



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 08:27 pm BST

PDB ID : 1UWL
Title : 1.76Å Structure of Urocanate Hydratase from Pseudomonas putida
Authors : Kessler, D.; Retey, J.; Schulz, G.E.
Deposited on : 2004-02-05
Resolution : 1.76 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
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

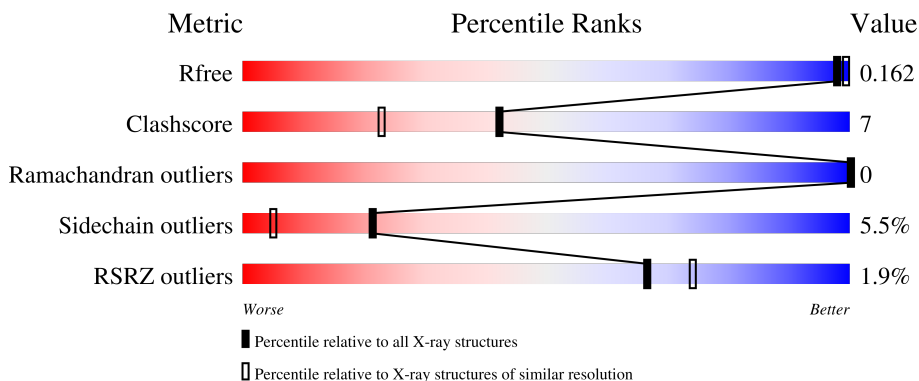
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	557	 2% 88% 9% ..
1	B	557	 2% 83% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9388 atoms, of which 6 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 UROCANATE HYDRATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	551	4226	2648	3	756	797	22	0	0	1
1	B	550	4225	2648	3	755	797	22	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

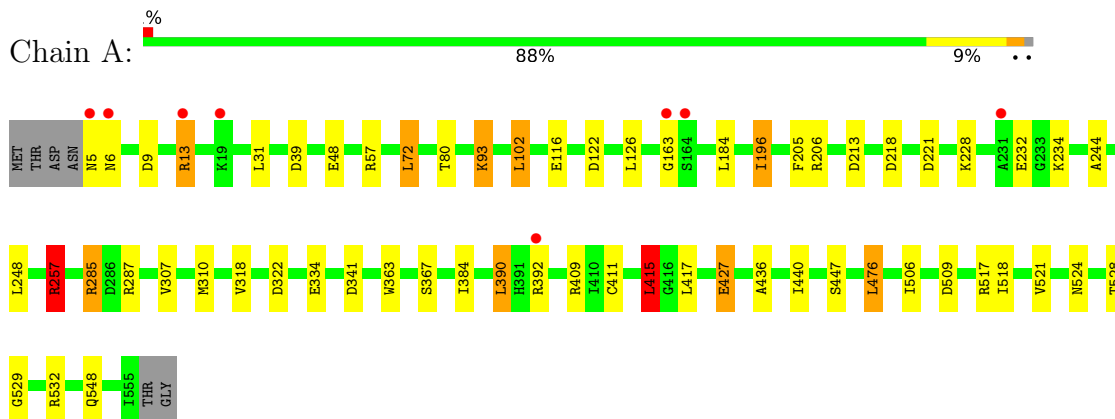
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SER	CYS	engineered mutation	UNP P25080
B	198	SER	CYS	engineered mutation	UNP P25080
A	6	ASN	LYS	conflict	UNP P25080
B	6	ASN	LYS	conflict	UNP P25080
A	164	SER	THR	conflict	UNP P25080
A	165	LEU	VAL	conflict	UNP P25080
A	167	GLY	ALA	conflict	UNP P25080
B	164	SER	THR	conflict	UNP P25080
B	165	LEU	VAL	conflict	UNP P25080
B	167	GLY	ALA	conflict	UNP P25080

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

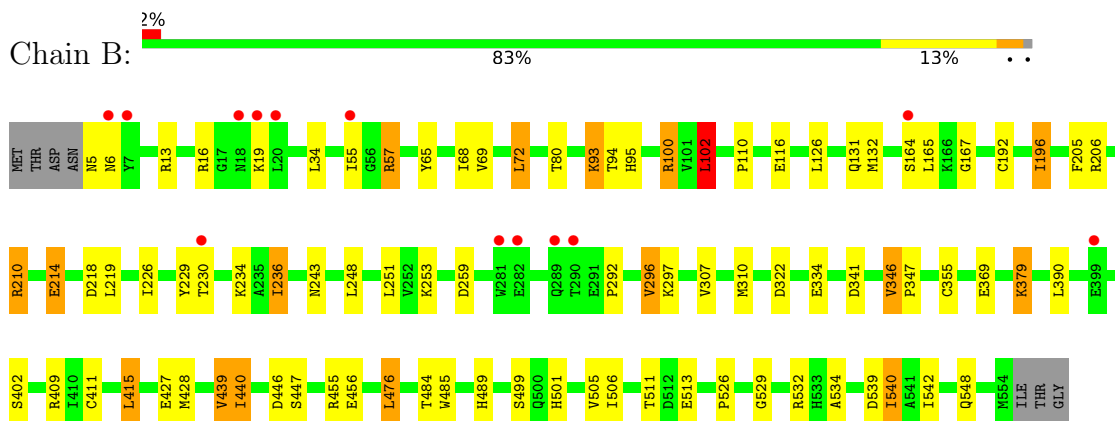
3 Residue-property plots [i](#)

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 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: UROCANATE HYDRATASE



- Molecule 1: UROCANATE HYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.43Å 71.62Å 129.12Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	24.33 – 1.76 24.31 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.33-1.76) 99.1 (24.31-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 1.76Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.189 0.163 , 0.162	Depositor DCC
R_{free} test set	4924 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: NAD

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	0.80	3/4316 (0.1%)	0.93	17/5859 (0.3%)
1	B	0.78	4/4315 (0.1%)	0.94	15/5857 (0.3%)
All	All	0.79	7/8631 (0.1%)	0.93	32/11716 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	GLU	CD-OE1	7.12	1.33	1.25
1	B	439	VAL	CB-CG2	-6.03	1.40	1.52
1	B	346	VAL	CB-CG1	-6.03	1.40	1.52
1	A	116	GLU	CD-OE2	5.57	1.31	1.25
1	A	427	GLU	CG-CD	5.35	1.59	1.51
1	A	116	GLU	CD-OE1	5.10	1.31	1.25
1	B	192	CYS	C-O	5.08	1.33	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	B	100	ARG	NE-CZ-NH1	12.17	126.38	120.30
1	A	509	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	341	ASP	CB-CG-OD2	7.47	125.02	118.30
1	A	257	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	57	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	B	539	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	72	LEU	CB-CG-CD1	6.81	122.58	111.00
1	B	100	ARG	CG-CD-NE	-6.70	97.73	111.80
1	B	57	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	341	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	9	ASP	CB-CG-OD2	6.23	123.91	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	57	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	322	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	476	LEU	CB-CG-CD1	5.82	120.90	111.00
1	A	122	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	287	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	39	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	409	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	259	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	415	LEU	CB-CG-CD2	5.67	120.63	111.00
1	B	446	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	257	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	218	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	485	TRP	CA-CB-CG	5.49	124.14	113.70
1	A	409	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	221	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	213	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	102	LEU	CB-CG-CD1	5.21	119.85	111.00
1	B	57	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	218	ASP	CB-CG-OD2	5.07	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4223	3	4124	41	0
1	B	4222	3	4124	74	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
3	A	443	0	0	8	0
3	B	406	0	0	11	0
All	All	9382	6	8300	116	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 7.

All (116) 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:163:GLY:O	3:A:2182:HOH:O	1.75	1.03
1:A:13:ARG:NH1	3:A:2016:HOH:O	2.00	0.93
1:B:68:ILE:HD12	1:B:69:VAL:N	1.84	0.92
1:B:540:ILE:HD13	3:B:2385:HOH:O	1.71	0.91
1:B:346:VAL:HG12	3:B:2346:HOH:O	1.71	0.90
1:B:94:THR:HG23	1:B:95:HIS:H	1.44	0.82
1:B:346:VAL:HG11	1:B:456:GLU:HA	1.62	0.82
1:B:34:LEU:CD2	1:B:68:ILE:HD13	2.11	0.81
1:B:369:GLU:OE1	3:B:2288:HOH:O	2.01	0.79
1:B:346:VAL:HG13	1:B:347:PRO:HD3	1.65	0.77
1:A:415:LEU:HD13	1:A:548:GLN:HG3	1.68	0.76
1:A:93:LYS:HZ2	1:A:93:LYS:H	1.32	0.75
1:A:506:ILE:HD13	1:A:521:VAL:HG11	1.70	0.74
1:B:226:ILE:O	1:B:230:THR:HG22	1.92	0.70
1:B:94:THR:HG23	1:B:95:HIS:N	2.06	0.69
1:A:517:ARG:O	1:A:521:VAL:HG12	1.92	0.68
1:B:346:VAL:HG13	1:B:347:PRO:CD	2.24	0.68
1:A:307:VAL:HG22	1:A:310:MET:HE3	1.76	0.67
1:B:229:TYR:CE2	1:B:236:ILE:HD12	2.30	0.67
1:A:390:LEU:HD12	1:A:390:LEU:O	1.95	0.67
1:B:369:GLU:HG3	3:B:2288:HOH:O	1.95	0.66
1:B:390:LEU:HD21	1:B:411:CYS:SG	2.35	0.66
1:B:534:ALA:HB1	1:B:542:ILE:HD13	1.79	0.65
1:B:34:LEU:HD21	1:B:68:ILE:CD1	2.27	0.65
1:A:390:LEU:HD13	3:A:2358:HOH:O	1.97	0.63
1:B:292:PRO:O	1:B:296:VAL:HG12	1.99	0.63
2:B:1555:NAD:C4N	3:B:2337:HOH:O	2.47	0.63
1:B:439:VAL:CG2	1:B:505:VAL:CG1	2.77	0.62
1:B:307:VAL:HG22	1:B:310:MET:CE	2.29	0.62
1:A:384:ILE:CD1	1:A:417:LEU:HD22	2.30	0.61
1:B:65:TYR:O	1:B:68:ILE:HG13	2.00	0.61
1:B:439:VAL:HG22	1:B:505:VAL:CG1	2.30	0.61
1:B:34:LEU:HD21	1:B:68:ILE:HD13	1.82	0.60
1:A:196:ILE:HD11	1:A:244:ALA:N	2.18	0.58
1:B:214:GLU:CG	1:B:236:ILE:HD11	2.33	0.58
1:B:164:SER:O	1:B:165:LEU:HB2	2.04	0.58
1:A:196:ILE:CD1	1:A:244:ALA:HB2	2.34	0.57
1:B:346:VAL:CG1	1:B:455:ARG:O	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TRP:HB3	1:A:440:ILE:HD13	1.87	0.57
1:B:540:ILE:HD13	1:B:540:ILE:H	1.70	0.57
1:A:506:ILE:CD1	1:A:521:VAL:HG11	2.33	0.57
1:B:415:LEU:HD13	1:B:548:GLN:HG3	1.87	0.57
1:B:439:VAL:C	1:B:440:ILE:HD12	2.25	0.57
1:A:390:LEU:HD11	1:A:411:CYS:SG	2.46	0.56
1:B:210:ARG:NH1	1:B:402:SER:OG	2.38	0.56
1:A:196:ILE:HD12	1:A:244:ALA:HB2	1.88	0.56
1:B:93:LYS:H	1:B:93:LYS:NZ	2.03	0.56
1:B:307:VAL:HA	1:B:310:MET:CE	2.36	0.56
1:A:80:THR:HG21	1:A:102:LEU:HD22	1.88	0.56
1:A:447:SER:OG	1:A:529:GLY:HA3	2.06	0.55
1:B:511:THR:HG22	1:B:513:GLU:OE2	2.06	0.55
1:B:540:ILE:CD1	3:B:2385:HOH:O	2.38	0.55
1:A:5:ASN:N	3:A:2003:HOH:O	2.39	0.54
1:A:384:ILE:HD12	1:A:417:LEU:HD13	1.89	0.54
1:B:196:ILE:HD11	1:B:243:ASN:C	2.28	0.54
1:A:257:ARG:CG	1:A:257:ARG:HH11	2.22	0.52
1:B:219:LEU:HD11	1:B:251:LEU:HD21	1.92	0.52
1:B:229:TYR:CD2	1:B:236:ILE:HG21	2.45	0.52
1:B:65:TYR:O	1:B:68:ILE:CD1	2.58	0.52
2:B:1555:NAD:C5N	3:B:2337:HOH:O	2.58	0.51
1:B:210:ARG:NH1	1:B:402:SER:CB	2.73	0.51
1:B:80:THR:OG1	1:B:94:THR:HG21	2.11	0.51
1:A:93:LYS:H	1:A:93:LYS:NZ	2.07	0.51
1:B:80:THR:HG21	1:B:102:LEU:HD22	1.93	0.51
1:B:489:HIS:HB2	1:B:501:HIS:CE1	2.46	0.51
1:B:229:TYR:CD2	1:B:236:ILE:CG2	2.94	0.50
1:A:384:ILE:HD11	1:A:417:LEU:HD22	1.93	0.50
1:B:167:GLY:O	1:B:230:THR:OG1	2.28	0.50
1:A:228:LYS:NZ	1:A:232:GLU:OE1	2.44	0.49
1:B:440:ILE:CD1	1:B:440:ILE:N	2.75	0.49
1:B:93:LYS:HE2	3:B:2094:HOH:O	2.13	0.48
1:B:307:VAL:HA	1:B:310:MET:HE2	1.94	0.48
1:A:6:ASN:O	1:A:48:GLU:HA	2.14	0.48
1:B:296:VAL:HG11	3:B:2120:HOH:O	2.14	0.48
1:B:511:THR:CG2	1:B:513:GLU:OE2	2.62	0.48
1:A:196:ILE:HD11	2:A:1555:NAD:H2A	1.96	0.47
1:B:346:VAL:HG11	1:B:455:ARG:O	2.14	0.47
1:A:31:LEU:C	1:A:31:LEU:HD23	2.35	0.47
1:B:369:GLU:CG	3:B:2288:HOH:O	2.60	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:HB3	1:B:102:LEU:HG	1.96	0.47
1:B:34:LEU:HD21	1:B:68:ILE:HD11	1.96	0.46
1:A:196:ILE:CD1	2:A:1555:NAD:H2A	2.45	0.46
1:B:68:ILE:CD1	1:B:69:VAL:HG23	2.45	0.46
1:B:415:LEU:HD23	1:B:526:PRO:HG2	1.98	0.46
1:A:234:LYS:HG3	3:A:2229:HOH:O	2.15	0.46
1:A:392:ARG:HG2	3:A:2339:HOH:O	2.15	0.45
1:B:346:VAL:HG11	1:B:456:GLU:CA	2.40	0.45
1:B:440:ILE:HD12	1:B:440:ILE:N	2.31	0.45
1:A:518:ILE:HA	1:A:521:VAL:CG1	2.47	0.45
1:B:68:ILE:HD12	1:B:69:VAL:HG23	1.98	0.45
1:A:13:ARG:NH1	3:A:2015:HOH:O	2.49	0.45
1:B:68:ILE:HD12	1:B:69:VAL:H	1.71	0.44
1:A:307:VAL:HA	1:A:310:MET:HE2	1.99	0.44
1:B:307:VAL:HA	1:B:310:MET:HE3	2.00	0.43
1:A:384:ILE:HD12	1:A:417:LEU:CD1	2.47	0.43
1:A:518:ILE:HA	1:A:521:VAL:HG12	1.99	0.43
1:B:68:ILE:O	1:B:72:LEU:HD22	2.17	0.43
1:B:164:SER:O	1:B:165:LEU:CB	2.67	0.43
1:B:447:SER:OG	1:B:529:GLY:HA3	2.19	0.43
1:B:307:VAL:HG22	1:B:310:MET:HE2	1.99	0.43
1:A:524:ASN:O	1:A:528:THR:HG23	2.19	0.43
1:B:484:THR:OG1	1:B:506:ILE:HD12	2.19	0.43
1:B:534:ALA:HB1	1:B:542:ILE:CD1	2.46	0.43
1:B:214:GLU:CD	1:B:236:ILE:HD11	2.38	0.43
1:A:307:VAL:HA	1:A:310:MET:CE	2.48	0.42
1:B:296:VAL:HG13	1:B:297:LYS:NZ	2.33	0.42
1:B:5:ASN:N	3:B:2002:HOH:O	2.51	0.42
1:B:34:LEU:CD2	1:B:68:ILE:CD1	2.84	0.42
1:A:285:ARG:NH2	3:A:2267:HOH:O	2.52	0.42
1:B:55:ILE:HD11	1:B:57:ARG:NH1	2.35	0.42
1:B:439:VAL:HG22	1:B:505:VAL:HG13	2.01	0.42
1:A:390:LEU:HD12	1:A:390:LEU:C	2.40	0.41
1:A:367:SER:HB3	1:A:436:ALA:HB3	2.03	0.40
1:B:131:GLN:HB3	1:B:132:MET:H	1.79	0.40
1:B:379:LYS:NZ	1:B:428:MET:SD	2.93	0.40
1:B:355:CYS:HB3	1:B:540:ILE:HG12	2.03	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	549/557 (99%)	532 (97%)	17 (3%)	0	100	100
1	B	548/557 (98%)	529 (96%)	19 (4%)	0	100	100
All	All	1097/1114 (98%)	1061 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	433/439 (99%)	414 (96%)	19 (4%)	28	8
1	B	433/439 (99%)	404 (93%)	29 (7%)	16	3
All	All	866/878 (99%)	818 (94%)	48 (6%)	21	5

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	72	LEU
1	A	93	LYS
1	A	102	LEU
1	A	126	LEU
1	A	184	LEU
1	A	196	ILE
1	A	205	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ARG
1	A	248	LEU
1	A	257	ARG
1	A	285	ARG
1	A	318	VAL
1	A	334	GLU
1	A	390	LEU
1	A	415	LEU
1	A	427	GLU
1	A	476	LEU
1	A	532	ARG
1	B	6	ASN
1	B	13	ARG
1	B	16	ARG
1	B	19	LYS
1	B	72	LEU
1	B	93	LYS
1	B	100	ARG
1	B	102	LEU
1	B	110	PRO
1	B	126	LEU
1	B	196	ILE
1	B	205	PHE
1	B	206	ARG
1	B	210	ARG
1	B	214	GLU
1	B	234	LYS
1	B	236	ILE
1	B	248	LEU
1	B	253	LYS
1	B	296	VAL
1	B	334	GLU
1	B	379	LYS
1	B	415	LEU
1	B	427	GLU
1	B	440	ILE
1	B	476	LEU
1	B	499	SER
1	B	532	ARG
1	B	540	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	241	HIS
1	B	264	GLN
1	B	316	GLN
1	B	500	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 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$
2	NAD	B	1555	-	42,48,48	1.71	5 (11%)	50,73,73	1.28	6 (12%)
2	NAD	A	1555	-	42,48,48	1.65	4 (9%)	50,73,73	1.33	5 (10%)

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
2	NAD	B	1555	-	-	5/26/62/62	0/5/5/5
2	NAD	A	1555	-	-	5/26/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1555	NAD	O7N-C7N	7.81	1.39	1.24
2	A	1555	NAD	O7N-C7N	7.65	1.38	1.24
2	B	1555	NAD	C2A-N3A	4.07	1.38	1.32
2	A	1555	NAD	C2A-N3A	3.46	1.37	1.32
2	A	1555	NAD	C2A-N1A	2.99	1.39	1.33
2	B	1555	NAD	O4D-C1D	2.52	1.44	1.41
2	A	1555	NAD	O4B-C1B	2.47	1.44	1.41
2	B	1555	NAD	O2B-C2B	-2.46	1.37	1.43
2	B	1555	NAD	C2A-N1A	2.28	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1555	NAD	N3A-C2A-N1A	-4.44	121.75	128.68
2	B	1555	NAD	N3A-C2A-N1A	-4.26	122.01	128.68
2	A	1555	NAD	C6N-N1N-C2N	-3.37	118.90	121.97
2	A	1555	NAD	C3N-C7N-N7N	3.30	121.71	117.75
2	B	1555	NAD	O4D-C1D-C2D	-3.16	102.31	106.93
2	A	1555	NAD	O7N-C7N-N7N	-2.74	118.68	122.58
2	B	1555	NAD	C2N-C3N-C4N	2.30	120.86	118.26
2	B	1555	NAD	C3N-C7N-N7N	2.19	120.38	117.75
2	A	1555	NAD	C5N-C4N-C3N	-2.18	117.76	120.34
2	B	1555	NAD	C6N-N1N-C2N	-2.17	119.99	121.97
2	B	1555	NAD	C5N-C4N-C3N	-2.09	117.86	120.34

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1555	NAD	O4D-C1D-N1N-C2N
2	A	1555	NAD	O4D-C1D-N1N-C6N
2	A	1555	NAD	C2D-C1D-N1N-C2N
2	A	1555	NAD	C2D-C1D-N1N-C6N
2	B	1555	NAD	O4D-C1D-N1N-C2N
2	B	1555	NAD	O4D-C1D-N1N-C6N
2	B	1555	NAD	C2D-C1D-N1N-C2N

Continued on next page...

Continued from previous page...

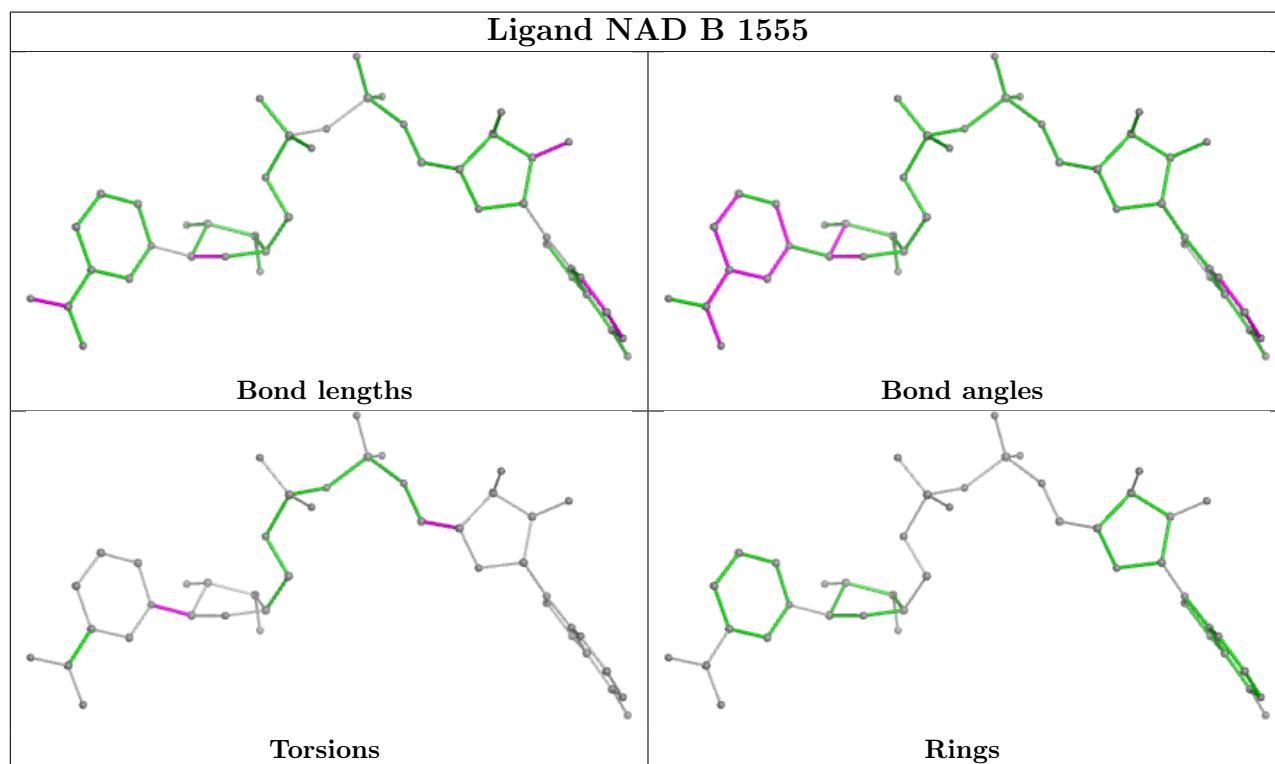
Mol	Chain	Res	Type	Atoms
2	B	1555	NAD	C2D-C1D-N1N-C6N
2	A	1555	NAD	O4B-C4B-C5B-O5B
2	B	1555	NAD	O4B-C4B-C5B-O5B

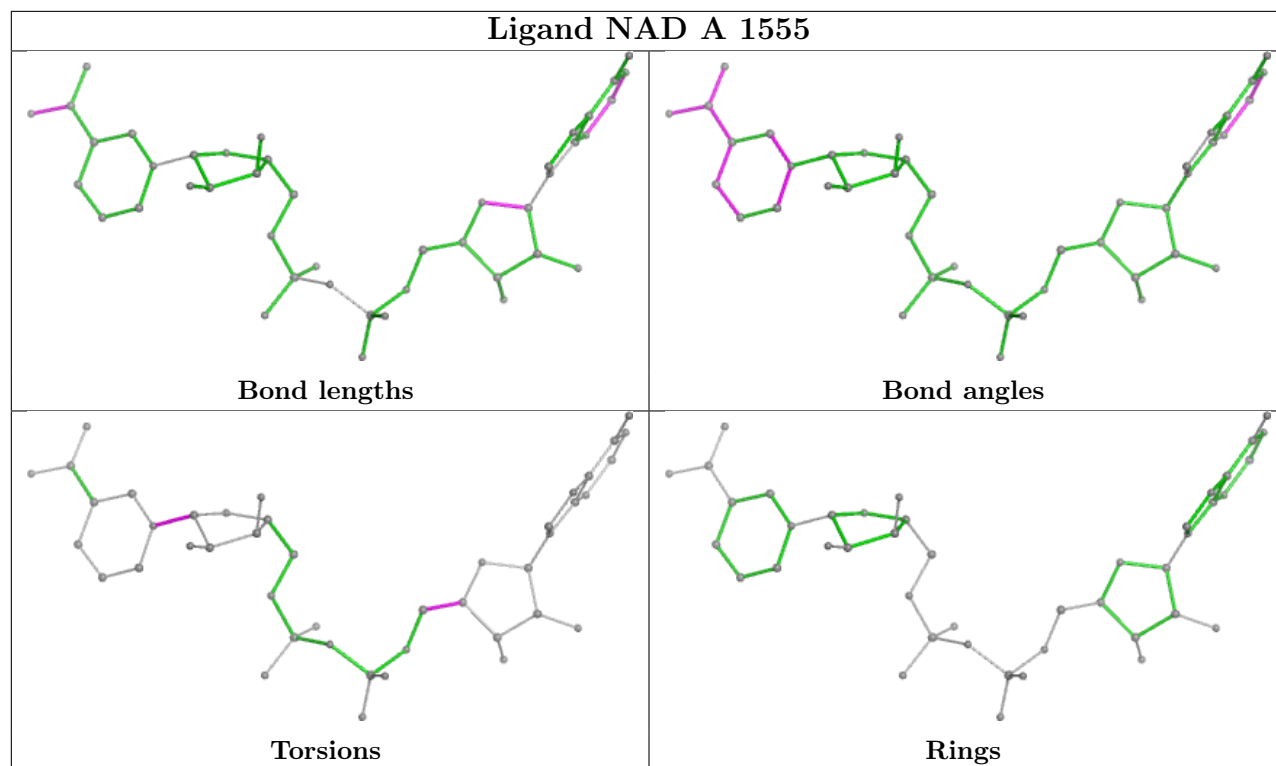
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1555	NAD	2	0
2	A	1555	NAD	2	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

6.1 Protein, DNA and RNA chains

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	551/557 (98%)	-0.09	8 (1%) 73 80	8, 12, 22, 30	0
1	B	550/557 (98%)	0.09	13 (2%) 59 65	7, 14, 25, 36	0
All	All	1101/1114 (98%)	-0.00	21 (1%) 66 74	7, 13, 24, 36	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	LYS	4.1
1	B	164	SER	4.0
1	A	164	SER	4.0
1	A	5	ASN	3.9
1	B	7	TYR	3.7
1	B	289	GLN	3.4
1	B	6	ASN	3.4
1	B	282	GLU	3.0
1	A	392	ARG	2.8
1	A	19	LYS	2.8
1	A	13	ARG	2.7
1	A	163	GLY	2.5
1	B	20	LEU	2.5
1	B	18	ASN	2.3
1	A	6	ASN	2.3
1	A	231	ALA	2.3
1	B	230	THR	2.2
1	B	281	TRP	2.2
1	B	55	ILE	2.1
1	B	290	THR	2.1
1	B	399	GLU	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

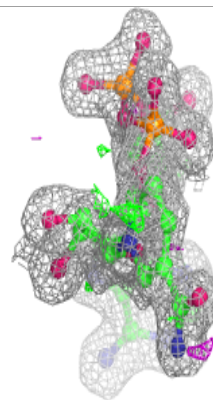
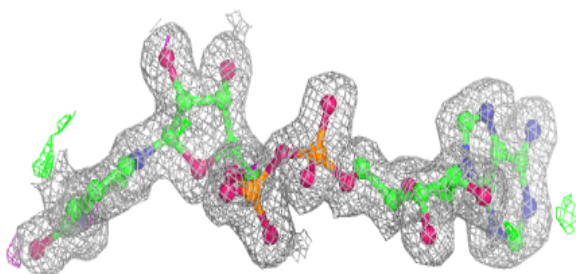
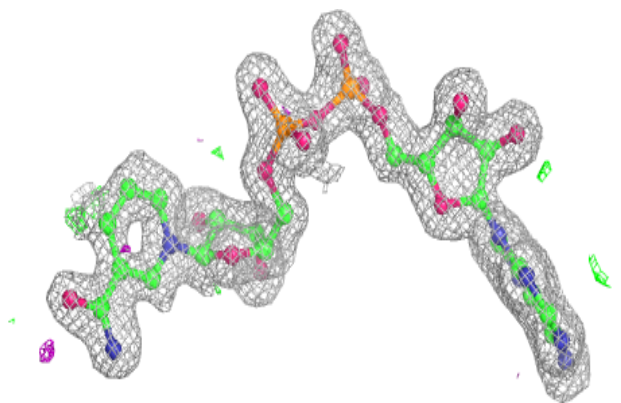
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	B	1555	44/44	0.96	0.09	11,14,19,22	0
2	NAD	A	1555	44/44	0.97	0.08	8,11,15,17	0

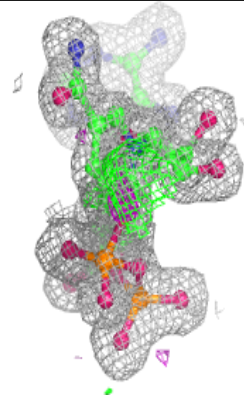
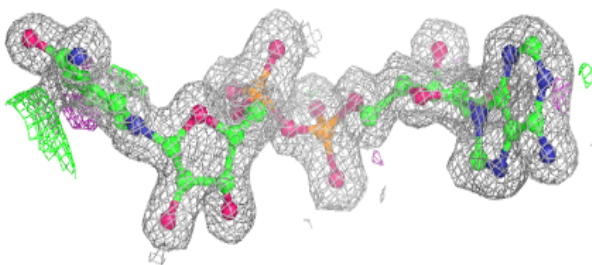
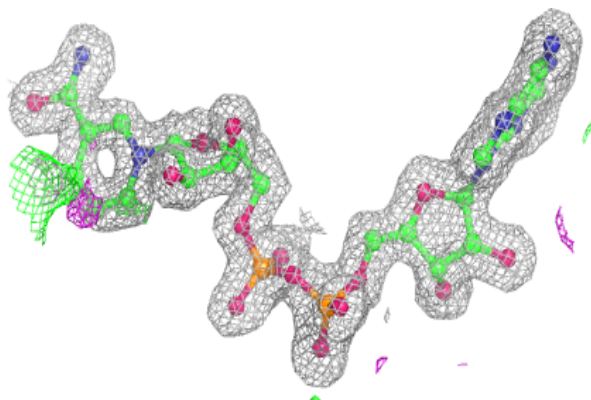
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 1555:

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

**Electron density around NAD A 1555:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.