



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:44 AM UTC

PDB ID : 5GZ6 / pdb_00005gz6
Title : Structure of D-amino acid dehydrogenase in complex with NADPH and 2-ket
o-6-aminocaproic acid
Authors : Sakuraba, H.; Seto, T.; Hayashi, J.; Akita, H.; Yoneda, K.; Ohshima, T.
Deposited on : 2016-09-26
Resolution : 1.74 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

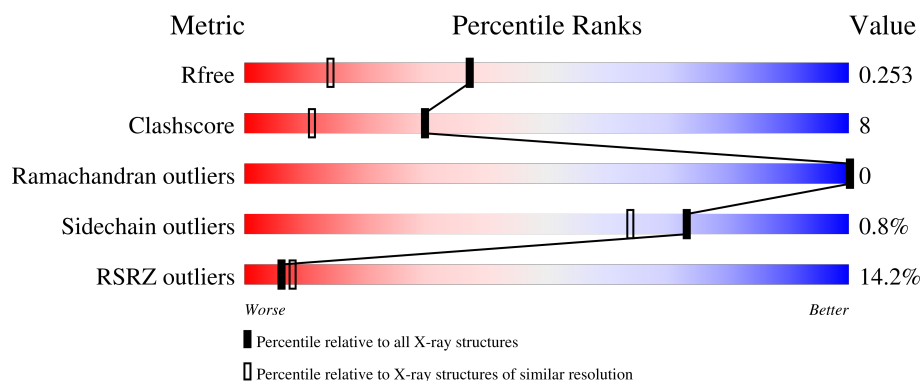
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	326	13% 81% 15% ..
1	B	326	14% 74% 20% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5400 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 Meso-diaminopimelate D-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2465	1563	422	472	8			
1	B	316	Total	C	N	O	S	0	1	0
			2466	1564	424	470	8			

There are 14 discrepancies between the modelled and reference sequences:

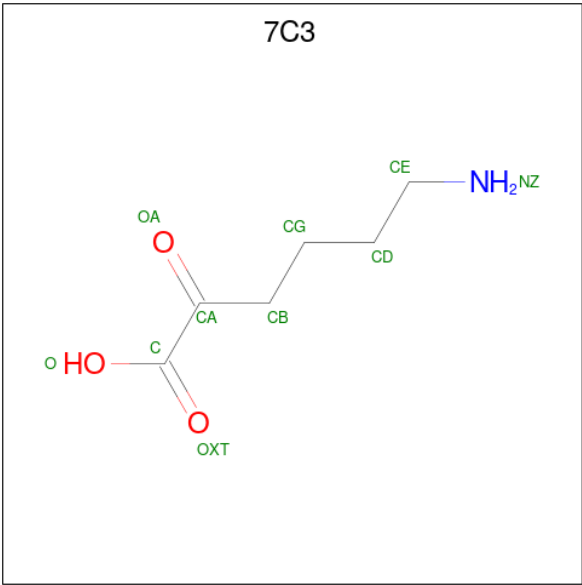
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	ASP	engineered mutation	UNP G1UII1
A	154	LEU	GLN	engineered mutation	UNP G1UII1
A	158	GLY	ASP	engineered mutation	UNP G1UII1
A	173	ILE	THR	engineered mutation	UNP G1UII1
A	199	MET	ARG	engineered mutation	UNP G1UII1
A	224	PHE	TYR	engineered mutation	UNP G1UII1
A	249	ASN	HIS	engineered mutation	UNP G1UII1
B	94	ALA	ASP	engineered mutation	UNP G1UII1
B	154	LEU	GLN	engineered mutation	UNP G1UII1
B	158	GLY	ASP	engineered mutation	UNP G1UII1
B	173	ILE	THR	engineered mutation	UNP G1UII1
B	199	MET	ARG	engineered mutation	UNP G1UII1
B	224	PHE	TYR	engineered mutation	UNP G1UII1
B	249	ASN	HIS	engineered mutation	UNP G1UII1

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 3 is 6-azanyl-2-oxidanylidene-hexanoic acid (CCD ID: 7C3) (formula: C₆H₁₁NO₃).



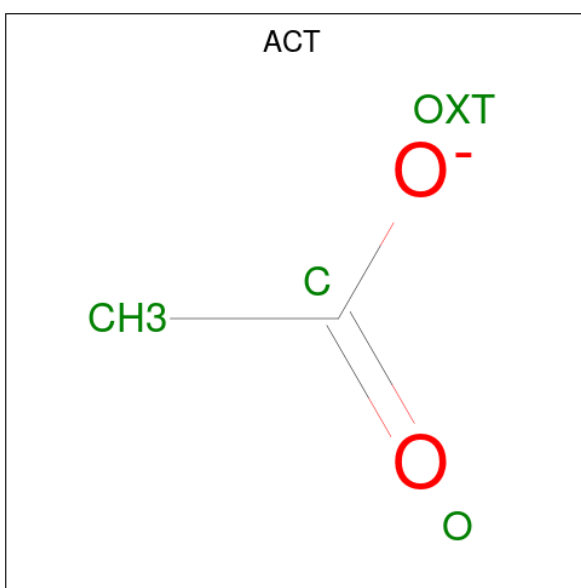
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

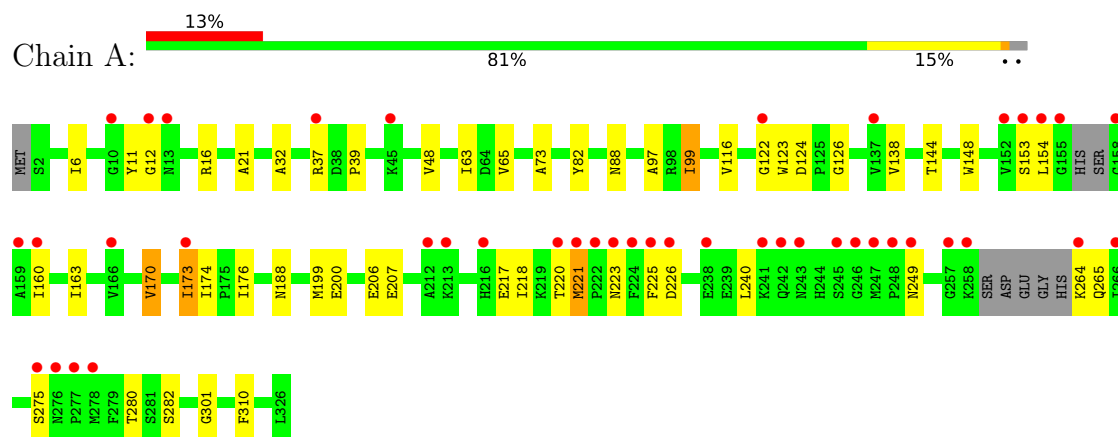
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total 213	O 213	0	0
6	B	184	Total 184	O 184	0	0

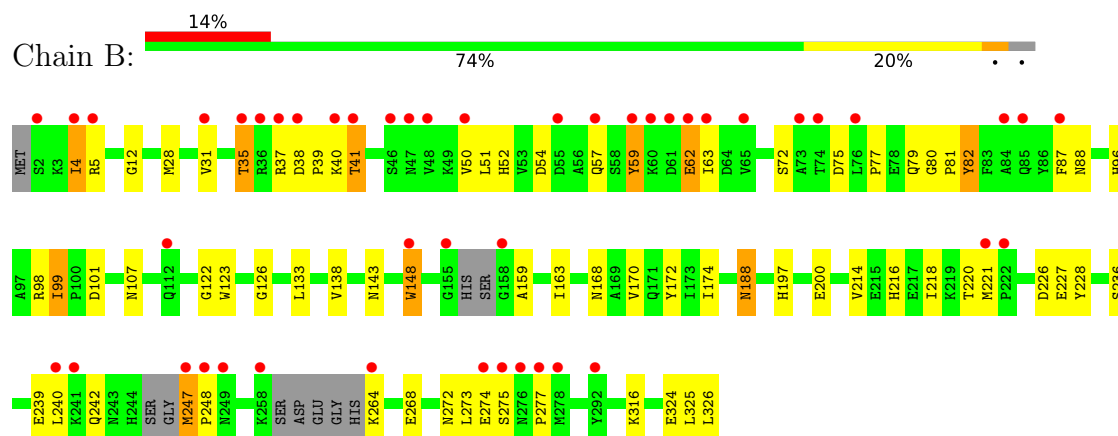
3 Residue-property plots

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: Meso-diaminopimelate D-dehydrogenase



- Molecule 1: Meso-diaminopimelate D-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.84Å 94.77Å 138.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.74 50.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.74) 99.7 (50.00-1.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.207 , 0.250 0.222 , 0.253	Depositor DCC
R_{free} test set	3782 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5400	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: NDP, SO4, 7C3, ACT

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	1.46	16/2514 (0.6%)	1.24	9/3400 (0.3%)
1	B	1.33	13/2514 (0.5%)	1.31	19/3398 (0.6%)
All	All	1.40	29/5028 (0.6%)	1.27	28/6798 (0.4%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	ILE	CA-CB	11.98	1.62	1.53
1	A	188	ASN	C-O	6.49	1.26	1.23
1	A	188	ASN	N-CA	-6.36	1.41	1.46
1	A	170	VAL	C-O	6.32	1.30	1.23
1	B	170	VAL	N-CA	6.24	1.53	1.46
1	A	21	ALA	CA-C	-6.09	1.45	1.52
1	B	41	THR	CA-C	6.06	1.61	1.52
1	B	163	ILE	C-O	-6.02	1.17	1.24
1	B	268	GLU	C-O	6.01	1.30	1.24
1	B	170	VAL	C-O	5.74	1.30	1.23
1	A	207	GLU	CA-C	-5.73	1.45	1.52
1	A	97	ALA	C-O	5.69	1.31	1.24
1	B	272	ASN	CA-C	5.67	1.59	1.52
1	B	50	VAL	CA-CB	-5.67	1.47	1.53
1	A	63	ILE	N-CA	5.65	1.52	1.46
1	B	31	VAL	CA-C	-5.64	1.46	1.53
1	A	144	THR	N-CA	5.57	1.52	1.46
1	B	172	TYR	C-O	5.47	1.30	1.23
1	B	188	ASN	C-O	-5.33	1.21	1.23
1	A	82	TYR	C-O	5.26	1.30	1.24
1	A	249	ASN	N-CA	-5.17	1.39	1.45
1	B	12	GLY	C-O	-5.17	1.18	1.23
1	B	107	ASN	C-O	-5.16	1.18	1.24
1	A	176	ILE	N-CA	5.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	C-N	5.12	1.39	1.33
1	A	65	VAL	CA-CB	5.08	1.61	1.54
1	B	168	ASN	C-O	-5.07	1.17	1.23
1	A	6	ILE	CA-C	-5.07	1.46	1.52
1	A	218	ILE	CA-CB	5.04	1.60	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASP	N-CA-C	10.93	123.19	111.28
1	B	324	GLU	N-CA-C	7.64	119.69	111.36
1	B	80	GLY	CA-C-N	-7.59	111.90	119.56
1	B	80	GLY	C-N-CA	-7.59	111.90	119.56
1	B	79	GLN	N-CA-C	7.48	119.51	111.36
1	B	325	LEU	N-CA-C	7.41	122.99	113.88
1	B	99	ILE	CA-C-N	-7.38	110.85	119.05
1	B	99	ILE	C-N-CA	-7.38	110.85	119.05
1	B	35	THR	N-CA-C	7.13	121.02	109.40
1	B	63	ILE	N-CA-C	7.11	118.13	108.17
1	B	72	SER	N-CA-C	6.72	118.69	111.36
1	B	242	GLN	N-CA-C	6.25	117.89	111.14
1	B	62	GLU	N-CA-C	6.18	118.10	111.36
1	A	301	GLY	CA-C-O	-5.96	117.81	122.52
1	B	75	ASP	N-CA-C	5.90	117.38	111.07
1	A	221	MET	CA-C-N	-5.77	113.60	119.83
1	A	221	MET	C-N-CA	-5.77	113.60	119.83
1	A	173	ILE	N-CA-C	-5.74	100.15	108.36
1	A	12	GLY	N-CA-C	-5.71	103.85	112.41
1	A	73	ALA	N-CA-C	5.43	116.88	111.07
1	B	4	ILE	N-CA-C	-5.34	102.70	109.80
1	A	310	PHE	N-CA-C	5.29	117.79	111.71
1	B	316	LYS	N-CA-C	5.22	117.86	110.50
1	B	59	TYR	N-CA-C	5.16	119.07	112.26
1	B	88	ASN	N-CA-C	-5.09	102.33	109.96
1	B	82	TYR	N-CA-C	5.08	116.67	111.03
1	A	138	VAL	N-CA-C	5.07	115.84	110.72
1	A	206	GLU	N-CA-C	-5.03	103.89	110.53

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	2465	0	2435	32	0
1	B	2466	0	2438	58	0
2	A	48	0	26	5	0
3	A	10	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	4	0	3	0	0
6	A	213	0	0	0	0
6	B	184	0	0	1	0
All	All	5400	0	4902	84	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 8.

All (84) 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:B:247:MET:HG3	1:B:248:PRO:CD	1.67	1.23
1:B:247:MET:CG	1:B:248:PRO:HD2	1.84	1.07
1:B:247:MET:HG3	1:B:248:PRO:HD2	1.05	1.04
1:B:38:ASP:O	1:B:41:THR:HG22	1.66	0.94
1:B:247:MET:CG	1:B:248:PRO:CD	2.43	0.92
1:B:148:TRP:H	1:B:197:HIS:HE1	1.18	0.91
1:B:148:TRP:H	1:B:197:HIS:CE1	1.96	0.84
1:A:174:ILE:HD12	1:A:200:GLU:HG3	1.57	0.83
1:A:124:ASP:H	2:A:1001:NDP:H72N	1.24	0.82
1:B:159:ALA:HB1	1:B:221:MET:HE3	1.61	0.82
1:A:173:ILE:HG12	1:A:199:MET:SD	2.25	0.77
1:B:247:MET:HG3	1:B:248:PRO:HD3	1.64	0.77
1:B:247:MET:CB	1:B:248:PRO:CD	2.63	0.75
1:A:88:ASN:HD22	1:A:116:VAL:H	1.37	0.72
1:B:159:ALA:CB	1:B:221:MET:HE3	2.23	0.69
1:B:247:MET:CG	1:B:248:PRO:HD3	2.23	0.68
1:B:247:MET:CB	1:B:248:PRO:HD3	2.22	0.68
1:B:247:MET:HB2	1:B:248:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:HB3	6:B:3103:HOH:O	1.95	0.65
1:B:159:ALA:HB3	1:B:221:MET:CE	2.28	0.63
1:B:159:ALA:CB	1:B:221:MET:CE	2.76	0.63
1:A:170:VAL:HG22	1:A:240:LEU:HD11	1.81	0.63
1:A:160:ILE:HG13	1:A:221:MET:HE1	1.81	0.62
1:B:159:ALA:HB3	1:B:221:MET:HE1	1.80	0.61
1:A:223:ASN:OD1	1:A:225:PHE:N	2.34	0.61
1:B:57:GLN:HG3	1:B:82:TYR:OH	2.01	0.60
1:A:280:THR:OG1	2:A:1001:NDP:H41N	2.02	0.59
1:B:38:ASP:OD1	1:B:40:LYS:HG2	2.02	0.59
1:A:220:THR:HG22	1:A:220:THR:O	2.02	0.59
1:B:5:ARG:HD2	1:B:62:GLU:O	2.03	0.59
1:B:5:ARG:NH1	1:B:62:GLU:O	2.35	0.59
1:B:4:ILE:HB	1:B:28:MET:HG2	1.87	0.57
1:B:148:TRP:N	1:B:197:HIS:HE1	1.96	0.56
1:B:240:LEU:C	1:B:240:LEU:HD23	2.31	0.56
1:B:52:HIS:CD2	1:B:54:ASP:H	2.23	0.56
1:B:122:GLY:O	1:B:126:GLY:HA3	2.05	0.55
1:A:99:ILE:HG21	1:B:326:LEU:HD23	1.88	0.55
1:A:275:SER:CB	1:B:264:LYS:O	2.55	0.54
1:B:174:ILE:CD1	1:B:200:GLU:OE1	2.56	0.54
1:B:174:ILE:HD12	1:B:200:GLU:CD	2.33	0.54
1:A:153:SER:O	1:A:154:LEU:HG	2.07	0.54
1:B:96:HIS:HA	1:B:99:ILE:HD12	1.90	0.54
1:A:124:ASP:N	2:A:1001:NDP:H72N	2.00	0.53
2:A:1001:NDP:H42N	3:A:1002:7C3:CB	2.38	0.53
1:A:122:GLY:O	1:A:126:GLY:HA3	2.11	0.51
1:B:5:ARG:NH1	1:B:62:GLU:C	2.69	0.51
1:B:35:THR:HG23	1:B:37[B]:ARG:O	2.12	0.50
1:B:77:PRO:O	1:B:81:PRO:HD2	2.12	0.50
1:A:223:ASN:O	1:A:226:ASP:OD1	2.30	0.49
1:B:35:THR:HG23	1:B:37[A]:ARG:O	2.12	0.49
1:B:133:LEU:C	1:B:133:LEU:HD23	2.37	0.49
1:A:37:ARG:HE	2:A:1001:NDP:C2A	2.26	0.49
1:B:35:THR:OG1	1:B:37[B]:ARG:NE	2.46	0.49
1:A:264:LYS:O	1:B:275:SER:CB	2.60	0.49
1:B:274:GLU:O	1:B:277:PRO:HD3	2.12	0.49
1:A:11:TYR:CZ	1:A:16:ARG:HG2	2.49	0.48
1:A:88:ASN:ND2	1:A:116:VAL:H	2.07	0.48
1:B:236:SER:OG	1:B:239:GLU:HG3	2.14	0.48
1:A:123:TRP:CD1	1:A:123:TRP:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:HG3	1:B:228:TYR:CD2	2.50	0.47
1:A:217:GLU:O	1:A:221:MET:HB2	2.15	0.46
1:B:5:ARG:NH1	1:B:62:GLU:HA	2.30	0.46
1:B:273:LEU:HB3	1:B:277:PRO:HG2	1.98	0.45
1:B:52:HIS:HD2	1:B:54:ASP:H	1.63	0.45
1:B:216:HIS:O	1:B:220:THR:HG23	2.17	0.45
1:B:98:ARG:NH1	1:B:101:ASP:OD2	2.49	0.45
1:A:199:MET:HB3	1:A:199:MET:HE3	1.68	0.44
1:A:275:SER:HB2	1:B:264:LYS:O	2.17	0.43
1:A:37:ARG:O	1:A:39:PRO:HD3	2.18	0.43
1:A:153:SER:C	1:A:154:LEU:HG	2.42	0.43
1:B:143:ASN:HD22	1:B:188:ASN:HD22	1.65	0.43
1:B:123:TRP:C	1:B:123:TRP:CD1	2.95	0.43
1:A:160:ILE:HA	1:A:163:ILE:HD12	2.01	0.43
1:B:214:VAL:O	1:B:218:ILE:HG13	2.20	0.42
1:A:264:LYS:O	1:B:275:SER:HB2	2.18	0.42
1:A:170:VAL:CG2	1:A:240:LEU:HD11	2.48	0.42
1:B:77:PRO:O	1:B:81:PRO:CD	2.68	0.42
1:A:282:SER:HB2	1:B:138:VAL:HG13	2.01	0.42
1:A:265:GLN:NE2	1:B:277:PRO:HA	2.35	0.41
1:B:38:ASP:CG	1:B:40:LYS:HG2	2.45	0.41
1:B:51:LEU:HD13	1:B:59:TYR:CE1	2.56	0.41
1:A:32:ALA:HA	1:A:48:VAL:CG2	2.50	0.41
1:A:154:LEU:HD12	1:A:154:LEU:O	2.21	0.41
1:B:39:PRO:HG3	1:B:51:LEU:C	2.46	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	312/326 (96%)	308 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	309/326 (95%)	303 (98%)	6 (2%)	0	100	100
All	All	621/652 (95%)	611 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	265/272 (97%)	264 (100%)	1 (0%)	84	79
1	B	265/272 (97%)	262 (99%)	3 (1%)	65	50
All	All	530/544 (97%)	526 (99%)	4 (1%)	73	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	TRP
1	B	87	PHE
1	B	148	TRP
1	B	247	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	85	GLN
1	A	88	ASN
1	A	131	ASN
1	A	265	GLN
1	B	13	ASN
1	B	52	HIS
1	B	85	GLN
1	B	131	ASN

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Mol	Chain	Res	Type
1	B	143	ASN
1	B	197	HIS
1	B	233	HIS
1	B	243	ASN
1	B	249	ASN

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](#)

5 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	7C3	A	1002	-	9,9,9	2.10	1 (11%)	10,10,10	2.06	3 (30%)
4	SO4	A	1003	-	4,4,4	0.77	0	6,6,6	0.37	0
5	ACT	B	3001	-	3,3,3	0.79	0	3,3,3	1.02	0
2	NDP	A	1001	-	51,52,52	1.25	7 (13%)	71,80,80	1.61	13 (18%)
4	SO4	B	3002	-	4,4,4	0.52	0	6,6,6	0.79	0

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	7C3	A	1002	-	-	1/9/9/9	-
2	NDP	A	1001	-	-	3/34/77/77	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	7C3	CB-CA	5.65	1.57	1.51
2	A	1001	NDP	C5A-C4A	4.70	1.47	1.39
2	A	1001	NDP	C5A-C6A	2.52	1.48	1.41
2	A	1001	NDP	PN-O3	2.39	1.62	1.59
2	A	1001	NDP	C5A-N7A	-2.31	1.34	1.39
2	A	1001	NDP	PA-O3	2.25	1.61	1.59
2	A	1001	NDP	C8A-N7A	2.22	1.36	1.31
2	A	1001	NDP	C4A-N9A	-2.04	1.33	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NDP	C5A-C4A-N3A	-5.46	119.20	126.72
3	A	1002	7C3	CG-CB-CA	-4.78	104.27	113.58
2	A	1001	NDP	N3A-C4A-N9A	4.60	134.99	127.17
2	A	1001	NDP	C2B-C1B-N9A	-3.67	107.71	113.75
2	A	1001	NDP	C2A-N3A-C4A	3.62	120.68	111.83
2	A	1001	NDP	N3A-C2A-N1A	-3.56	123.19	128.58
2	A	1001	NDP	C4A-C5A-N7A	-3.05	107.10	110.58
2	A	1001	NDP	C4A-N9A-C8A	2.99	108.88	105.74
3	A	1002	7C3	OXT-C-CA	-2.89	118.22	121.81
2	A	1001	NDP	C6N-N1N-C2N	2.62	122.13	119.32
2	A	1001	NDP	C3D-C2D-C1D	2.30	105.81	101.46
2	A	1001	NDP	C5A-N7A-C8A	2.28	107.04	103.45
2	A	1001	NDP	C2A-N1A-C6A	2.27	122.47	118.73
3	A	1002	7C3	O-C-CA	2.22	119.76	113.59
2	A	1001	NDP	C6A-C5A-N7A	2.09	136.12	132.09
2	A	1001	NDP	C2D-C1D-N1N	-2.02	108.34	113.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

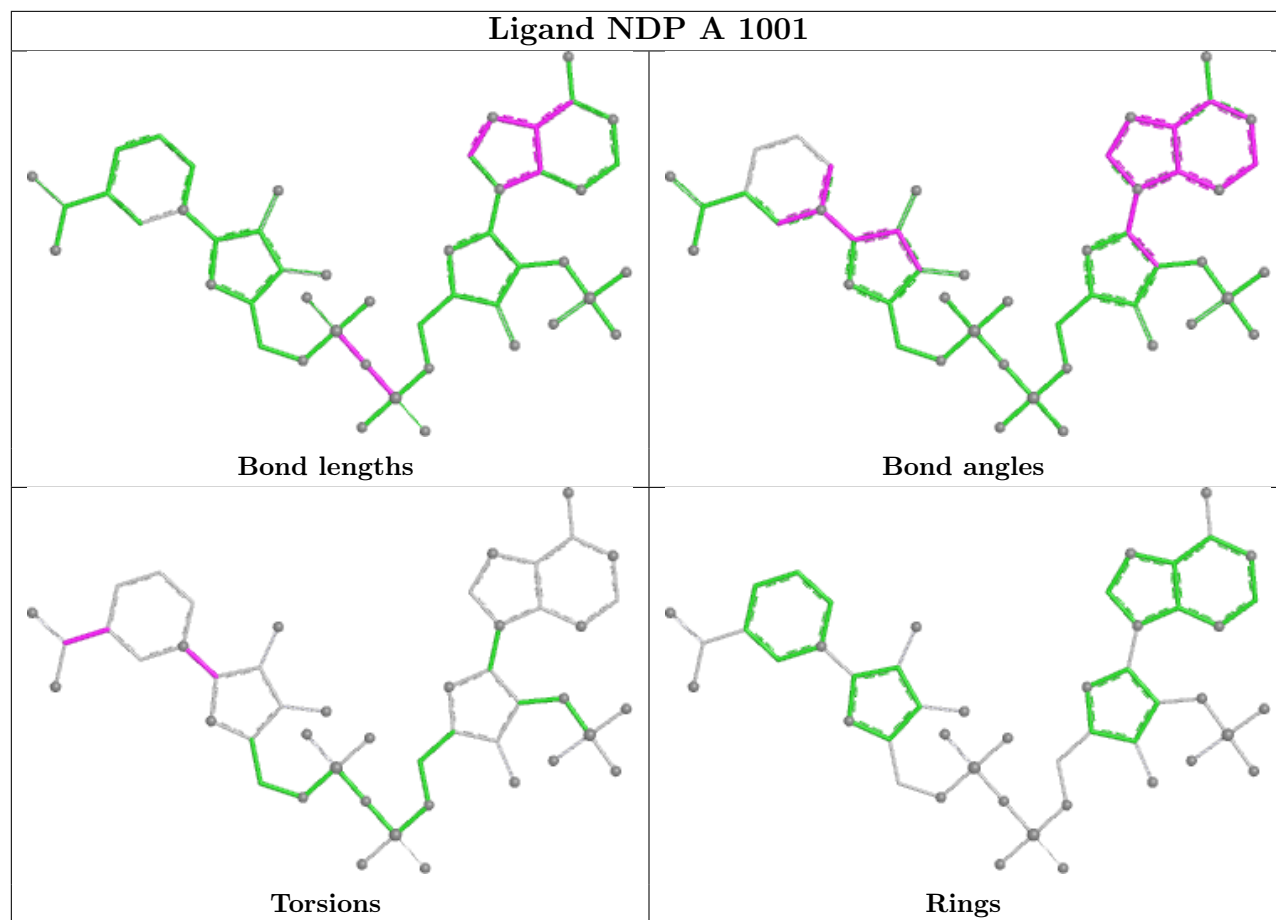
Mol	Chain	Res	Type	Atoms
3	A	1002	7C3	C-CA-CB-CG
2	A	1001	NDP	O4D-C1D-N1N-C2N
2	A	1001	NDP	C2N-C3N-C7N-N7N
2	A	1001	NDP	C2N-C3N-C7N-O7N

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	7C3	1	0
2	A	1001	NDP	5	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	318/326 (97%)	0.78	43 (13%) 7 9	17, 29, 66, 84	0
1	B	316/326 (96%)	0.96	47 (14%) 5 7	16, 34, 57, 86	1 (0%)
All	All	634/652 (97%)	0.87	90 (14%) 6 8	16, 32, 62, 86	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	LEU	7.9
1	A	220	THR	7.8
1	A	224	PHE	6.2
1	A	155	GLY	6.1
1	A	158	GLY	5.9
1	B	276	ASN	5.5
1	B	248	PRO	5.4
1	A	277	PRO	5.4
1	A	225	PHE	4.9
1	A	152	VAL	4.9
1	B	74	THR	4.5
1	B	4	ILE	4.4
1	A	153	SER	4.1
1	B	155	GLY	4.0
1	B	48	VAL	3.9
1	A	257	GLY	3.8
1	A	223	ASN	3.7
1	B	277	PRO	3.7
1	A	159	ALA	3.7
1	A	216	HIS	3.6
1	B	278	MET	3.6
1	A	222	PRO	3.5
1	B	148	TRP	3.5
1	B	2	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	46	SER	3.4
1	B	247	MET	3.3
1	A	245	SER	3.3
1	A	276	ASN	3.2
1	B	84	ALA	3.2
1	A	37	ARG	3.1
1	A	12	GLY	3.1
1	B	249	ASN	3.0
1	B	40	LYS	3.0
1	B	60	LYS	3.0
1	B	87	PHE	3.0
1	A	241	LYS	2.9
1	A	258	LYS	2.9
1	B	258	LYS	2.9
1	B	47	ASN	2.9
1	A	246	GLY	2.9
1	B	36	ARG	2.8
1	B	37[A]	ARG	2.8
1	B	59	TYR	2.8
1	A	160	ILE	2.8
1	B	275	SER	2.8
1	A	221	MET	2.8
1	A	275	SER	2.8
1	A	13	ASN	2.7
1	B	62	GLU	2.7
1	A	173	ILE	2.7
1	B	50	VAL	2.6
1	B	221	MET	2.6
1	B	35	THR	2.6
1	B	73	ALA	2.6
1	A	213	LYS	2.6
1	B	63	ILE	2.6
1	A	226	ASP	2.5
1	B	76	LEU	2.5
1	B	240	LEU	2.5
1	B	85	GLN	2.5
1	A	264	LYS	2.4
1	B	158	GLY	2.4
1	B	31	VAL	2.4
1	A	248	PRO	2.4
1	A	266	ILE	2.4
1	B	55	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLY	2.3
1	B	41	THR	2.3
1	B	274	GLU	2.3
1	A	212	ALA	2.3
1	B	5	ARG	2.3
1	A	45	LYS	2.3
1	B	292	TYR	2.3
1	B	222	PRO	2.2
1	A	137	VAL	2.2
1	B	57	GLN	2.2
1	B	61	ASP	2.2
1	A	247	MET	2.2
1	A	278	MET	2.2
1	B	241	LYS	2.2
1	A	166	VAL	2.1
1	B	112	GLN	2.1
1	A	249	ASN	2.1
1	A	243	ASN	2.1
1	A	238	GLU	2.1
1	A	242	GLN	2.1
1	B	38	ASP	2.0
1	A	122	GLY	2.0
1	B	65	VAL	2.0
1	B	264	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](#)

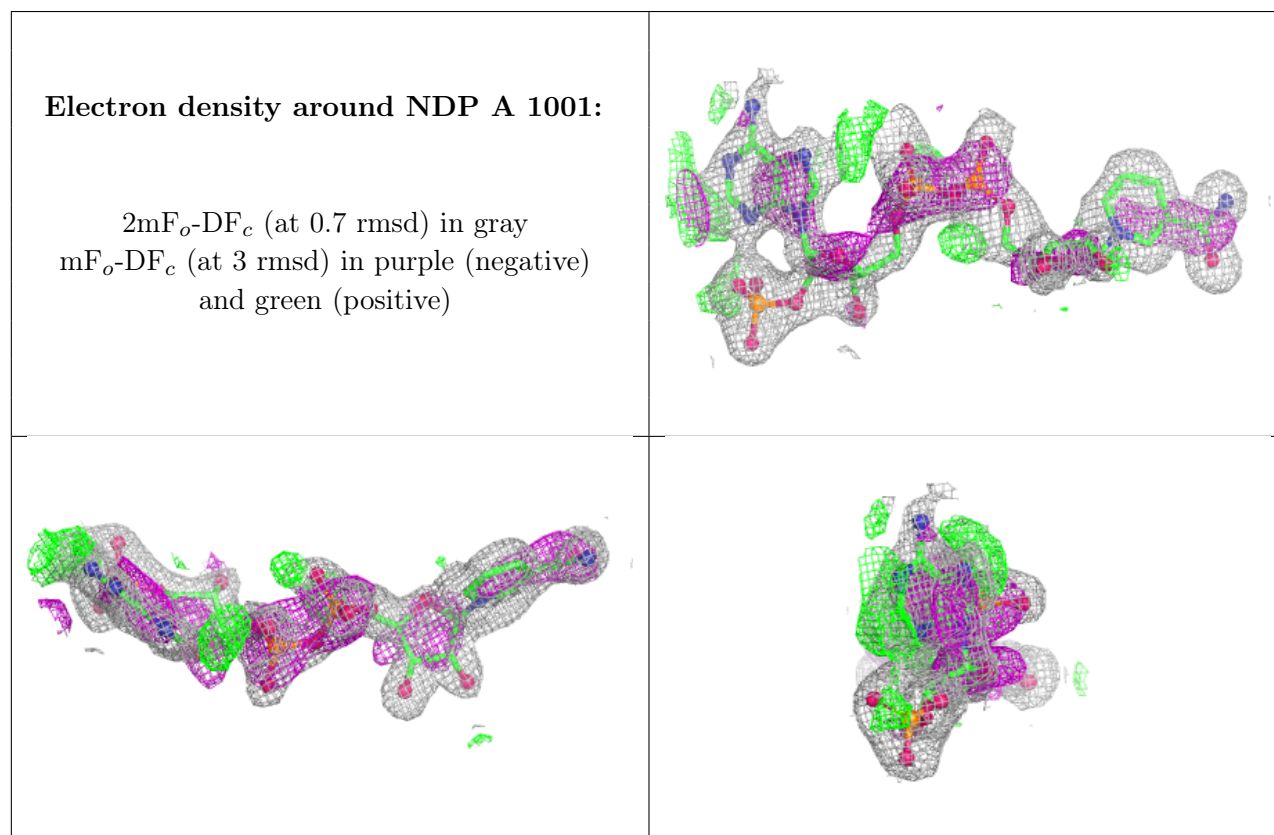
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	SO4	A	1003	5/5	0.68	0.17	50,53,59,62	0
3	7C3	A	1002	10/10	0.78	0.14	36,48,60,61	0
2	NDP	A	1001	48/48	0.82	0.14	20,35,41,45	0
5	ACT	B	3001	4/4	0.90	0.11	43,47,47,48	0
4	SO4	B	3002	5/5	0.91	0.09	51,54,59,63	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 ⓘ

There are no such residues in this entry.