZES, NAP

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	2.38	116/2575 (4.5%)	2.90	296/3496 (8.5%)

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	23

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	LEU	CG-CD2	-25.09	0.69	1.52
1	A	306	HIS	CA-CB	-14.25	1.29	1.53
1	A	224	ASP	CA-C	10.07	1.65	1.52
1	A	12	MET	CA-C	9.95	1.63	1.52
1	A	151	GLY	CA-C	9.04	1.64	1.51
1	A	311	PHE	CA-CB	8.70	1.66	1.53
1	A	2	SER	CA-C	8.64	1.64	1.52
1	A	211	PRO	CA-CB	-8.47	1.42	1.53
1	A	260	ILE	CA-C	8.06	1.61	1.52
1	A	289	LEU	C-N	7.88	1.45	1.33
1	A	163	HIS	CE1-NE2	7.53	1.40	1.32
1	A	78	LEU	N-CA	7.44	1.55	1.46
1	A	20	TRP	C-O	-7.38	1.15	1.24
1	A	144	MET	CA-CB	-7.33	1.42	1.53
1	A	27	VAL	N-CA	7.32	1.55	1.46
1	A	251	PHE	CA-C	7.32	1.62	1.52
1	A	83	HIS	ND1-CE1	7.25	1.39	1.32
1	A	222	PRO	CA-CB	7.20	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	LYS	CA-C	7.17	1.62	1.52
1	A	177	TYR	N-CA	7.15	1.54	1.46
1	A	296	ARG	CA-C	-7.08	1.43	1.52
1	A	87	LEU	C-N	7.08	1.42	1.33
1	A	153	VAL	C-O	-7.04	1.17	1.24
1	A	249	ILE	C-O	-7.01	1.16	1.24
1	A	22	SER	C-O	-6.98	1.15	1.24
1	A	127	SER	N-CA	6.97	1.55	1.46
1	A	37	VAL	CA-C	-6.95	1.44	1.52
1	A	297	VAL	CA-CB	6.80	1.63	1.54
1	A	145	GLU	CA-C	-6.79	1.43	1.52
1	A	221	LYS	N-CA	6.72	1.55	1.46
1	A	297	VAL	C-N	6.67	1.42	1.33
1	A	111	TRP	CA-CB	6.63	1.62	1.54
1	A	258	VAL	CA-CB	6.62	1.62	1.54
1	A	312	HIS	CG-CD2	6.61	1.43	1.35
1	A	265	THR	CA-C	-6.60	1.43	1.52
1	A	63	ARG	NE-CZ	6.55	1.40	1.33
1	A	30	ALA	CA-C	-6.53	1.44	1.52
1	A	88	VAL	C-O	6.36	1.31	1.24
1	A	236	ILE	CA-C	6.34	1.60	1.52
1	A	267	GLU	CA-CB	6.34	1.64	1.53
1	A	222	PRO	N-CD	6.33	1.56	1.47
1	A	83	HIS	CG-CD2	6.33	1.42	1.35
1	A	215	PRO	N-CA	6.32	1.54	1.47
1	A	206	VAL	N-CA	6.29	1.54	1.46
1	A	217	ARG	NE-CZ	6.27	1.40	1.33
1	A	125	ASP	C-N	6.24	1.42	1.33
1	A	31	VAL	C-O	-6.21	1.17	1.24
1	A	75	VAL	CA-C	6.14	1.59	1.52
1	A	210	SER	C-N	6.12	1.41	1.33
1	A	184	ILE	CA-C	6.10	1.60	1.52
1	A	10	ALA	CA-C	6.10	1.61	1.53
1	A	222	PRO	CA-C	6.09	1.61	1.52
1	A	46	HIS	CA-C	6.04	1.60	1.52
1	A	28	THR	C-N	6.03	1.42	1.34
1	A	109	ILE	CA-CB	6.03	1.61	1.54
1	A	12	MET	C-N	-5.97	1.25	1.33
1	A	175	LEU	CA-CB	5.95	1.60	1.52
1	A	142	ALA	C-O	5.93	1.31	1.24
1	A	125	ASP	C-O	-5.92	1.16	1.24
1	A	238	ALA	C-O	-5.91	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	LEU	C-O	-5.89	1.16	1.24
1	A	58	ILE	CB-CG2	-5.89	1.33	1.52
1	A	111	TRP	N-CA	5.88	1.50	1.45
1	A	233	ILE	N-CA	5.87	1.53	1.46
1	A	88	VAL	CA-CB	-5.87	1.48	1.54
1	A	210	SER	C-O	5.86	1.26	1.23
1	A	202	LYS	C-O	-5.85	1.16	1.24
1	A	125	ASP	N-CA	5.80	1.53	1.46
1	A	137	ILE	C-N	5.79	1.42	1.33
1	A	135	THR	CA-C	5.76	1.60	1.52
1	A	291	TYR	CA-C	5.76	1.60	1.52
1	A	274	LYS	CA-C	5.75	1.60	1.52
1	A	107	TYR	N-CA	5.73	1.53	1.46
1	A	187	HIS	CB-CG	5.72	1.58	1.50
1	A	97	SER	C-O	-5.69	1.17	1.24
1	A	87	LEU	CA-C	5.64	1.60	1.52
1	A	53	GLU	N-CA	-5.64	1.39	1.46
1	A	163	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	11	LYS	N-CA	-5.62	1.39	1.46
1	A	243	THR	C-N	5.58	1.41	1.33
1	A	306	HIS	CB-CG	5.58	1.57	1.50
1	A	15	LEU	CA-CB	5.56	1.61	1.53
1	A	75	VAL	N-CA	5.54	1.52	1.46
1	A	83	HIS	CE1-NE2	5.53	1.38	1.32
1	A	6	LEU	C-O	-5.52	1.16	1.23
1	A	187	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	206	VAL	C-O	-5.46	1.18	1.24
1	A	233	ILE	CA-CB	5.44	1.61	1.54
1	A	84	GLU	C-N	5.39	1.41	1.34
1	A	142	ALA	N-CA	-5.38	1.39	1.46
1	A	76	SER	N-CA	5.38	1.53	1.46
1	A	173	PRO	C-N	-5.33	1.26	1.33
1	A	170	LEU	N-CA	5.33	1.53	1.46
1	A	42	ILE	CA-C	-5.32	1.46	1.52
1	A	194	LYS	CA-C	5.26	1.59	1.52
1	A	48	TYR	C-N	5.25	1.40	1.33
1	A	137	ILE	N-CA	5.25	1.52	1.46
1	A	246	GLN	C-N	-5.23	1.27	1.33
1	A	122	PHE	N-CA	5.23	1.53	1.46
1	A	237	ALA	C-N	5.20	1.40	1.33
1	A	263	SER	N-CA	-5.20	1.39	1.45
1	A	147	LEU	C-O	-5.19	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLY	CA-C	5.18	1.59	1.51
1	A	31	VAL	N-CA	5.15	1.52	1.46
1	A	35	ILE	CA-C	5.10	1.59	1.52
1	A	292	ASN	CA-CB	5.07	1.62	1.53
1	A	293	ARG	CZ-NH2	5.07	1.40	1.33
1	A	96	LEU	CA-CB	-5.05	1.45	1.53
1	A	258	VAL	C-O	-5.05	1.18	1.24
1	A	262	LYS	C-N	5.05	1.39	1.33
1	A	220	ALA	CA-C	-5.02	1.47	1.53
1	A	127	SER	CA-C	5.02	1.59	1.52
1	A	295	TRP	CA-C	5.01	1.59	1.53
1	A	64	GLU	N-CA	5.01	1.52	1.46
1	A	187	HIS	N-CA	5.01	1.53	1.46
1	A	248	LEU	CA-C	5.00	1.59	1.52

All (296) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASP	CA-CB-CG	16.63	129.23	112.60
1	A	93	GLN	N-CA-C	12.66	124.61	111.07
1	A	101	LEU	CB-CG-CD2	-11.71	75.55	110.70
1	A	271	GLU	N-CA-C	11.47	124.88	111.11
1	A	189	TYR	N-CA-C	11.21	126.71	112.92
1	A	129	ASN	N-CA-C	11.17	125.64	110.55
1	A	158	ILE	CA-C-N	-11.15	107.94	122.77
1	A	158	ILE	C-N-CA	-11.15	107.94	122.77
1	A	188	PRO	CA-C-N	-10.62	105.65	122.65
1	A	188	PRO	C-N-CA	-10.62	105.65	122.65
1	A	315	PHE	CA-CB-CG	10.38	124.18	113.80
1	A	160	ASN	CA-CB-CG	10.16	122.77	112.60
1	A	272	ASN	CA-CB-CG	9.97	122.57	112.60
1	A	7	ASN	CA-CB-CG	9.85	122.44	112.60
1	A	3	ARG	CD-NE-CZ	-9.74	110.77	124.40
1	A	15	LEU	CA-C-N	-9.72	111.34	121.35
1	A	15	LEU	C-N-CA	-9.72	111.34	121.35
1	A	160	ASN	CA-C-N	9.71	139.18	121.70
1	A	160	ASN	C-N-CA	9.71	139.18	121.70
1	A	236	ILE	CA-C-N	9.55	133.85	120.29
1	A	236	ILE	C-N-CA	9.55	133.85	120.29
1	A	158	ILE	N-CA-C	9.52	121.44	108.11
1	A	300	LEU	CA-C-N	-9.31	107.62	122.24
1	A	300	LEU	C-N-CA	-9.31	107.62	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	N-CA-C	9.20	120.00	110.62
1	A	224	ASP	CB-CA-C	9.17	128.23	110.17
1	A	108	LEU	CA-C-N	-9.15	110.94	122.37
1	A	108	LEU	C-N-CA	-9.15	110.94	122.37
1	A	184	ILE	CA-C-N	-9.12	108.39	121.42
1	A	184	ILE	C-N-CA	-9.12	108.39	121.42
1	A	114	GLY	CA-C-N	-8.91	107.08	123.03
1	A	114	GLY	C-N-CA	-8.91	107.08	123.03
1	A	299	ALA	N-CA-C	8.78	129.51	110.80
1	A	259	VAL	CA-C-N	-8.75	105.94	122.13
1	A	259	VAL	C-N-CA	-8.75	105.94	122.13
1	A	14	ILE	N-CA-C	8.42	124.01	111.89
1	A	130	VAL	N-CA-C	8.42	120.33	109.30
1	A	97	SER	N-CA-C	8.40	122.51	111.75
1	A	98	ASP	CA-C-O	8.40	129.54	120.55
1	A	159	SER	N-CA-C	8.35	122.35	108.73
1	A	248	LEU	CA-C-N	8.31	131.09	120.70
1	A	248	LEU	C-N-CA	8.31	131.09	120.70
1	A	225	PRO	CA-C-O	8.23	130.66	121.36
1	A	264	VAL	CB-CA-C	-8.20	100.65	111.88
1	A	64	GLU	CA-CB-CG	8.19	130.48	114.10
1	A	306	HIS	CA-CB-CG	8.17	121.97	113.80
1	A	143	ALA	CA-C-O	8.17	129.37	119.49
1	A	267	GLU	CA-CB-CG	8.16	130.42	114.10
1	A	47	VAL	N-CA-C	8.15	121.24	111.05
1	A	74	ILE	N-CA-C	8.14	119.63	108.89
1	A	197	GLN	N-CA-C	8.12	121.57	112.97
1	A	64	GLU	N-CA-C	8.11	121.14	111.33
1	A	54	VAL	CA-C-O	8.11	129.70	121.27
1	A	304	THR	N-CA-C	8.04	122.35	112.54
1	A	217	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	A	225	PRO	N-CA-C	8.00	123.78	111.15
1	A	32	LYS	N-CA-C	7.92	119.92	111.28
1	A	201	SER	N-CA-CB	7.81	123.69	110.49
1	A	178	LYS	CA-C-N	-7.73	111.48	119.83
1	A	178	LYS	C-N-CA	-7.73	111.48	119.83
1	A	198	TYR	CA-C-N	-7.72	110.36	122.49
1	A	198	TYR	C-N-CA	-7.72	110.36	122.49
1	A	122	PHE	CA-CB-CG	7.72	121.52	113.80
1	A	65	GLN	N-CA-C	7.70	127.21	110.80
1	A	143	ALA	N-CA-C	7.70	121.77	112.38
1	A	42	ILE	CA-CB-CG2	-7.67	97.45	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	LYS	N-CA-C	7.64	120.50	111.71
1	A	184	ILE	N-CA-C	7.63	121.03	109.20
1	A	204	ILE	N-CA-CB	-7.60	98.70	111.23
1	A	296	ARG	NE-CZ-NH2	7.57	126.01	119.20
1	A	291	TYR	N-CA-C	7.56	121.94	112.87
1	A	247	VAL	CA-C-N	7.55	130.25	120.44
1	A	247	VAL	C-N-CA	7.55	130.25	120.44
1	A	260	ILE	N-CA-C	7.48	125.04	108.88
1	A	123	PRO	N-CA-CB	-7.46	97.16	103.36
1	A	81	THR	N-CA-C	7.46	121.82	112.87
1	A	104	LEU	N-CA-CB	-7.42	98.64	111.55
1	A	123	PRO	CB-CA-C	7.42	119.79	111.11
1	A	216	ASP	N-CA-C	7.41	121.17	112.72
1	A	141	TRP	N-CA-CB	-7.40	98.44	110.14
1	A	99	LEU	N-CA-C	7.40	120.22	111.71
1	A	113	THR	CA-C-O	7.40	129.57	120.25
1	A	80	CYS	CA-C-N	7.38	134.73	120.99
1	A	80	CYS	C-N-CA	7.38	134.73	120.99
1	A	227	LEU	CA-C-N	-7.38	110.39	120.28
1	A	227	LEU	C-N-CA	-7.38	110.39	120.28
1	A	297	VAL	CA-CB-CG1	7.38	122.94	110.40
1	A	300	LEU	N-CA-C	7.33	126.41	110.80
1	A	17	LEU	CD1-CG-CD2	-7.31	94.71	110.80
1	A	286	THR	CA-C-O	7.29	128.37	120.20
1	A	194	LYS	CA-C-N	-7.27	110.06	122.56
1	A	194	LYS	C-N-CA	-7.27	110.06	122.56
1	A	16	GLY	N-CA-C	7.26	121.77	110.96
1	A	12	MET	CG-SD-CE	-7.21	85.03	100.90
1	A	248	LEU	N-CA-C	7.16	118.73	111.07
1	A	34	ALA	CA-C-O	7.14	127.99	120.42
1	A	98	ASP	N-CA-CB	7.13	120.69	110.13
1	A	146	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	190	LEU	N-CA-CB	7.05	121.85	110.77
1	A	206	VAL	N-CA-C	7.05	118.28	107.99
1	A	237	ALA	N-CA-C	7.01	119.01	111.36
1	A	128	GLY	N-CA-C	7.00	129.77	113.18
1	A	59	GLN	N-CA-C	6.99	119.49	111.11
1	A	52	ASN	CA-C-O	6.98	128.02	120.20
1	A	264	VAL	N-CA-C	6.96	118.83	112.29
1	A	28	THR	N-CA-C	6.94	118.49	111.07
1	A	84	GLU	CB-CG-CD	-6.93	100.82	112.60
1	A	108	LEU	N-CA-C	6.91	120.71	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	PHE	N-CA-C	6.89	120.36	109.81
1	A	256	ASN	CA-CB-CG	-6.89	105.71	112.60
1	A	124	LEU	N-CA-C	6.89	120.90	109.95
1	A	232	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	A	217	ARG	CD-NE-CZ	6.85	133.99	124.40
1	A	220	ALA	CA-C-N	-6.82	105.17	121.80
1	A	220	ALA	C-N-CA	-6.82	105.17	121.80
1	A	176	LYS	N-CA-C	6.79	119.69	111.82
1	A	26	GLN	N-CA-C	6.76	121.68	113.17
1	A	264	VAL	O-C-N	6.74	128.16	122.09
1	A	140	THR	CA-C-O	6.73	127.02	118.54
1	A	39	TYR	CB-CA-C	-6.73	100.17	110.26
1	A	198	TYR	CB-CA-C	6.71	121.66	109.99
1	A	10	ALA	N-CA-C	6.68	120.28	110.59
1	A	60	GLU	N-CA-C	6.68	121.02	113.01
1	A	190	LEU	N-CA-C	6.66	119.26	108.34
1	A	210	SER	CB-CA-C	-6.65	104.46	110.71
1	A	116	LYS	O-C-N	6.64	127.35	121.18
1	A	175	LEU	N-CA-C	6.57	119.14	108.63
1	A	63	ARG	CB-CA-C	6.51	121.93	110.85
1	A	242	LYS	CB-CG-CD	6.49	126.23	111.30
1	A	233	ILE	N-CA-C	6.49	117.12	110.82
1	A	301	LEU	CA-C-O	6.46	125.95	118.77
1	A	124	LEU	CA-C-O	6.46	128.46	121.16
1	A	83	HIS	CA-C-O	6.45	127.32	119.38
1	A	87	LEU	N-CA-C	6.43	121.21	113.23
1	A	293	ARG	N-CA-C	6.42	120.79	113.15
1	A	275	VAL	N-CA-C	6.41	118.67	111.88
1	A	125	ASP	N-CA-C	6.41	124.44	110.80
1	A	152	LEU	CA-C-N	-6.38	113.50	122.75
1	A	152	LEU	C-N-CA	-6.38	113.50	122.75
1	A	150	GLU	CA-C-N	-6.35	108.97	121.41
1	A	150	GLU	C-N-CA	-6.35	108.97	121.41
1	A	22	SER	CA-C-N	-6.33	115.04	119.66
1	A	22	SER	C-N-CA	-6.33	115.04	119.66
1	A	178	LYS	N-CA-C	6.32	119.03	110.31
1	A	54	VAL	N-CA-C	6.31	116.99	110.36
1	A	100	LYS	CA-C-O	6.31	128.63	120.81
1	A	20	TRP	CA-C-N	6.30	133.58	121.54
1	A	20	TRP	C-N-CA	6.30	133.58	121.54
1	A	180	ALA	CA-C-O	6.30	127.19	120.70
1	A	243	THR	N-CA-C	6.29	119.72	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	CA-C-O	6.28	127.23	120.20
1	A	287	THR	CA-CB-CG2	6.27	121.17	110.50
1	A	103	TYR	N-CA-C	6.27	118.30	108.96
1	A	72	LEU	N-CA-C	6.24	118.84	110.35
1	A	140	THR	CB-CA-C	-6.23	100.99	109.28
1	A	268	ARG	CA-C-N	-6.19	112.66	120.77
1	A	268	ARG	C-N-CA	-6.19	112.66	120.77
1	A	253	MET	CA-C-O	6.12	127.06	120.20
1	A	306	HIS	N-CA-C	6.11	119.21	110.10
1	A	269	ILE	N-CA-CB	-6.11	104.21	110.62
1	A	147	LEU	N-CA-C	6.09	119.55	111.75
1	A	22	SER	CA-C-O	6.09	123.25	119.29
1	A	61	LYS	N-CA-C	6.07	119.15	111.69
1	A	121	PHE	N-CA-C	6.05	123.69	110.80
1	A	147	LEU	CA-C-O	6.04	126.96	120.20
1	A	207	THR	N-CA-C	6.03	118.51	108.20
1	A	169	ILE	CA-C-N	-6.01	110.88	122.06
1	A	169	ILE	C-N-CA	-6.01	110.88	122.06
1	A	222	PRO	CB-CA-C	6.00	121.47	111.56
1	A	183	GLN	CA-CB-CG	-5.97	102.15	114.10
1	A	2	SER	N-CA-C	5.97	123.52	110.80
1	A	170	LEU	N-CA-C	5.97	120.56	113.28
1	A	296	ARG	N-CA-C	5.97	118.89	110.23
1	A	295	TRP	N-CA-C	5.97	119.14	107.57
1	A	41	HIS	N-CA-CB	-5.96	101.21	110.57
1	A	277	ASP	N-CA-C	5.96	118.57	111.71
1	A	63	ARG	CA-C-N	-5.96	112.22	120.38
1	A	63	ARG	C-N-CA	-5.96	112.22	120.38
1	A	250	ARG	CD-NE-CZ	-5.96	116.06	124.40
1	A	9	GLY	CA-C-O	5.94	124.83	118.95
1	A	84	GLU	CB-CA-C	-5.94	98.60	110.42
1	A	170	LEU	CA-C-O	5.92	126.23	119.18
1	A	272	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	305	SER	CA-C-O	5.92	126.22	119.18
1	A	184	ILE	O-C-N	-5.91	116.62	122.76
1	A	314	GLU	CA-C-N	-5.91	111.07	121.70
1	A	314	GLU	C-N-CA	-5.91	111.07	121.70
1	A	133	SER	O-C-N	5.84	130.40	123.33
1	A	221	LYS	N-CA-C	5.82	122.67	109.81
1	A	125	ASP	CA-C-O	-5.81	112.20	120.51
1	A	150	GLU	N-CA-C	5.80	120.22	113.20
1	A	162	ASN	N-CA-C	5.80	118.93	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	GLY	N-CA-C	5.78	126.87	113.18
1	A	251	PHE	N-CA-C	5.77	122.56	109.81
1	A	222	PRO	CA-C-N	-5.75	110.56	121.54
1	A	222	PRO	C-N-CA	-5.75	110.56	121.54
1	A	110	HIS	O-C-N	5.75	128.21	122.12
1	A	196	ILE	N-CA-C	5.74	116.20	110.23
1	A	68	LYS	CA-CB-CG	-5.74	102.62	114.10
1	A	303	CYS	CA-C-O	5.74	126.36	119.59
1	A	283	GLN	CA-C-O	5.73	126.99	120.00
1	A	217	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	A	108	LEU	CA-C-O	5.70	126.75	120.71
1	A	70	GLU	N-CA-C	5.69	122.93	110.80
1	A	84	GLU	CA-C-N	-5.69	112.07	120.38
1	A	84	GLU	C-N-CA	-5.69	112.07	120.38
1	A	196	ILE	CA-CB-CG2	5.69	120.17	110.50
1	A	2	SER	CA-C-O	5.69	128.64	120.51
1	A	239	LYS	CA-C-O	5.68	126.51	120.10
1	A	32	LYS	CB-CA-C	-5.67	101.37	110.79
1	A	30	ALA	O-C-N	5.67	128.21	122.09
1	A	224	ASP	O-C-N	-5.64	114.83	121.32
1	A	294	ASN	N-CA-C	5.64	119.74	112.86
1	A	201	SER	CB-CA-C	-5.64	99.20	110.42
1	A	179	PRO	CB-CA-C	5.63	118.73	111.64
1	A	276	PHE	CA-C-N	5.62	128.37	120.28
1	A	276	PHE	C-N-CA	5.62	128.37	120.28
1	A	192	GLN	N-CA-C	5.62	119.09	111.17
1	A	4	LEU	CA-C-N	5.61	131.25	122.17
1	A	4	LEU	C-N-CA	5.61	131.25	122.17
1	A	237	ALA	CB-CA-C	-5.60	101.33	110.85
1	A	146	GLU	CB-CA-C	5.60	120.08	110.79
1	A	245	ALA	CA-C-N	-5.60	112.21	120.38
1	A	245	ALA	C-N-CA	-5.60	112.21	120.38
1	A	40	ARG	CD-NE-CZ	-5.60	116.56	124.40
1	A	236	ILE	CA-CB-CG1	5.54	119.82	110.40
1	A	244	THR	N-CA-CB	5.54	118.04	110.01
1	A	222	PRO	N-CA-C	5.53	123.87	112.47
1	A	27	VAL	N-CA-C	5.49	120.08	112.35
1	A	68	LYS	N-CA-C	5.48	119.17	109.96
1	A	63	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	A	135	THR	CA-C-N	-5.45	112.40	121.89
1	A	135	THR	C-N-CA	-5.45	112.40	121.89
1	A	53	GLU	CA-CB-CG	-5.45	103.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ASP	CA-C-O	5.42	126.21	119.97
1	A	143	ALA	N-CA-CB	-5.42	101.11	110.32
1	A	161	PHE	N-CA-C	5.41	126.14	111.00
1	A	227	LEU	CB-CA-C	-5.37	101.56	110.68
1	A	185	GLU	N-CA-C	5.36	118.66	110.20
1	A	92	CYS	CA-C-N	-5.35	113.48	120.44
1	A	92	CYS	C-N-CA	-5.35	113.48	120.44
1	A	219	TRP	CA-C-O	5.35	130.35	122.38
1	A	230	ASP	N-CA-C	5.34	117.36	109.62
1	A	104	LEU	CB-CA-C	5.34	120.73	109.79
1	A	174	GLY	CA-C-N	-5.33	113.00	122.07
1	A	174	GLY	C-N-CA	-5.33	113.00	122.07
1	A	298	CYS	N-CA-C	5.32	119.91	113.41
1	A	116	LYS	CA-C-N	5.31	126.48	119.84
1	A	116	LYS	C-N-CA	5.31	126.48	119.84
1	A	244	THR	N-CA-C	5.30	116.74	111.07
1	A	309	TYR	CA-CB-CG	-5.30	104.36	113.90
1	A	44	CYS	N-CA-C	5.28	118.27	110.46
1	A	45	ALA	O-C-N	-5.28	118.24	123.46
1	A	297	VAL	N-CA-C	5.27	118.70	113.53
1	A	22	SER	N-CA-C	5.26	117.88	108.47
1	A	268	ARG	CB-CA-C	5.25	120.20	109.55
1	A	258	VAL	N-CA-C	5.24	115.45	108.11
1	A	299	ALA	CA-C-O	-5.24	113.02	120.51
1	A	102	ASP	CB-CA-C	5.21	118.71	109.65
1	A	177	TYR	N-CA-C	5.21	117.93	109.24
1	A	144	MET	N-CA-C	5.20	120.27	113.30
1	A	241	ASN	N-CA-C	5.20	121.88	110.80
1	A	293	ARG	CA-C-N	-5.20	114.89	123.05
1	A	293	ARG	C-N-CA	-5.20	114.89	123.05
1	A	18	GLY	N-CA-C	5.19	117.89	111.93
1	A	141	TRP	CA-C-O	5.18	126.00	120.20
1	A	263	SER	CA-C-O	-5.16	115.76	121.33
1	A	139	ASP	N-CA-C	5.16	119.14	113.21
1	A	133	SER	CA-C-O	-5.15	114.42	120.60
1	A	246	GLN	N-CA-C	5.15	118.34	111.75
1	A	300	LEU	CA-C-O	5.14	127.86	120.51
1	A	265	THR	CA-C-N	5.14	124.58	119.24
1	A	265	THR	C-N-CA	5.14	124.58	119.24
1	A	33	VAL	CA-C-O	-5.13	115.08	120.57
1	A	101	LEU	CA-C-N	-5.13	113.39	122.26
1	A	101	LEU	C-N-CA	-5.13	113.39	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	PRO	N-CA-CB	5.12	107.79	103.19
1	A	64	GLU	CA-C-N	5.11	131.30	121.54
1	A	64	GLU	C-N-CA	5.11	131.30	121.54
1	A	46	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	104	LEU	CA-C-N	-5.09	112.69	121.66
1	A	104	LEU	C-N-CA	-5.09	112.69	121.66
1	A	261	PRO	N-CA-C	5.09	119.56	111.26
1	A	41	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	39	TYR	N-CA-CB	5.08	117.53	109.71
1	A	105	ASP	N-CA-C	5.07	119.52	113.23
1	A	249	ILE	N-CA-C	5.07	115.21	110.30
1	A	40	ARG	CA-C-N	5.05	129.97	123.00
1	A	40	ARG	C-N-CA	5.05	129.97	123.00
1	A	248	LEU	N-CA-CB	-5.05	102.68	110.01
1	A	235	ALA	N-CA-C	5.05	117.56	111.40
1	A	89	LYS	N-CA-C	5.04	121.53	110.80
1	A	71	GLU	CB-CG-CD	-5.04	104.04	112.60
1	A	286	THR	O-C-N	-5.03	116.47	122.20
1	A	69	ARG	N-CA-C	5.02	121.48	110.80
1	A	103	TYR	O-C-N	-5.00	117.35	123.10

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	112	PRO	Peptide
1	A	121	PHE	Sidechain
1	A	126	GLU	Peptide
1	A	160	ASN	Peptide
1	A	163	HIS	Peptide
1	A	189	TYR	Peptide,Sidechain
1	A	195	LEU	Peptide
1	A	198	TYR	Sidechain
1	A	199	CYS	Peptide
1	A	201	SER	Peptide
1	A	202	LYS	Peptide
1	A	209	TYR	Sidechain
1	A	221	LYS	Peptide
1	A	222	PRO	Peptide
1	A	224	ASP	Peptide
1	A	291	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	298	CYS	Peptide
1	A	3	ARG	Sidechain
1	A	309	TYR	Sidechain
1	A	63	ARG	Sidechain
1	A	82	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	2513	0	2528	150	0
2	A	48	0	25	6	0
3	A	26	0	11	3	0
4	A	186	0	0	20	0
All	All	2773	0	2564	153	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 30.

All (153) 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:58:ILE:HG21	4:A:502:HOH:O	1.63	0.98
1:A:27:VAL:HG23	4:A:524:HOH:O	1.71	0.89
1:A:85:LYS:HB2	1:A:143:ALA:HB2	1.59	0.84
1:A:115:PHE:HZ	1:A:121:PHE:O	1.64	0.81
1:A:81:THR:HG23	1:A:115:PHE:HE2	1.46	0.79
1:A:60:GLU:O	1:A:64:GLU:HB2	1.86	0.74
1:A:106:LEU:HD21	1:A:181:VAL:HG11	1.70	0.73
1:A:98:ASP:HA	4:A:505:HOH:O	1.90	0.71
1:A:58:ILE:CG2	4:A:502:HOH:O	2.31	0.71
1:A:35:ILE:HG23	1:A:40:ARG:HH12	1.58	0.68
1:A:83:HIS:O	1:A:140:THR:HG22	1.93	0.68
1:A:85:LYS:HA	1:A:88:VAL:HG23	1.75	0.68
1:A:8:ASN:ND2	1:A:155:ALA:HB2	2.09	0.67
1:A:15:LEU:HD12	1:A:276:PHE:CZ	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HA	1:A:292:ASN:OD1	1.94	0.66
1:A:115:PHE:CZ	1:A:121:PHE:O	2.49	0.66
1:A:96:LEU:HD21	1:A:104:LEU:HB2	1.78	0.65
1:A:81:THR:HG23	1:A:115:PHE:CE2	2.30	0.64
1:A:48:TYR:O	4:A:518:HOH:O	2.14	0.64
1:A:104:LEU:HD11	1:A:107:TYR:CD1	2.33	0.63
1:A:17:LEU:O	1:A:42:ILE:HG22	2.01	0.61
1:A:179:PRO:O	1:A:204:ILE:HG12	2.00	0.61
1:A:161:PHE:CE2	1:A:165:GLN:HB3	2.36	0.60
1:A:77:LYS:HD2	1:A:110:HIS:CD2	2.36	0.60
1:A:291:TYR:N	1:A:291:TYR:CD1	2.69	0.59
1:A:167:GLU:HA	1:A:170:LEU:HD11	1.85	0.59
1:A:185:GLU:HB3	1:A:209:TYR:CE1	2.38	0.59
1:A:184:ILE:HD13	1:A:195:LEU:HD21	1.85	0.58
1:A:110:HIS:O	1:A:159:SER:HB3	2.04	0.58
1:A:195:LEU:HB3	1:A:315:PHE:HB2	1.85	0.58
1:A:160:ASN:HB3	1:A:183:GLN:O	2.04	0.57
1:A:255:ARG:HD3	4:A:392:HOH:O	2.04	0.57
1:A:217:ARG:O	1:A:219:TRP:N	2.38	0.56
1:A:230:ASP:O	1:A:233:ILE:HG22	2.05	0.56
1:A:189:TYR:OH	1:A:230:ASP:OD1	2.24	0.55
1:A:136:ASN:HB3	1:A:139:ASP:HB2	1.87	0.55
1:A:82:TYR:HA	4:A:416:HOH:O	2.06	0.55
1:A:233:ILE:HD11	1:A:248:LEU:CD1	2.37	0.55
1:A:296:ARG:HD3	1:A:311:PHE:CD2	2.42	0.54
1:A:290:SER:N	4:A:515:HOH:O	2.41	0.54
1:A:291:TYR:N	1:A:291:TYR:HD1	2.04	0.54
1:A:189:TYR:HD1	1:A:291:TYR:O	1.90	0.54
1:A:188:PRO:HD2	1:A:227:LEU:HD11	1.88	0.54
1:A:250:ARG:O	1:A:253:MET:HG2	2.07	0.54
1:A:108:LEU:HD22	1:A:108:LEU:N	2.24	0.53
1:A:115:PHE:HZ	1:A:121:PHE:C	2.16	0.53
1:A:172:LYS:O	1:A:175:LEU:HB2	2.09	0.53
1:A:231:PRO:HA	1:A:234:LYS:CE	2.38	0.53
1:A:295:TRP:HB2	4:A:514:HOH:O	2.08	0.53
1:A:161:PHE:HE2	1:A:165:GLN:HB3	1.74	0.52
1:A:259:VAL:O	1:A:261:PRO:HD2	2.10	0.52
1:A:183:GLN:HG3	1:A:207:THR:HB	1.92	0.52
1:A:113:THR:HG21	3:A:351:ZES:BR3	2.65	0.52
1:A:164:LEU:O	1:A:168:MET:HG3	2.10	0.52
1:A:57:ALA:O	1:A:61:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:O	1:A:248:LEU:HB2	2.10	0.52
1:A:309:TYR:HE2	4:A:376:HOH:O	1.92	0.52
1:A:306:HIS:CG	4:A:517:HOH:O	2.62	0.51
1:A:156:ILE:HD11	1:A:177:TYR:HB3	1.93	0.51
1:A:275:VAL:HG23	1:A:278:PHE:CE1	2.46	0.51
1:A:219:TRP:HZ2	1:A:298:CYS:HA	1.76	0.51
1:A:85:LYS:NZ	1:A:139:ASP:HB3	2.25	0.51
1:A:141:TRP:HA	1:A:141:TRP:CE3	2.47	0.50
1:A:85:LYS:HB2	1:A:143:ALA:CB	2.38	0.50
1:A:151:GLY:C	4:A:535:HOH:O	2.54	0.49
1:A:85:LYS:HE3	1:A:139:ASP:O	2.11	0.49
1:A:233:ILE:HD11	1:A:248:LEU:HD13	1.93	0.49
1:A:161:PHE:H	1:A:310:PRO:HB3	1.77	0.49
1:A:146:GLU:O	1:A:150:GLU:HG3	2.13	0.49
1:A:14:ILE:HA	4:A:357:HOH:O	2.13	0.48
1:A:3:ARG:HG3	1:A:13:PRO:HA	1.95	0.48
1:A:64:GLU:O	1:A:65:GLN:HB2	2.12	0.48
1:A:193:GLU:O	1:A:196:ILE:HB	2.12	0.48
1:A:103:TYR:CE2	1:A:154:LYS:HE2	2.48	0.48
1:A:217:ARG:HD2	1:A:219:TRP:NE1	2.28	0.48
1:A:20:TRP:HB2	2:A:350:NAP:H2D	1.96	0.48
1:A:132:PRO:HB3	1:A:306:HIS:HD2	1.77	0.48
1:A:147:LEU:HD23	1:A:152:LEU:HD13	1.94	0.48
1:A:231:PRO:HA	1:A:234:LYS:HE2	1.95	0.48
1:A:209:TYR:CD1	2:A:350:NAP:C5N	2.97	0.47
1:A:275:VAL:HG23	1:A:278:PHE:HE1	1.78	0.47
1:A:233:ILE:HA	1:A:236:ILE:HG12	1.96	0.47
1:A:192:GLN:HG3	4:A:493:HOH:O	2.14	0.47
1:A:178:LYS:HG2	1:A:179:PRO:HD2	1.96	0.47
1:A:197:GLN:O	1:A:201:SER:HB3	2.15	0.47
1:A:252:PRO:O	1:A:257:LEU:HB2	2.15	0.47
1:A:65:GLN:HG3	1:A:65:GLN:O	2.15	0.47
1:A:180:ALA:O	1:A:204:ILE:HG23	2.15	0.46
1:A:252:PRO:HG3	1:A:259:VAL:HG13	1.98	0.46
1:A:99:LEU:HD12	4:A:490:HOH:O	2.16	0.46
1:A:251:PHE:HZ	1:A:289:LEU:HD23	1.81	0.46
2:A:350:NAP:O3X	2:A:350:NAP:H3B	2.15	0.46
1:A:115:PHE:CE2	1:A:123:PRO:HD3	2.51	0.45
1:A:54:VAL:O	1:A:58:ILE:HD12	2.16	0.45
1:A:151:GLY:HA2	4:A:535:HOH:O	2.15	0.45
1:A:248:LEU:O	1:A:252:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HE3	1:A:144:MET:HB3	1.71	0.45
1:A:160:ASN:N	1:A:161:PHE:HB2	2.32	0.45
1:A:28:THR:HA	1:A:57:ALA:HB2	1.99	0.45
2:A:350:NAP:C7N	3:A:351:ZES:O32	2.65	0.45
1:A:198:TYR:O	1:A:198:TYR:CD2	2.69	0.45
1:A:214:SER:O	1:A:217:ARG:HG2	2.17	0.44
1:A:189:TYR:HB2	1:A:295:TRP:HE3	1.83	0.44
1:A:231:PRO:HA	1:A:234:LYS:HE3	1.99	0.44
1:A:136:ASN:O	1:A:137:ILE:C	2.60	0.44
1:A:79:TRP:CE3	1:A:79:TRP:HA	2.53	0.44
1:A:109:ILE:HD11	1:A:144:MET:SD	2.58	0.44
1:A:188:PRO:HG3	1:A:251:PHE:CE2	2.53	0.44
1:A:189:TYR:CE1	1:A:291:TYR:HB3	2.53	0.43
1:A:80:CYS:SG	1:A:111:TRP:HB2	2.58	0.43
1:A:189:TYR:HE1	1:A:291:TYR:HB3	1.83	0.43
1:A:61:LYS:HA	1:A:61:LYS:HD2	1.72	0.43
1:A:115:PHE:C	1:A:115:PHE:CD2	2.95	0.43
1:A:250:ARG:NH1	1:A:275:VAL:O	2.52	0.43
1:A:68:LYS:O	1:A:69:ARG:C	2.62	0.43
1:A:132:PRO:HB3	1:A:306:HIS:CD2	2.53	0.43
1:A:130:VAL:HB	4:A:475:HOH:O	2.17	0.43
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.62	0.43
1:A:289:LEU:HB2	4:A:515:HOH:O	2.17	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.85	0.43
1:A:249:ILE:HD11	1:A:272:ASN:OD1	2.19	0.43
1:A:31:VAL:HG21	1:A:54:VAL:HG13	2.01	0.43
1:A:115:PHE:C	1:A:115:PHE:HD2	2.26	0.43
1:A:141:TRP:O	1:A:145:GLU:HG3	2.19	0.43
1:A:22:SER:HA	1:A:23:PRO:HD3	1.91	0.42
1:A:168:MET:HB3	1:A:168:MET:HE2	1.82	0.42
1:A:306:HIS:CB	4:A:517:HOH:O	2.68	0.42
1:A:259:VAL:HG12	1:A:261:PRO:HD3	2.01	0.42
1:A:75:VAL:HG13	1:A:108:LEU:HD21	2.02	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.85	0.42
1:A:189:TYR:CD1	1:A:291:TYR:O	2.72	0.42
1:A:243:THR:O	1:A:247:VAL:HG23	2.20	0.42
1:A:300:LEU:HD23	1:A:301:LEU:N	2.35	0.42
1:A:125:ASP:HB3	1:A:127:SER:C	2.45	0.41
1:A:138:LEU:O	1:A:141:TRP:HB3	2.20	0.41
1:A:306:HIS:O	1:A:309:TYR:HB2	2.21	0.41
1:A:99:LEU:HB3	1:A:101:LEU:HG	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TRP:CE3	1:A:144:MET:SD	3.14	0.41
1:A:144:MET:CB	1:A:147:LEU:HD12	2.51	0.41
1:A:255:ARG:HD2	1:A:289:LEU:HD21	2.02	0.41
1:A:262:LYS:O	2:A:350:NAP:H8A	2.20	0.41
1:A:187:HIS:HD2	1:A:189:TYR:N	2.18	0.41
1:A:300:LEU:HB2	3:A:351:ZES:C18	2.50	0.41
1:A:136:ASN:OD1	1:A:138:LEU:HD12	2.20	0.41
1:A:144:MET:HG3	4:A:389:HOH:O	2.20	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HG21	1.59	0.41
1:A:82:TYR:CD2	1:A:82:TYR:N	2.89	0.41
1:A:185:GLU:HB3	1:A:209:TYR:CD1	2.55	0.40
1:A:85:LYS:HZ1	1:A:139:ASP:HB3	1.84	0.40
1:A:12:MET:HE3	1:A:12:MET:HB2	1.89	0.40
1:A:230:ASP:HA	1:A:231:PRO:HD3	1.79	0.40
1:A:306:HIS:ND1	1:A:308:ASP:N	2.70	0.40
2:A:350:NAP:O3X	2:A:350:NAP:C3B	2.68	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	313/316 (99%)	243 (78%)	40 (13%)	30 (10%)	0 0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	121	PHE
1	A	135	THR
1	A	161	PHE
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	201	SER
1	A	218	PRO
1	A	224	ASP
1	A	241	ASN
1	A	299	ALA
1	A	300	LEU
1	A	125	ASP
1	A	137	ILE
1	A	164	LEU
1	A	282	SER
1	A	21	LYS
1	A	89	LYS
1	A	126	GLU
1	A	202	LYS
1	A	234	LYS
1	A	267	GLU
1	A	292	ASN
1	A	62	LEU
1	A	223	GLU
1	A	120	GLU
1	A	160	ASN
1	A	112	PRO
1	A	221	LYS
1	A	222	PRO
1	A	236	ILE

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	279/281 (99%)	209 (75%)	70 (25%)	0 1

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	ASN
1	A	21	LYS
1	A	22	SER
1	A	26	GLN
1	A	33	VAL
1	A	39	TYR
1	A	42	ILE
1	A	56	VAL
1	A	63	ARG
1	A	65	GLN
1	A	69	ARG
1	A	72	LEU
1	A	74	ILE
1	A	77	LYS
1	A	78	LEU
1	A	82	TYR
1	A	85	LYS
1	A	93	GLN
1	A	94	LYS
1	A	99	LEU
1	A	101	LEU
1	A	104	LEU
1	A	108	LEU
1	A	113	THR
1	A	115	PHE
1	A	119	LYS
1	A	123	PRO
1	A	134	ASP
1	A	138	LEU
1	A	144	MET
1	A	146	GLU
1	A	153	VAL
1	A	154	LYS
1	A	156	ILE
1	A	160	ASN
1	A	164	LEU
1	A	167	GLU
1	A	175	LEU
1	A	176	LYS
1	A	178	LYS
1	A	181	VAL

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Mol	Chain	Res	Type
1	A	186	CYS
1	A	189	TYR
1	A	190	LEU
1	A	192	GLN
1	A	193	GLU
1	A	194	LYS
1	A	195	LEU
1	A	196	ILE
1	A	197	GLN
1	A	199	CYS
1	A	202	LYS
1	A	218	PRO
1	A	229	GLU
1	A	239	LYS
1	A	248	LEU
1	A	253	MET
1	A	259	VAL
1	A	271	GLU
1	A	279	GLU
1	A	280	LEU
1	A	297	VAL
1	A	300	LEU
1	A	301	LEU
1	A	305	SER
1	A	307	LYS
1	A	313	GLU
1	A	315	PHE

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	7	ASN
1	A	26	GLN
1	A	59	GLN
1	A	83	HIS
1	A	93	GLN
1	A	187	HIS
1	A	197	GLN
1	A	200	GLN
1	A	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	ZES	A	351	-	28,28,28	2.42	11 (39%)	41,41,41	1.73	7 (17%)
2	NAP	A	350	-	50,52,52	3.72	20 (40%)	71,80,80	2.14	28 (39%)

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	ZES	A	351	-	-	0/8/8/8	0/3/3/3
2	NAP	A	350	-	-	8/35/67/67	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAP	C4N-C3N	11.36	1.56	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAP	PA-O3	-11.23	1.47	1.59
2	A	350	NAP	C2N-N1N	10.39	1.46	1.35
2	A	350	NAP	PN-O3	-8.69	1.50	1.59
2	A	350	NAP	C6N-N1N	7.34	1.52	1.35
3	A	351	ZES	C27-C28	6.92	1.65	1.51
2	A	350	NAP	C5N-C4N	5.71	1.48	1.38
2	A	350	NAP	P2B-O2B	-5.33	1.50	1.59
2	A	350	NAP	C5D-C4D	3.95	1.63	1.51
3	A	351	ZES	C12-N11	-3.87	1.32	1.38
3	A	351	ZES	C19-C18	-3.76	1.31	1.37
3	A	351	ZES	C12-N13	3.74	1.42	1.37
2	A	350	NAP	C3N-C7N	-3.69	1.45	1.50
2	A	350	NAP	O3D-C3D	3.58	1.51	1.43
3	A	351	ZES	C6-CL6	-3.17	1.67	1.74
2	A	350	NAP	O2B-C2B	-3.13	1.33	1.44
2	A	350	NAP	O4D-C4D	-3.05	1.38	1.45
2	A	350	NAP	C5B-C4B	2.82	1.60	1.51
3	A	351	ZES	C14-C15	2.80	1.56	1.51
2	A	350	NAP	C2B-C1B	-2.79	1.46	1.53
3	A	351	ZES	C4-N13	-2.76	1.36	1.41
3	A	351	ZES	C10-N11	-2.73	1.34	1.40
2	A	350	NAP	O2D-C2D	2.66	1.49	1.43
2	A	350	NAP	C8A-N9A	-2.62	1.33	1.37
3	A	351	ZES	C14-N11	-2.48	1.43	1.47
3	A	351	ZES	C27-N13	-2.39	1.41	1.46
2	A	350	NAP	PN-O5D	-2.34	1.50	1.59
3	A	351	ZES	O32-C28	2.34	1.38	1.30
2	A	350	NAP	C2N-C3N	-2.31	1.35	1.39
2	A	350	NAP	P2B-O1X	2.24	1.57	1.50
2	A	350	NAP	C4A-N3A	2.10	1.38	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	NAP	C5N-C4N-C3N	-6.17	114.30	120.36
2	A	350	NAP	C3N-C7N-N7N	6.12	125.28	117.74
2	A	350	NAP	O3B-C3B-C2B	4.60	124.05	111.19
3	A	351	ZES	C10-N11-C12	-4.31	122.18	125.33
3	A	351	ZES	C3-C10-N11	4.24	121.47	115.26
2	A	350	NAP	O2N-PN-O5D	-3.99	89.49	107.57
3	A	351	ZES	C2-C3-C4	3.94	123.33	118.81
3	A	351	ZES	C4-C3-C10	-3.73	116.09	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	NAP	C5A-C4A-N3A	-3.40	122.04	126.72
2	A	350	NAP	C2N-C3N-C4N	3.36	122.17	118.26
2	A	350	NAP	C6N-C5N-C4N	3.24	124.11	119.45
2	A	350	NAP	C6A-C5A-N7A	3.05	137.97	132.09
3	A	351	ZES	BR3-C20-C19	-3.01	114.98	119.23
2	A	350	NAP	C4N-C3N-C7N	-2.97	112.97	121.06
2	A	350	NAP	P2B-O2B-C2B	-2.96	115.54	123.43
2	A	350	NAP	O2B-P2B-O1X	-2.92	98.93	109.33
2	A	350	NAP	O7N-C7N-N7N	-2.92	118.40	122.62
2	A	350	NAP	C3B-C2B-C1B	2.90	108.36	102.81
2	A	350	NAP	N6A-C6A-N1A	-2.90	111.92	118.38
3	A	351	ZES	C14-C15-C22	2.70	125.46	120.12
2	A	350	NAP	N3A-C2A-N1A	-2.69	124.51	128.58
2	A	350	NAP	O7N-C7N-C3N	-2.69	116.31	119.60
2	A	350	NAP	C2B-C1B-N9A	-2.66	109.38	113.75
2	A	350	NAP	O3-PN-O1N	2.65	118.67	110.70
2	A	350	NAP	O2D-C2D-C3D	2.63	120.24	111.82
2	A	350	NAP	C4A-C5A-N7A	-2.62	107.58	110.58
2	A	350	NAP	O2A-PA-O3	2.61	114.33	107.27
2	A	350	NAP	C2A-N3A-C4A	2.58	118.13	111.83
3	A	351	ZES	C21-C22-C15	-2.37	118.29	121.39
2	A	350	NAP	C5A-C6A-N1A	2.34	123.45	117.51
2	A	350	NAP	C4A-N9A-C8A	-2.26	103.36	105.74
2	A	350	NAP	C5A-C4A-N9A	2.17	108.17	105.81
2	A	350	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
2	A	350	NAP	O4B-C1B-C2B	-2.05	103.06	106.59
2	A	350	NAP	C6A-C5A-C4A	-2.01	114.43	117.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

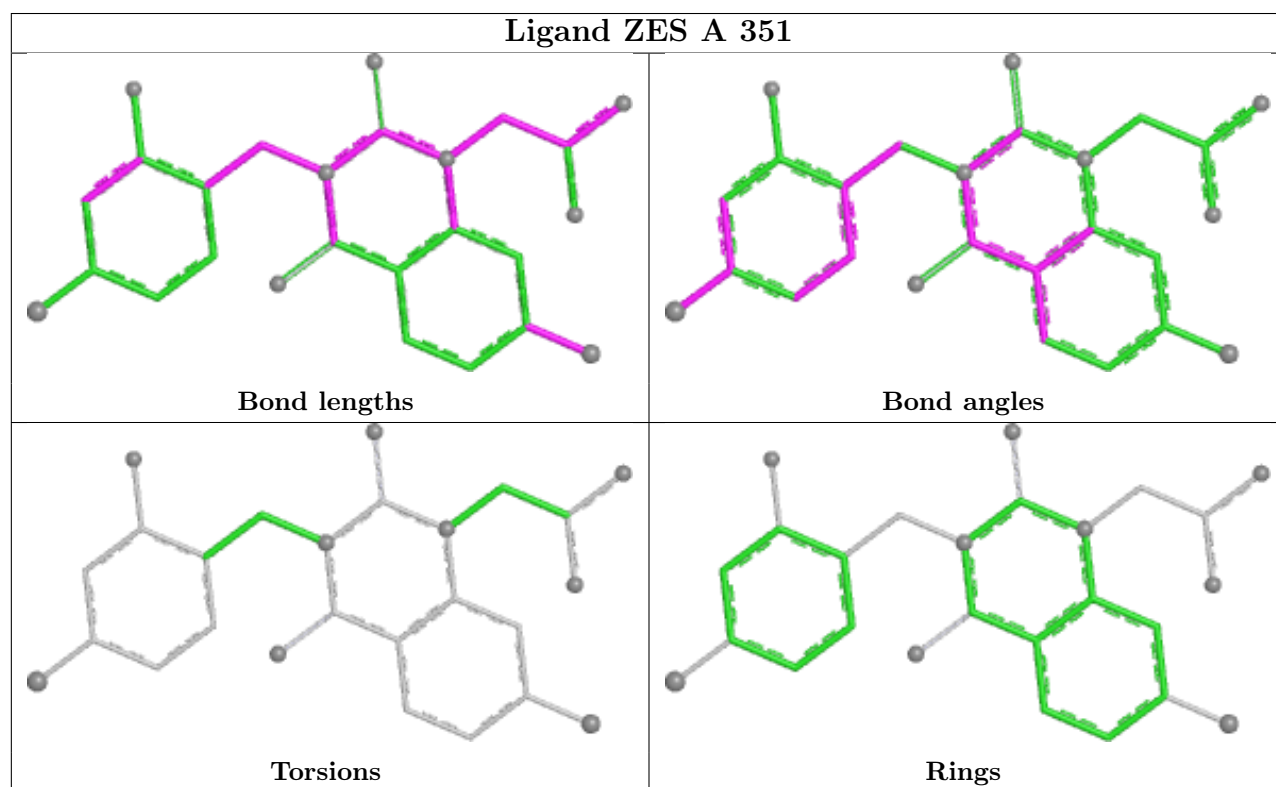
Mol	Chain	Res	Type	Atoms
2	A	350	NAP	PA-O3-PN-O5D
2	A	350	NAP	O4D-C1D-N1N-C6N
2	A	350	NAP	C3B-C2B-O2B-P2B
2	A	350	NAP	C1B-C2B-O2B-P2B
2	A	350	NAP	C4D-C5D-O5D-PN
2	A	350	NAP	PN-O3-PA-O1A
2	A	350	NAP	PN-O3-PA-O2A
2	A	350	NAP	PA-O3-PN-O2N

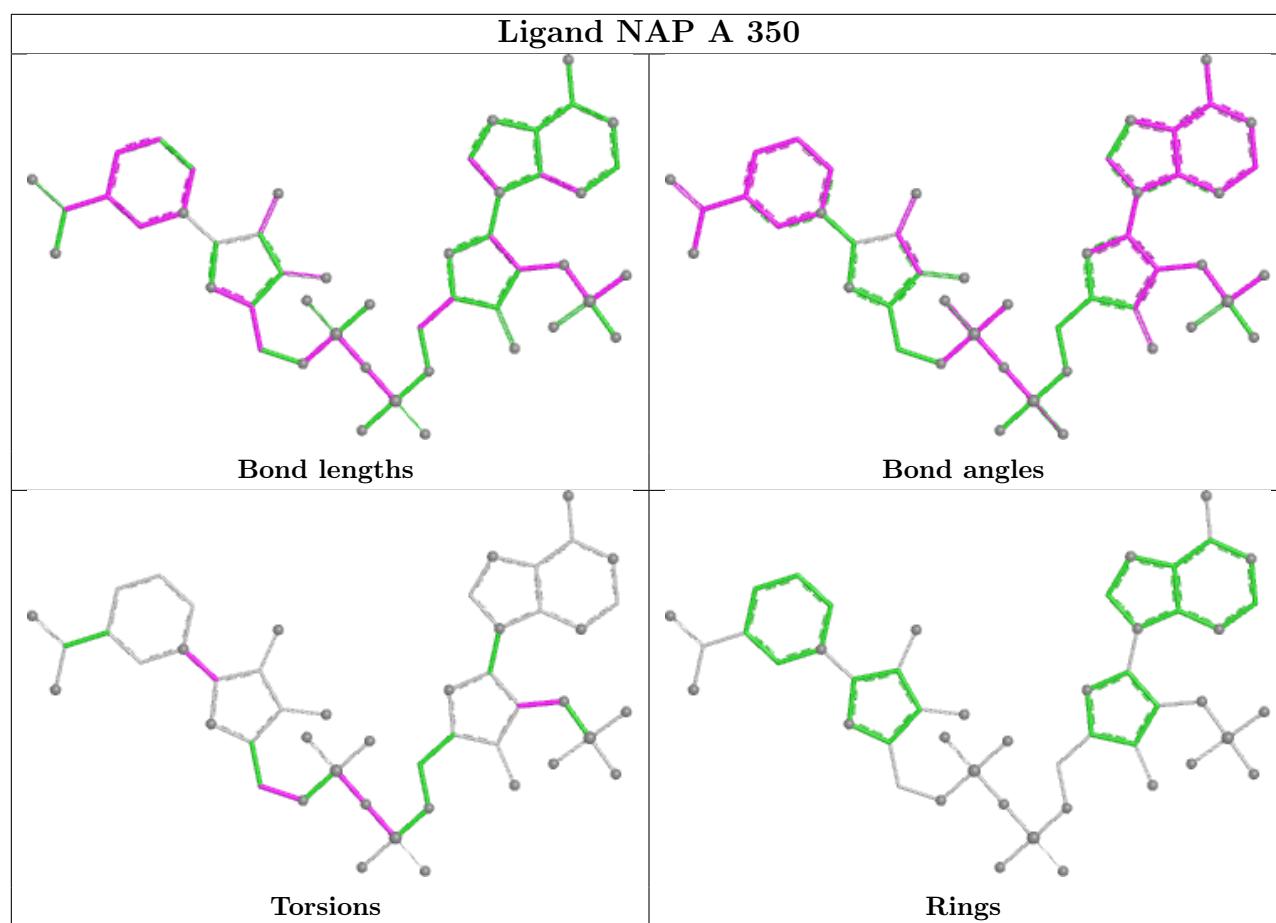
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	ZES	3	0
2	A	350	NAP	6	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	315/316 (99%)	-0.69	0 100 100	3, 11, 20, 27	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](#)

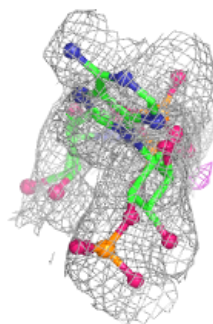
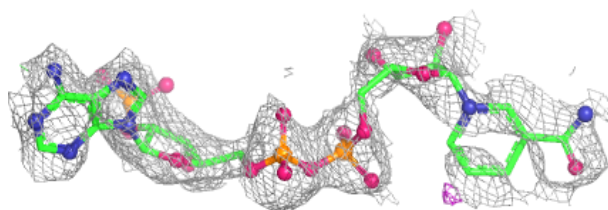
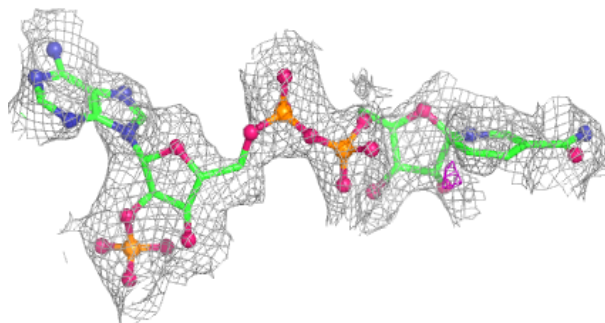
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	A	350	48/48	0.98	0.06	2,11,21,23	0
3	ZES	A	351	26/26	0.99	0.05	2,8,13,19	0

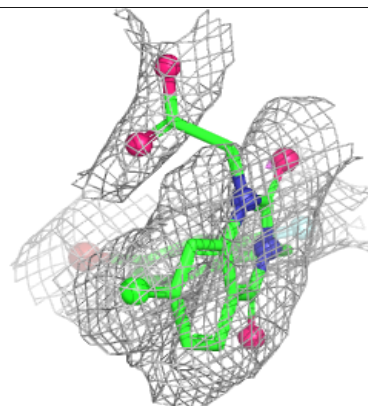
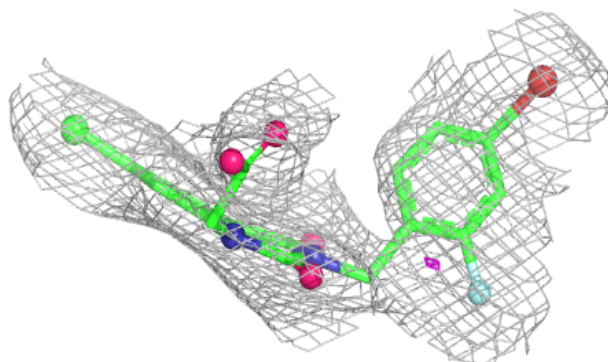
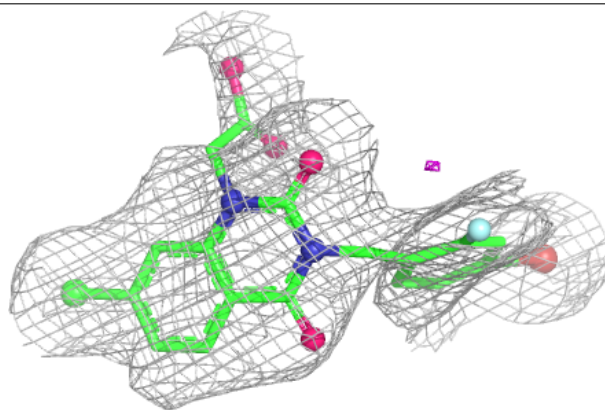
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 350:

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

**Electron density around ZES A 351:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.