



Full wwPDB X-ray Structure Validation Report i

Jun 12, 2024 – 03:22 AM EDT

PDB ID : 1IEI
Title : CRYSTAL STRUCTURE OF HUMAN ALDOSE REDUCTASE COMPLEXED 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

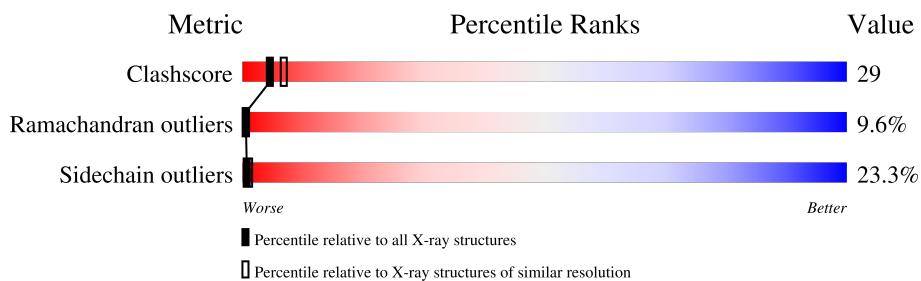
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

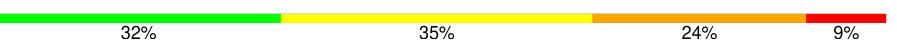
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Mol	Chain	Length	Quality of chain			
1	A	316		32%	35%	24% 9%

2 Entry composition (i)

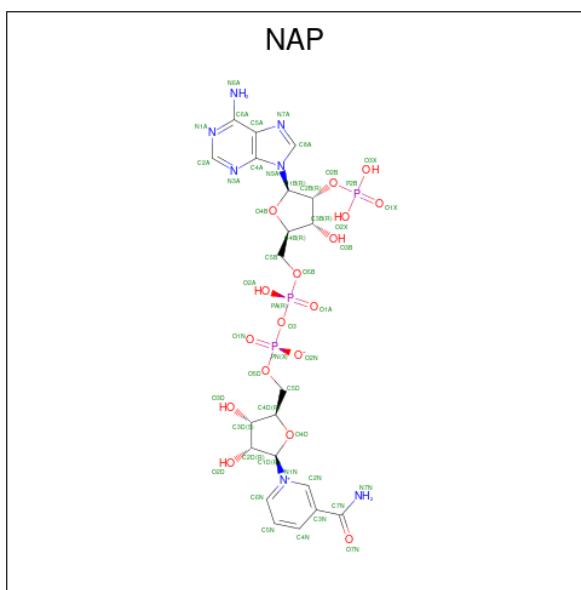
There are 4 unique types of molecules in this entry. The entry contains 2773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

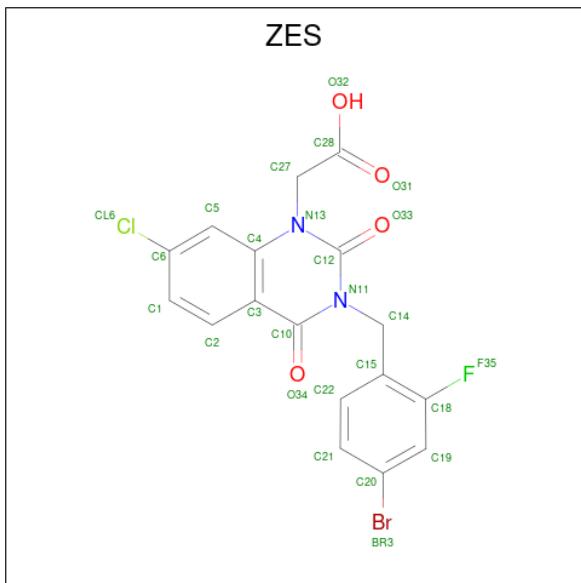
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2513	1615	424	462	12	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is [3-(4-BROMO-2-FLUORO-BENZYL)-7-CHLORO-2,4-DIOXO-3,4-DIHYDRO-2H-QUINAZOLIN-1-YL]-ACETIC ACID (three-letter code: ZES) (formula: C₁₇H₁₁BrClFN₂O₄).



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

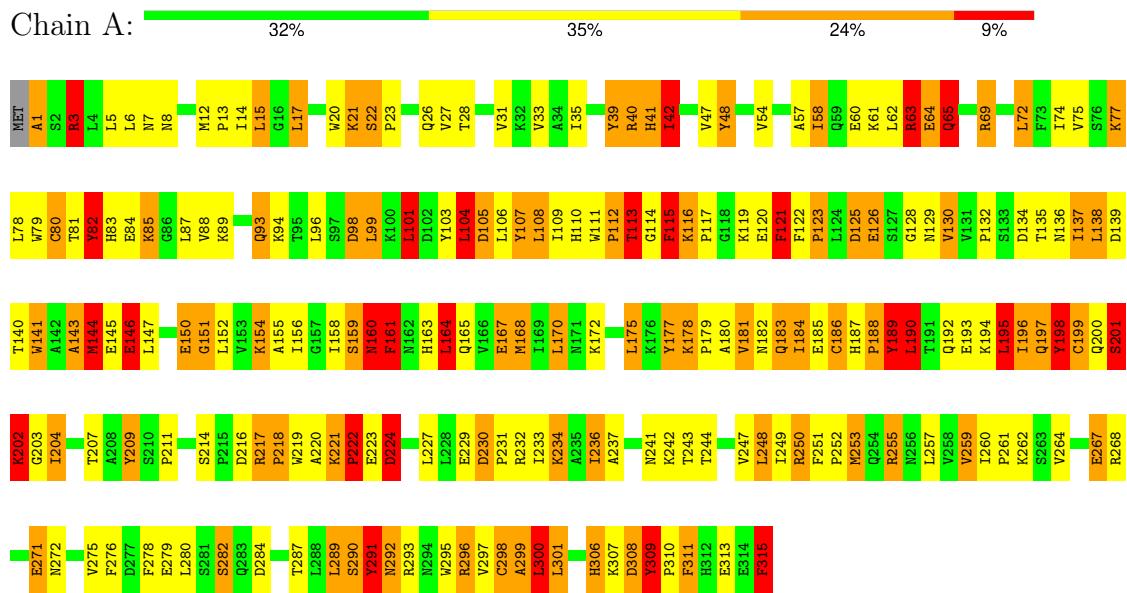
- Molecule 4 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ALDOSE REDUCTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.40 Å 47.97 Å 47.66 Å 76.20° 76.70° 67.50°	Depositor
Resolution (Å)	10.00 – 2.50 32.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 45.9 (32.34-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	12.82 (at 2.00 Å)	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)	0.28 , 134.0	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	1.76	21/2575 (0.8%)	2.23	101/3496 (2.9%)

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	23

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	LEU	CG-CD2	-22.19	0.69	1.51
1	A	306	HIS	CA-CB	-10.90	1.29	1.53
1	A	151	GLY	CA-C	7.98	1.64	1.51
1	A	39	TYR	CE2-CZ	6.88	1.47	1.38
1	A	58	ILE	CB-CG2	-6.37	1.33	1.52
1	A	222	PRO	N-CD	6.26	1.56	1.47
1	A	311	PHE	CG-CD1	5.93	1.47	1.38
1	A	122	PHE	CG-CD1	5.91	1.47	1.38
1	A	211	PRO	CA-CB	-5.79	1.42	1.53
1	A	282	SER	CB-OG	-5.58	1.34	1.42
1	A	63	ARG	NE-CZ	5.54	1.40	1.33
1	A	291	TYR	CE2-CZ	5.49	1.45	1.38
1	A	311	PHE	CA-CB	5.48	1.66	1.53
1	A	144	MET	CA-CB	-5.42	1.42	1.53
1	A	293	ARG	CZ-NH2	5.37	1.40	1.33
1	A	217	ARG	NE-CZ	5.30	1.40	1.33
1	A	222	PRO	CA-CB	5.22	1.64	1.53
1	A	267	GLU	CG-CD	5.16	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	TYR	CG-CD1	5.10	1.45	1.39
1	A	146	GLU	CG-CD	5.10	1.59	1.51
1	A	289	LEU	C-N	5.02	1.45	1.34

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	LEU	CB-CG-CD2	-20.85	75.55	111.00
1	A	217	ARG	NE-CZ-NH1	18.41	129.50	120.30
1	A	217	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	309	TYR	CB-CG-CD1	-11.44	114.14	121.00
1	A	296	ARG	NE-CZ-NH2	11.42	126.01	120.30
1	A	232	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	A	12	MET	CG-SD-CE	-9.48	85.03	100.20
1	A	69	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	3	ARG	CD-NE-CZ	-9.17	110.77	123.60
1	A	224	ASP	CB-CA-C	8.92	128.23	110.40
1	A	201	SER	N-CA-CB	8.79	123.69	110.50
1	A	115	PHE	CB-CG-CD1	-8.25	115.03	120.80
1	A	297	VAL	CA-CB-CG1	8.03	122.94	110.90
1	A	105	ASP	CB-CG-OD2	7.95	125.46	118.30
1	A	82	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	A	64	GLU	CA-CB-CG	7.76	130.48	113.40
1	A	267	GLU	CA-CB-CG	7.74	130.42	113.40
1	A	40	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	217	ARG	CD-NE-CZ	7.42	133.99	123.60
1	A	198	TYR	CG-CD1-CE1	-7.34	115.43	121.30
1	A	216	ASP	CA-CB-CG	7.20	129.23	113.40
1	A	160	ASN	C-N-CA	6.99	139.18	121.70
1	A	315	PHE	CB-CG-CD2	-6.98	115.92	120.80
1	A	299	ALA	N-CA-C	6.85	129.51	111.00
1	A	232	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	141	TRP	N-CA-CB	-6.75	98.44	110.60
1	A	42	ILE	CA-CB-CG2	-6.72	97.45	110.90
1	A	128	GLY	N-CA-C	6.67	129.77	113.10
1	A	220	ALA	C-N-CA	-6.61	105.17	121.70
1	A	198	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	A	188	PRO	C-N-CA	-6.42	105.65	121.70
1	A	47	VAL	CG1-CB-CG2	6.42	121.17	110.90
1	A	143	ALA	N-CA-CB	-6.42	101.11	110.10
1	A	64	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	A	150	GLU	C-N-CA	-6.35	108.97	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	VAL	C-N-CA	-6.31	105.94	121.70
1	A	287	THR	CA-CB-CG2	6.26	121.17	112.40
1	A	309	TYR	CG-CD2-CE2	-6.22	116.33	121.30
1	A	189	TYR	CD1-CE1-CZ	-6.17	114.25	119.80
1	A	259	VAL	CG1-CB-CG2	6.03	120.54	110.90
1	A	65	GLN	N-CA-C	6.00	127.21	111.00
1	A	268	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	284	ASP	CB-CG-OD2	6.00	123.69	118.30
1	A	104	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	198	TYR	CG-CD2-CE2	-5.94	116.55	121.30
1	A	84	GLU	CB-CA-C	-5.90	98.60	110.40
1	A	104	LEU	N-CA-CB	-5.88	98.64	110.40
1	A	105	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	237	ALA	CB-CA-C	-5.85	101.33	110.10
1	A	114	GLY	C-N-CA	-5.85	107.08	121.70
1	A	189	TYR	N-CA-C	5.82	126.71	111.00
1	A	63	ARG	CB-CA-C	5.76	121.93	110.40
1	A	87	LEU	CB-CG-CD2	5.75	120.78	111.00
1	A	115	PHE	CD1-CG-CD2	5.74	125.77	118.30
1	A	177	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	A	201	SER	CB-CA-C	-5.74	99.20	110.10
1	A	190	LEU	N-CA-CB	5.72	121.85	110.40
1	A	300	LEU	N-CA-C	5.71	126.41	111.00
1	A	264	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	255	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	300	LEU	C-N-CA	-5.63	107.62	121.70
1	A	198	TYR	CB-CA-C	5.63	121.66	110.40
1	A	242	LYS	CB-CG-CD	5.63	126.23	111.60
1	A	161	PHE	N-CA-C	5.61	126.14	111.00
1	A	98	ASP	N-CA-CB	5.61	120.69	110.60
1	A	291	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	230	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	104	LEU	CB-CA-C	5.54	120.73	110.20
1	A	168	MET	CG-SD-CE	-5.54	91.34	100.20
1	A	203	GLY	N-CA-C	5.51	126.87	113.10
1	A	158	ILE	C-N-CA	-5.51	107.94	121.70
1	A	107	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	308	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	177	TYR	CG-CD2-CE2	-5.47	116.92	121.30
1	A	39	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	A	129	ASN	N-CA-C	5.42	125.64	111.00
1	A	250	ARG	CD-NE-CZ	-5.39	116.06	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	THR	CA-C-N	-5.37	105.46	116.20
1	A	186	CYS	CA-CB-SG	5.37	123.66	114.00
1	A	33	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	A	184	ILE	C-N-CA	-5.33	108.39	121.70
1	A	17	LEU	CD1-CG-CD2	-5.26	94.71	110.50
1	A	204	ILE	N-CA-CB	-5.26	98.70	110.80
1	A	198	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	A	159	SER	N-CA-CB	5.24	118.36	110.50
1	A	15	LEU	C-N-CA	-5.22	111.34	122.30
1	A	41	HIS	N-CA-CB	-5.22	101.21	110.60
1	A	80	CYS	C-N-CA	5.21	134.73	121.70
1	A	260	ILE	N-CA-C	5.20	125.04	111.00
1	A	39	TYR	CD1-CG-CD2	5.18	123.59	117.90
1	A	130	VAL	CA-CB-CG1	5.14	118.61	110.90
1	A	271	GLU	N-CA-C	5.14	124.88	111.00
1	A	39	TYR	CB-CA-C	-5.12	100.17	110.40
1	A	183	GLN	CA-CB-CG	-5.11	102.15	113.40
1	A	48	TYR	CG-CD1-CE1	-5.11	117.22	121.30
1	A	290	SER	N-CA-CB	5.11	118.16	110.50
1	A	93	GLN	N-CA-C	5.04	124.61	111.00
1	A	216	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	1	ALA	O-C-N	5.04	130.76	122.70
1	A	308	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	40	ARG	CD-NE-CZ	-5.03	116.56	123.60

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	Sidechain,Peptide
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	221	LYS	Peptide
1	A	222	PRO	Peptide
1	A	224	ASP	Peptide
1	A	291	TYR	Sidechain
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 [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2528	144	0
2	A	48	0	25	7	0
3	A	26	0	11	3	0
4	A	186	0	0	20	0
All	All	2773	0	2564	147	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 29.

All (147) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:115:PHE:HZ	1:A:121:PHE:C	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:151:GLY:C	4:A:535:HOH:O	2.54	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:137:ILE:O	1:A:140:THR:OG1	2.34	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: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:250:ARG:NH1	1:A:275:VAL:O	2.52	0.43
1:A:48:TYR:HE2	2:A:350:NAP:HO2N	1.65	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: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: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: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
1:A:141:TRP:CE3	1:A:144:MET:SD	3.14	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [\(i\)](#)

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	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
1	A	201	SER
1	A	218	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [\(i\)](#)

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%)	214 (77%)	65 (23%)	1 1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	SER
1	A	26	GLN
1	A	39	TYR
1	A	41	HIS
1	A	42	ILE
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	105	ASP
1	A	108	LEU
1	A	113	THR
1	A	115	PHE
1	A	116	LYS
1	A	119	LYS
1	A	123	PRO
1	A	125	ASP
1	A	134	ASP
1	A	138	LEU
1	A	144	MET
1	A	146	GLU
1	A	154	LYS
1	A	160	ASN
1	A	164	LEU
1	A	167	GLU
1	A	170	LEU
1	A	175	LEU
1	A	178	LYS
1	A	181	VAL
1	A	182	ASN
1	A	186	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	189	TYR
1	A	190	LEU
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	248	LEU
1	A	253	MET
1	A	271	GLU
1	A	279	GLU
1	A	280	LEU
1	A	301	LEU
1	A	307	LYS
1	A	309	TYR
1	A	313	GLU
1	A	315	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	93	GLN
1	A	182	ASN
1	A	187	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	24,28,28	3.27	10 (41%)	33,41,41	2.88	8 (24%)
2	NAP	A	350	-	46,52,52	3.84	17 (36%)	61,80,80	2.15	20 (32%)

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	-	-	1/8/8/8	0/3/3/3
2	NAP	A	350	-	-	8/31/67/67	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	ZES	C27-C28	12.08	1.65	1.51
2	A	350	NAP	C4N-C3N	11.36	1.56	1.39
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
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	C3-C4	-3.87	1.38	1.41
3	A	351	ZES	C19-C18	-3.76	1.31	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	C27-N13	-3.49	1.41	1.49
3	A	351	ZES	C4-N13	-3.41	1.36	1.40
3	A	351	ZES	C6-CL6	-3.17	1.67	1.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAP	O2B-C2B	-3.13	1.33	1.44
3	A	351	ZES	C14-N11	-3.08	1.43	1.48
2	A	350	NAP	O4D-C4D	-3.05	1.38	1.45
2	A	350	NAP	C5B-C4B	2.82	1.60	1.51
2	A	350	NAP	O2D-C2D	2.66	1.49	1.43
3	A	351	ZES	C14-C15	2.54	1.56	1.51
3	A	351	ZES	C10-N11	-2.41	1.34	1.38
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

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	351	ZES	C2-C3-C4	11.96	123.33	117.89
3	A	351	ZES	C3-C10-N11	8.12	121.47	116.13
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
2	A	350	NAP	O2N-PN-O5D	-3.99	89.49	107.57
3	A	351	ZES	C14-C15-C18	-3.69	116.41	121.22
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	N3A-C2A-N1A	-3.07	124.51	128.67
3	A	351	ZES	BR3-C20-C19	-3.01	114.98	119.23
2	A	350	NAP	N6A-C6A-N1A	-3.00	111.92	118.33
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	C5A-C6A-N6A	2.83	124.63	120.31
2	A	350	NAP	O7N-C7N-C3N	-2.69	116.31	119.60
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	O2A-PA-O3	2.61	114.33	107.27
3	A	351	ZES	C4-C3-C10	-2.51	116.09	119.39
3	A	351	ZES	C21-C22-C15	-2.37	118.29	121.39
3	A	351	ZES	C1-C2-C3	-2.19	118.26	121.62
2	A	350	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
2	A	350	NAP	O4B-C1B-C2B	-2.08	103.06	106.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	351	ZES	C14-C15-C22	2.00	125.46	121.04

There are no chirality outliers.

All (9) torsion outliers are listed below:

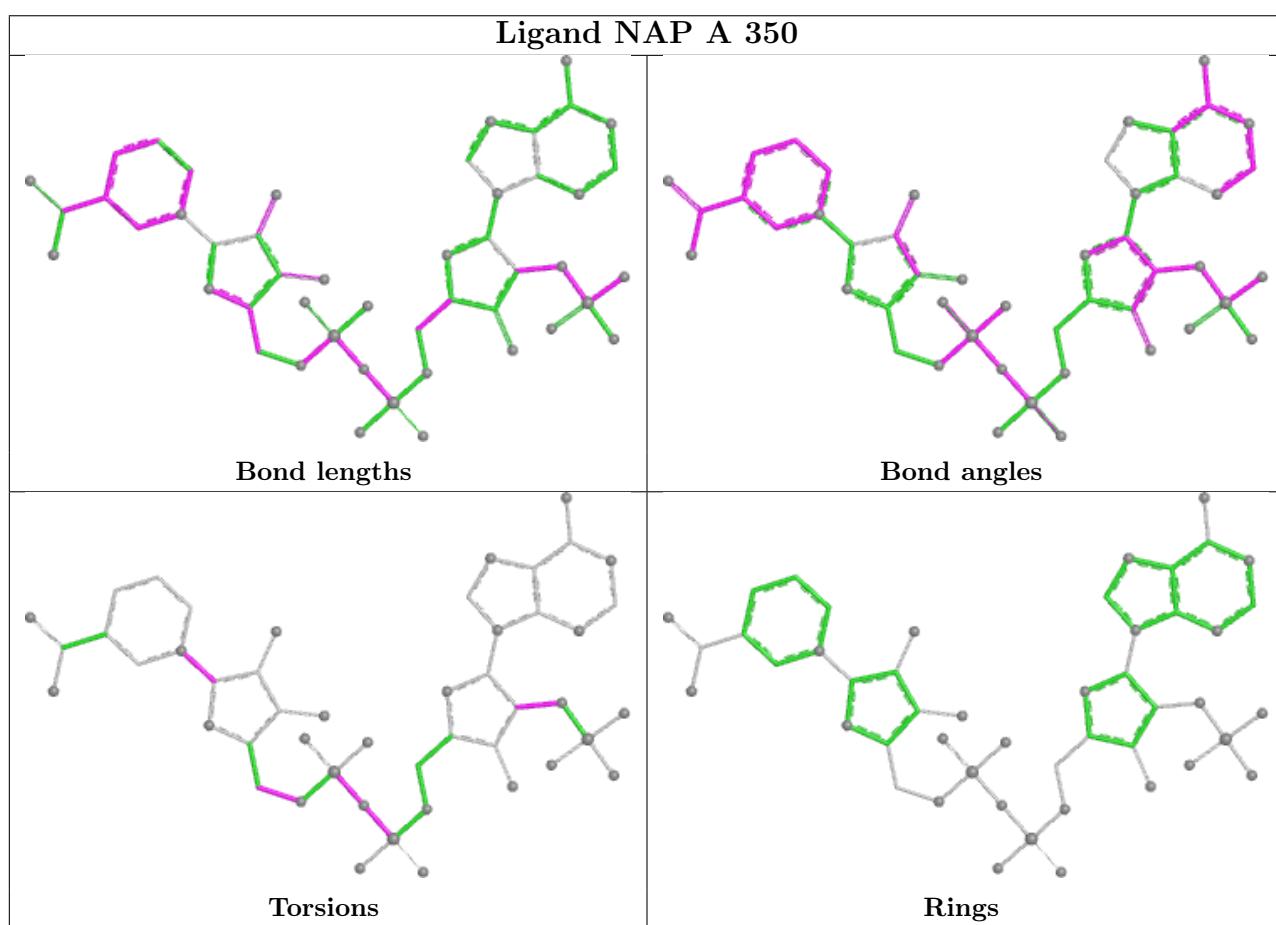
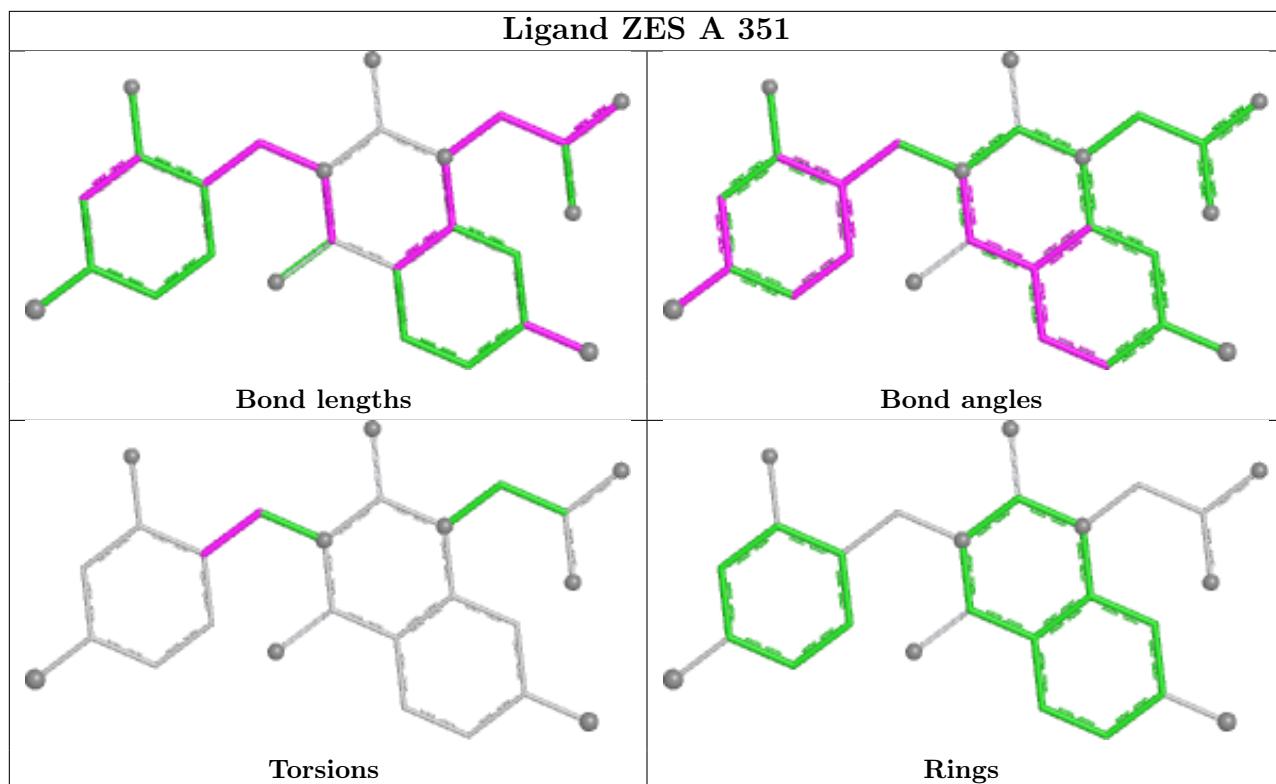
Mol	Chain	Res	Type	Atoms
2	A	350	NAP	PA-O3-PN-O5D
2	A	350	NAP	O4D-C1D-N1N-C6N
2	A	350	NAP	C3B-C2B-O2B-P2B
2	A	350	NAP	C1B-C2B-O2B-P2B
3	A	351	ZES	N11-C14-C15-C18
2	A	350	NAP	C4D-C5D-O5D-PN
2	A	350	NAP	PN-O3-PA-O1A
2	A	350	NAP	PN-O3-PA-O2A
2	A	350	NAP	PA-O3-PN-O2N

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	ZES	3	0
2	A	350	NAP	7	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 [\(i\)](#)

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

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

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

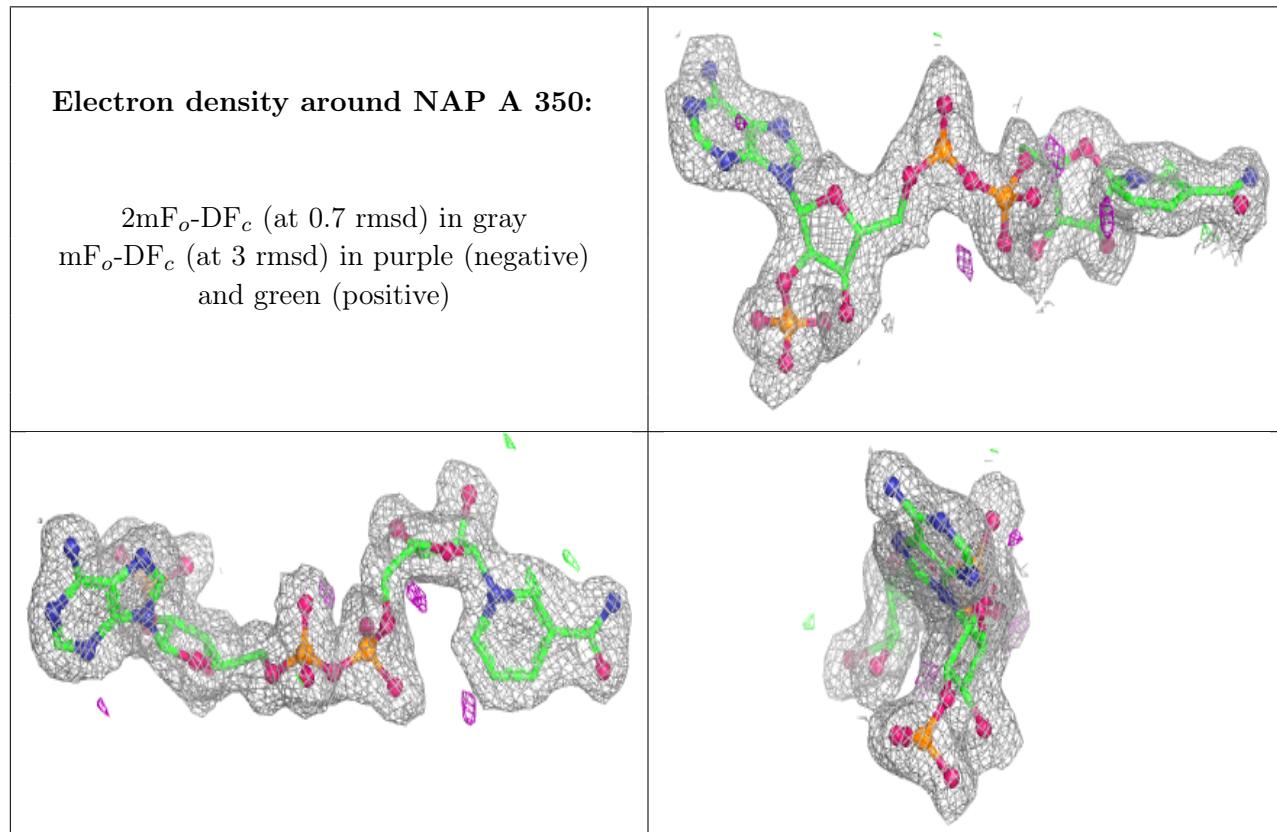
6.3 Carbohydrates [\(i\)](#)

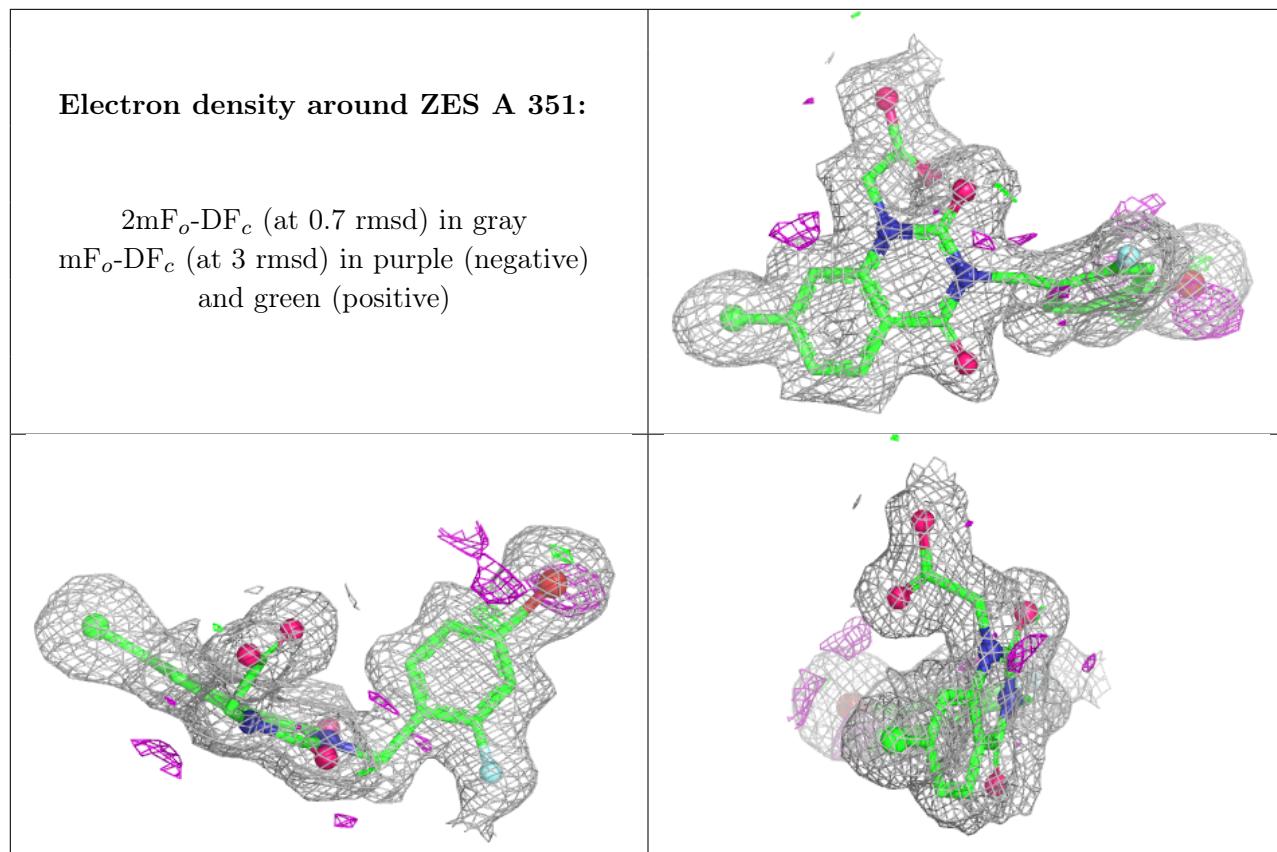
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

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

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





6.5 Other polymers [\(i\)](#)

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