



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:44 AM UTC

PDB ID : 1AZ2 / pdb_00001az2
Title : CITRATE BOUND, C298A/W219Y MUTANT HUMAN ALDOSE REDUCTASE
Authors : Harrison, D.H.; Bohren, K.M.; Ringe, D.; Petsko, G.A.; Gabbay, K.H.
Deposited on : 1997-11-24
Resolution : 2.90 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

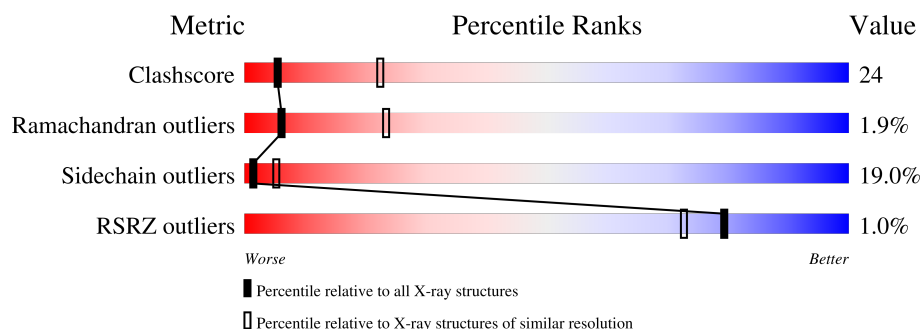
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	315	44% 43% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	700	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2570 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	314	2509	1612	423	463	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	TYR	TRP	engineered mutation	UNP P15121
A	298	ALA	CYS	engineered mutation	UNP P15121

- 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
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).

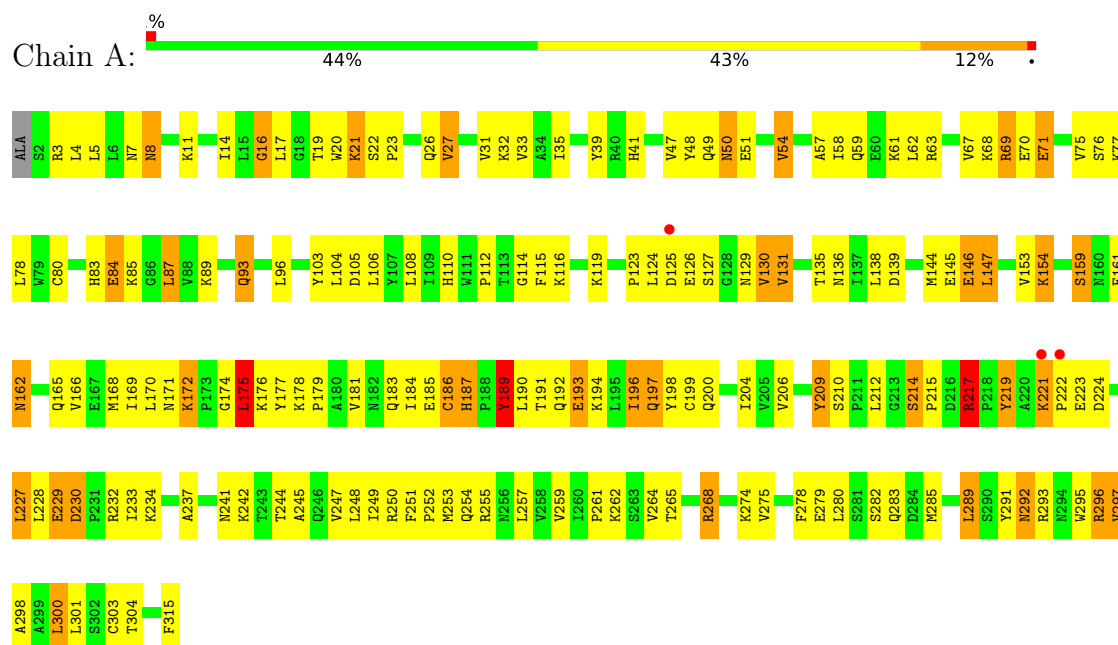


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.03Å 67.17Å 92.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (10.00-2.90) 94.0 (10.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.68Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available) 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2570	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, 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	1.23	17/2570 (0.7%)	1.12	8/3489 (0.2%)

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	8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	SER	C-O	-11.56	1.18	1.23
1	A	139	ASP	C-O	-7.96	1.15	1.24
1	A	16	GLY	C-O	-6.42	1.15	1.23
1	A	196	ILE	C-O	-6.04	1.17	1.24
1	A	189	TYR	C-O	-5.87	1.16	1.24
1	A	199	CYS	C-O	-5.84	1.17	1.24
1	A	159	SER	C-O	-5.83	1.17	1.23
1	A	32	LYS	C-O	-5.70	1.17	1.24
1	A	71	GLU	C-O	-5.53	1.17	1.24
1	A	153	VAL	C-O	-5.47	1.18	1.24
1	A	181	VAL	C-O	-5.24	1.17	1.24
1	A	168	MET	SD-CE	5.15	1.92	1.79
1	A	93	GLN	C-O	-5.12	1.17	1.24
1	A	51	GLU	C-O	-5.07	1.17	1.24
1	A	114	GLY	C-O	-5.07	1.18	1.23
1	A	125	ASP	C-O	5.04	1.29	1.23
1	A	268	ARG	C-O	-5.02	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	CA-C-N	7.89	129.71	119.84
1	A	131	VAL	C-N-CA	7.89	129.71	119.84
1	A	230	ASP	CA-C-N	7.03	127.33	119.32
1	A	230	ASP	C-N-CA	7.03	127.33	119.32
1	A	49	GLN	N-CA-C	6.17	120.14	112.24
1	A	217	ARG	CA-C-N	5.67	126.04	119.47
1	A	217	ARG	C-N-CA	5.67	126.04	119.47
1	A	131	VAL	N-CA-C	5.51	113.37	108.63

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLU	Peptide
1	A	175	LEU	Mainchain
1	A	189	TYR	Sidechain
1	A	198	TYR	Sidechain
1	A	209	TYR	Sidechain
1	A	217	ARG	Sidechain
1	A	39	TYR	Sidechain
1	A	69	ARG	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	2509	0	2524	122	0
2	A	48	0	25	8	0
3	A	13	0	5	2	0
All	All	2570	0	2554	122	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 24.

All (122) 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:116:LYS:HE3	1:A:131:VAL:HG11	1.52	0.91
1:A:215:PRO:HD2	2:A:316:NAP:H4B	1.60	0.81
1:A:84:GLU:HG2	1:A:87:LEU:HD22	1.60	0.80
1:A:221:LYS:HB3	1:A:222:PRO:HD2	1.62	0.79
1:A:68:LYS:HE2	1:A:71:GLU:HG3	1.64	0.77
1:A:214:SER:O	1:A:217:ARG:HD3	1.85	0.77
1:A:250:ARG:HE	1:A:254:GLN:HE21	1.30	0.77
1:A:169:ILE:O	1:A:175:LEU:HG	1.90	0.72
1:A:253:MET:HE1	1:A:275:VAL:HG21	1.73	0.70
1:A:215:PRO:HD2	2:A:316:NAP:C4B	2.24	0.68
1:A:206:VAL:HB	1:A:257:LEU:HD22	1.76	0.67
1:A:58:ILE:O	1:A:62:LEU:HG	1.94	0.67
1:A:193:GLU:O	1:A:197:GLN:HB2	1.96	0.66
1:A:196:ILE:O	1:A:200:GLN:HG3	1.95	0.66
1:A:212:LEU:HD22	1:A:228:LEU:HD21	1.80	0.64
1:A:84:GLU:CG	1:A:87:LEU:HD22	2.28	0.63
1:A:136:ASN:HD22	1:A:138:LEU:H	1.44	0.63
1:A:183:GLN:NE2	2:A:316:NAP:H71N	1.96	0.63
1:A:16:GLY:HA3	1:A:41:HIS:CD2	2.34	0.63
1:A:300:LEU:HD13	1:A:303:CYS:HB2	1.80	0.62
1:A:298:ALA:HB1	3:A:700:CIT:O2	1.98	0.62
1:A:217:ARG:HG3	1:A:219:TYR:CE2	2.34	0.62
1:A:250:ARG:NE	1:A:254:GLN:HE21	1.96	0.62
1:A:262:LYS:O	2:A:316:NAP:H8A	2.01	0.61
1:A:145:GLU:HG2	1:A:177:TYR:HB2	1.81	0.61
1:A:253:MET:HE1	1:A:275:VAL:CG2	2.31	0.60
1:A:4:LEU:HD21	1:A:14:ILE:HD12	1.84	0.59
1:A:251:PHE:CZ	1:A:289:LEU:HD13	2.38	0.59
1:A:178:LYS:HE3	1:A:204:ILE:HD13	1.83	0.59
1:A:285:MET:O	1:A:289:LEU:HB2	2.03	0.59
1:A:187:HIS:HB2	1:A:227:LEU:HD21	1.84	0.58
1:A:227:LEU:HD12	1:A:227:LEU:H	1.69	0.56
1:A:23:PRO:HG2	1:A:26:GLN:HB2	1.87	0.56
1:A:221:LYS:HB3	1:A:222:PRO:CD	2.34	0.56
1:A:254:GLN:HE22	1:A:280:LEU:H	1.51	0.56
1:A:217:ARG:HD2	1:A:297:VAL:HG13	1.87	0.56
1:A:57:ALA:O	1:A:61:LYS:HG2	2.07	0.55
1:A:116:LYS:HB2	1:A:131:VAL:HG12	1.89	0.55
1:A:35:ILE:CD1	1:A:61:LYS:HG3	2.37	0.55
1:A:144:MET:HA	1:A:147:LEU:HD22	1.90	0.54
1:A:68:LYS:HG2	1:A:71:GLU:HG3	1.89	0.54
1:A:22:SER:HB3	1:A:27:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HB	1:A:268:ARG:HG3	1.88	0.53
1:A:20:TRP:HB2	1:A:48:TYR:CZ	2.44	0.53
1:A:221:LYS:HB2	1:A:224:ASP:CG	2.34	0.53
1:A:127:SER:HB2	1:A:129:ASN:OD1	2.09	0.53
1:A:176:LYS:HG2	1:A:177:TYR:CE2	2.43	0.53
1:A:221:LYS:HD3	1:A:224:ASP:OD1	2.08	0.52
1:A:232:ARG:HB3	1:A:291:TYR:OH	2.09	0.52
1:A:123:PRO:O	1:A:130:VAL:HA	2.09	0.52
1:A:22:SER:HB3	1:A:27:VAL:CG2	2.40	0.51
1:A:227:LEU:HD12	1:A:227:LEU:N	2.26	0.51
1:A:249:ILE:HG22	1:A:253:MET:HE3	1.93	0.51
1:A:230:ASP:HB3	1:A:233:ILE:HB	1.92	0.51
1:A:251:PHE:HB3	1:A:252:PRO:HD3	1.93	0.50
1:A:191:THR:HG23	1:A:292:ASN:HB2	1.93	0.50
1:A:233:ILE:HG22	1:A:244:THR:HG23	1.94	0.50
1:A:172:LYS:O	1:A:175:LEU:HB2	2.11	0.50
1:A:185:GLU:OE2	1:A:296:ARG:HA	2.12	0.50
1:A:162:ASN:C	1:A:162:ASN:HD22	2.19	0.50
1:A:219:TYR:CD1	1:A:219:TYR:N	2.79	0.50
1:A:105:ASP:HA	1:A:154:LYS:HB2	1.93	0.50
1:A:27:VAL:HG11	1:A:50:ASN:HB2	1.94	0.49
1:A:124:LEU:HA	1:A:129:ASN:O	2.12	0.49
1:A:145:GLU:HG2	1:A:177:TYR:HD2	1.78	0.49
1:A:174:GLY:O	1:A:176:LYS:N	2.45	0.48
1:A:244:THR:O	1:A:248:LEU:HG	2.13	0.48
1:A:27:VAL:HG13	1:A:54:VAL:HG23	1.96	0.48
1:A:4:LEU:CD2	1:A:14:ILE:HD12	2.44	0.47
1:A:21:LYS:HB2	1:A:21:LYS:NZ	2.29	0.47
1:A:229:GLU:HA	1:A:234:LYS:HE3	1.96	0.47
1:A:19:THR:O	1:A:22:SER:HB2	2.15	0.47
1:A:237:ALA:HA	1:A:247:VAL:HG21	1.95	0.47
1:A:35:ILE:HD13	1:A:61:LYS:HG3	1.97	0.47
1:A:115:PHE:CZ	1:A:303:CYS:SG	3.07	0.47
1:A:185:GLU:HG2	1:A:186:CYS:N	2.28	0.47
1:A:242:LYS:HE3	1:A:278:PHE:CD1	2.49	0.47
1:A:110:HIS:O	1:A:159:SER:HB3	2.15	0.47
1:A:227:LEU:C	1:A:229:GLU:H	2.23	0.47
1:A:96:LEU:HD21	1:A:104:LEU:HG	1.97	0.46
1:A:68:LYS:CG	1:A:71:GLU:HG3	2.46	0.46
1:A:75:VAL:HG13	1:A:106:LEU:HB3	1.97	0.46
1:A:251:PHE:HZ	1:A:289:LEU:HD13	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:O	1:A:170:LEU:HG	2.15	0.46
1:A:176:LYS:HG2	1:A:177:TYR:CD2	2.51	0.46
1:A:293:ARG:O	1:A:293:ARG:HG2	2.16	0.45
1:A:217:ARG:HD3	1:A:217:ARG:H	1.82	0.45
1:A:31:VAL:HB	1:A:57:ALA:CB	2.47	0.45
1:A:115:PHE:CE1	1:A:303:CYS:SG	3.10	0.45
1:A:123:PRO:HB2	1:A:131:VAL:HB	1.98	0.45
1:A:136:ASN:ND2	1:A:138:LEU:H	2.13	0.45
1:A:210:SER:H	2:A:316:NAP:H51N	1.82	0.44
1:A:221:LYS:HB2	1:A:224:ASP:OD1	2.17	0.44
1:A:48:TYR:HE1	3:A:700:CIT:O6	1.99	0.44
1:A:185:GLU:HB2	1:A:209:TYR:CE1	2.53	0.44
1:A:189:TYR:HA	1:A:292:ASN:HA	2.00	0.44
1:A:262:LYS:HB2	2:A:316:NAP:O3D	2.18	0.44
1:A:179:PRO:HB2	1:A:204:ILE:HD12	2.00	0.44
1:A:47:VAL:HG11	1:A:110:HIS:CE1	2.53	0.43
1:A:183:GLN:NE2	2:A:316:NAP:H2N	2.33	0.43
1:A:251:PHE:O	1:A:255:ARG:HG3	2.18	0.43
1:A:77:LYS:HA	1:A:108:LEU:O	2.18	0.43
1:A:20:TRP:CE3	1:A:21:LYS:HE3	2.53	0.43
1:A:35:ILE:HD12	1:A:61:LYS:HG3	1.99	0.43
1:A:80:CYS:HB2	1:A:115:PHE:CD2	2.53	0.43
1:A:8:ASN:HD22	1:A:8:ASN:H	1.66	0.43
1:A:210:SER:H	2:A:316:NAP:C5D	2.32	0.43
1:A:103:TYR:CD1	1:A:154:LYS:HD2	2.54	0.42
1:A:20:TRP:HB2	1:A:48:TYR:CE1	2.55	0.42
1:A:3:ARG:HB3	1:A:11:LYS:HB3	2.01	0.42
1:A:47:VAL:CG1	1:A:110:HIS:CE1	3.03	0.42
1:A:68:LYS:HG2	1:A:71:GLU:OE1	2.19	0.42
1:A:214:SER:O	1:A:217:ARG:CD	2.63	0.41
1:A:259:VAL:HG22	1:A:261:PRO:HD3	2.02	0.41
1:A:161:PHE:CD2	1:A:165:GLN:HB3	2.56	0.41
1:A:190:LEU:HB2	1:A:295:TRP:O	2.20	0.41
1:A:212:LEU:CD2	1:A:245:ALA:HA	2.50	0.41
1:A:169:ILE:H	1:A:169:ILE:HD12	1.86	0.41
1:A:27:VAL:CG1	1:A:54:VAL:HG23	2.51	0.41
1:A:112:PRO:HG3	1:A:161:PHE:CD1	2.55	0.41
1:A:162:ASN:HB2	1:A:315:PHE:OXT	2.21	0.41
1:A:89:LYS:HA	1:A:147:LEU:HD11	2.04	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	312/315 (99%)	283 (91%)	23 (7%)	6 (2%)	6	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	A	221	LYS
1	A	186	CYS
1	A	241	ASN
1	A	223	GLU
1	A	297	VAL

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	279/279 (100%)	226 (81%)	53 (19%)	1	5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASN
1	A	8	ASN
1	A	17	LEU
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	27	VAL
1	A	33	VAL
1	A	50	ASN
1	A	54	VAL
1	A	59	GLN
1	A	63	ARG
1	A	67	VAL
1	A	69	ARG
1	A	70	GLU
1	A	76	SER
1	A	78	LEU
1	A	83	HIS
1	A	84	GLU
1	A	85	LYS
1	A	87	LEU
1	A	93	GLN
1	A	119	LYS
1	A	126	GLU
1	A	130	VAL
1	A	135	THR
1	A	146	GLU
1	A	147	LEU
1	A	154	LYS
1	A	162	ASN
1	A	171	ASN
1	A	172	LYS
1	A	175	LEU
1	A	184	ILE
1	A	187	HIS
1	A	192	GLN
1	A	193	GLU
1	A	194	LYS
1	A	197	GLN
1	A	217	ARG
1	A	219	TYR
1	A	227	LEU
1	A	229	GLU
1	A	264	VAL
1	A	274	LYS
1	A	279	GLU
1	A	282	SER
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	289	LEU
1	A	292	ASN
1	A	296	ARG
1	A	300	LEU
1	A	301	LEU
1	A	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	41	HIS
1	A	50	ASN
1	A	52	ASN
1	A	65	GLN
1	A	93	GLN
1	A	136	ASN
1	A	160	ASN
1	A	162	ASN
1	A	163	HIS
1	A	183	GLN
1	A	254	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](#)

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	CIT	A	700	-	12,12,12	4.92	7 (58%)	17,17,17	3.14	11 (64%)
2	NAP	A	316	-	50,52,52	1.54	6 (12%)	71,80,80	2.25	24 (33%)

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	CIT	A	700	-	-	5/16/16/16	-
2	NAP	A	316	-	-	11/35/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	CIT	C2-C3	14.11	1.71	1.54
3	A	700	CIT	C4-C3	7.20	1.62	1.54
2	A	316	NAP	C2N-N1N	5.81	1.41	1.35
2	A	316	NAP	C6N-N1N	3.36	1.43	1.35
2	A	316	NAP	C4A-N9A	-3.16	1.31	1.37
2	A	316	NAP	C5A-N7A	-2.85	1.33	1.39
3	A	700	CIT	O1-C1	2.79	1.31	1.22
2	A	316	NAP	PN-O3	2.62	1.62	1.59
3	A	700	CIT	C4-C5	2.61	1.58	1.50
3	A	700	CIT	O6-C6	-2.47	1.21	1.30
3	A	700	CIT	O2-C1	-2.31	1.23	1.30
3	A	700	CIT	C2-C1	2.28	1.57	1.50
2	A	316	NAP	PA-O1A	-2.12	1.43	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	CIT	O6-C6-C3	7.73	127.97	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	NAP	O4D-C4D-C5D	-6.57	88.28	109.33
2	A	316	NAP	N3A-C2A-N1A	-5.97	119.55	128.58
3	A	700	CIT	O7-C3-C4	-5.69	96.40	109.38
2	A	316	NAP	O2A-PA-O3	5.45	122.00	107.27
2	A	316	NAP	C5A-C4A-N3A	-4.53	120.48	126.72
2	A	316	NAP	C2A-N3A-C4A	4.01	121.62	111.83
2	A	316	NAP	C6A-C5A-N7A	-3.96	124.46	132.09
2	A	316	NAP	O2N-PN-O3	3.87	117.74	107.27
2	A	316	NAP	N3A-C4A-N9A	3.77	133.58	127.17
2	A	316	NAP	O4B-C1B-N9A	3.68	115.16	108.09
2	A	316	NAP	O2X-P2B-O2B	-3.62	91.74	105.85
2	A	316	NAP	C6N-N1N-C2N	-3.35	119.02	121.88
3	A	700	CIT	O5-C6-C3	-3.13	116.03	122.09
3	A	700	CIT	C4-C3-C6	3.08	116.84	110.03
3	A	700	CIT	C2-C3-C6	-3.07	103.25	110.03
2	A	316	NAP	C4A-C5A-N7A	3.04	114.05	110.58
3	A	700	CIT	O2-C1-C2	3.01	123.89	114.35
3	A	700	CIT	C4-C3-C2	2.97	116.93	109.31
2	A	316	NAP	C3N-C7N-N7N	-2.90	114.17	117.74
2	A	316	NAP	C4A-N9A-C1B	-2.90	119.86	126.63
2	A	316	NAP	C4A-N9A-C8A	2.81	108.69	105.74
3	A	700	CIT	O1-C1-C2	-2.76	115.14	122.95
2	A	316	NAP	O5B-C5B-C4B	-2.56	100.28	108.99
2	A	316	NAP	C4D-O4D-C1D	2.46	112.18	109.92
3	A	700	CIT	O6-C6-O5	-2.46	115.99	123.86
3	A	700	CIT	O3-C5-C4	-2.38	116.21	122.95
2	A	316	NAP	O3X-P2B-O2X	2.35	116.62	107.80
2	A	316	NAP	O4B-C4B-C3B	2.27	109.65	105.15
2	A	316	NAP	O7N-C7N-C3N	2.24	122.33	119.60
2	A	316	NAP	O3D-C3D-C4D	2.22	117.47	111.08
2	A	316	NAP	C6N-N1N-C1D	2.16	123.96	119.73
2	A	316	NAP	O3-PA-O1A	-2.14	104.28	110.70
2	A	316	NAP	C2A-N1A-C6A	2.10	122.18	118.73
3	A	700	CIT	O7-C3-C6	2.08	111.91	108.96

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	316	NAP	C5B-O5B-PA-O2A
2	A	316	NAP	C5B-O5B-PA-O3
2	A	316	NAP	C5D-O5D-PN-O3

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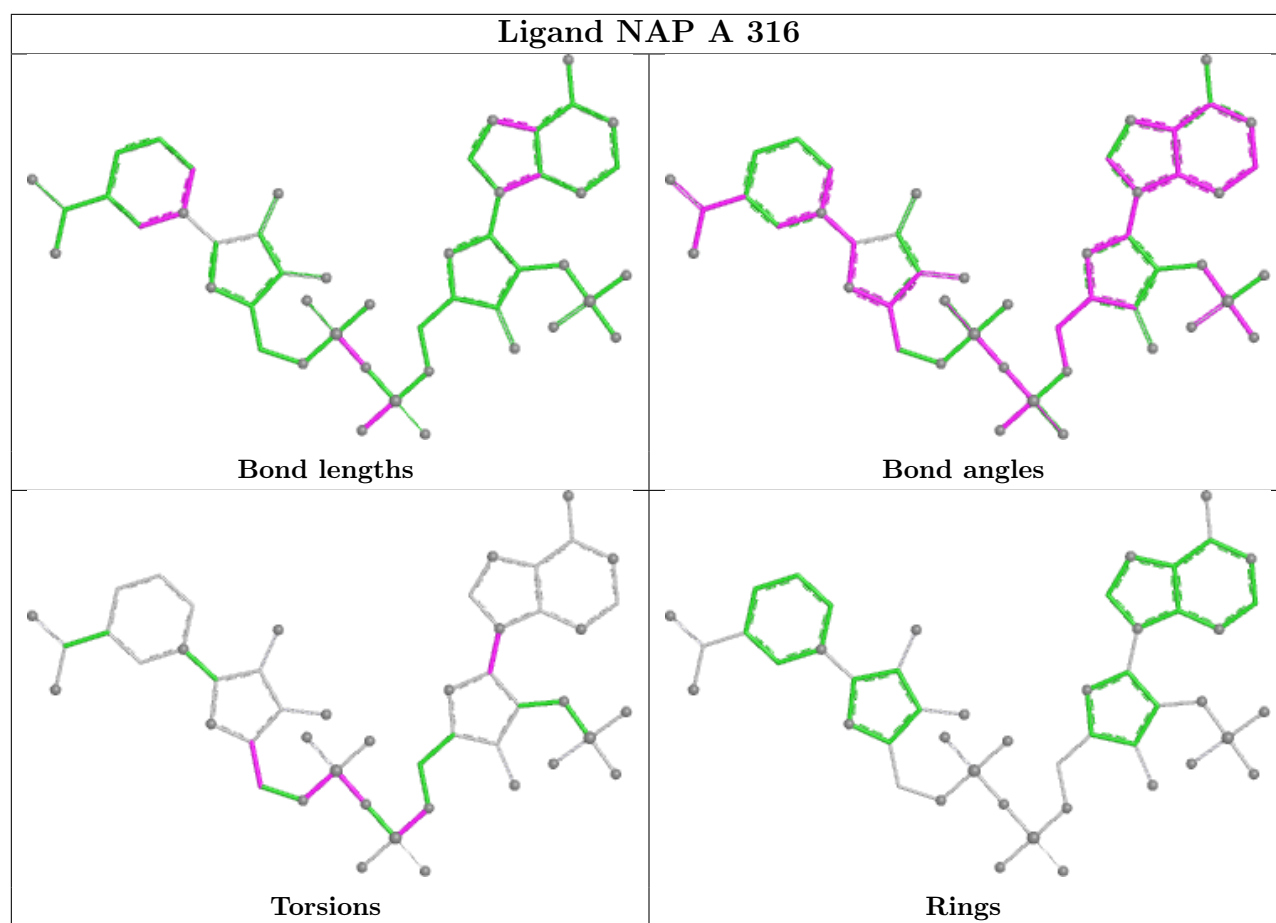
Mol	Chain	Res	Type	Atoms
2	A	316	NAP	C5D-O5D-PN-O2N
3	A	700	CIT	C2-C3-C6-O5
3	A	700	CIT	C2-C3-C6-O6
3	A	700	CIT	O7-C3-C6-O5
3	A	700	CIT	O7-C3-C6-O6
2	A	316	NAP	O4D-C4D-C5D-O5D
2	A	316	NAP	PA-O3-PN-O1N
3	A	700	CIT	O7-C3-C4-C5
2	A	316	NAP	PA-O3-PN-O5D
2	A	316	NAP	C5B-O5B-PA-O1A
2	A	316	NAP	C5D-O5D-PN-O1N
2	A	316	NAP	C2B-C1B-N9A-C8A
2	A	316	NAP	O4B-C1B-N9A-C8A

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	CIT	2	0
2	A	316	NAP	8	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	314/315 (99%)	-0.29	3 (0%) 79 73	18, 19, 20, 20	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	3.0
1	A	222	PRO	2.4
1	A	221	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

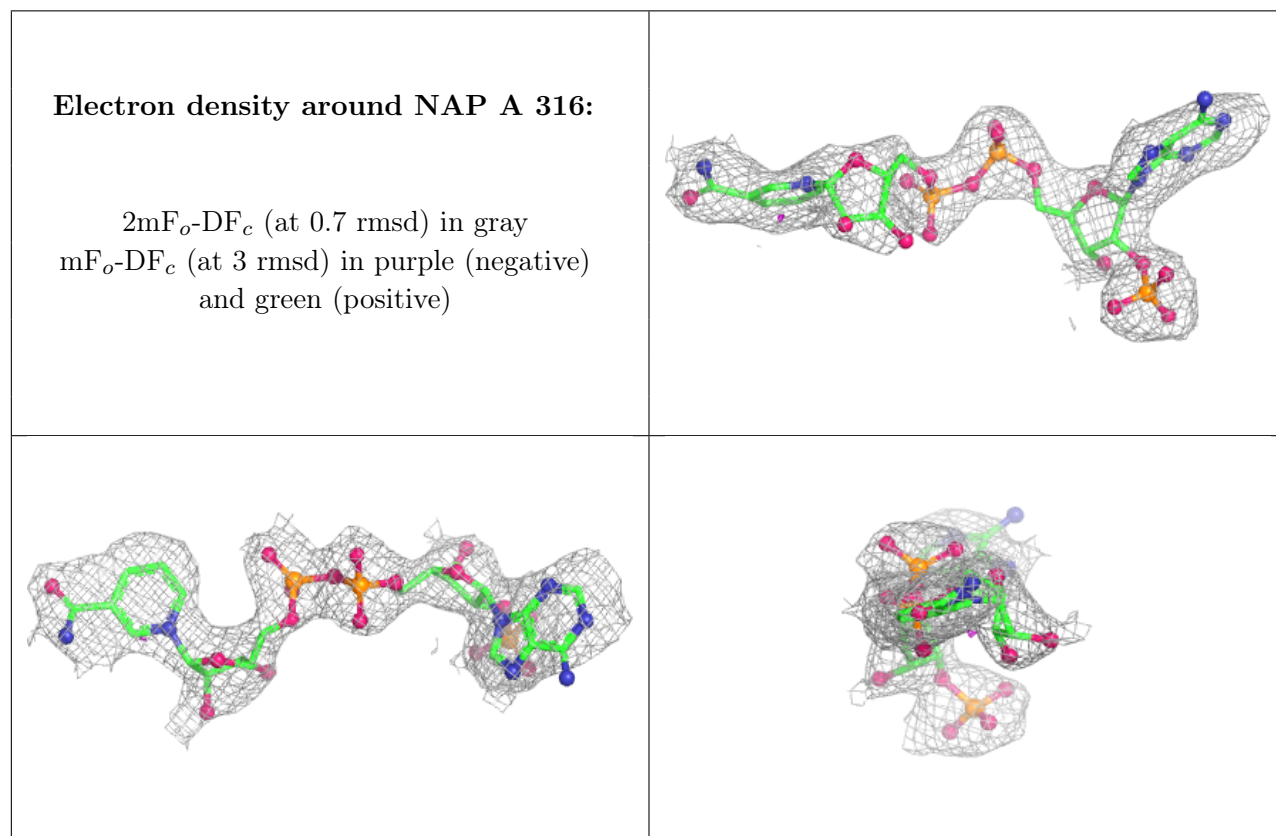
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIT	A	700	13/13	0.83	0.12	32,32,32,32	0
2	NAP	A	316	48/48	0.96	0.08	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.