



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:59 pm BST

PDB ID : 3FR8
Title : rice Ketolacid reductoisomerase in complex with Mg²⁺-NADPH
Authors : Leung, E.W.W.; Guddat, L.W.
Deposited on : 2009-01-08
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

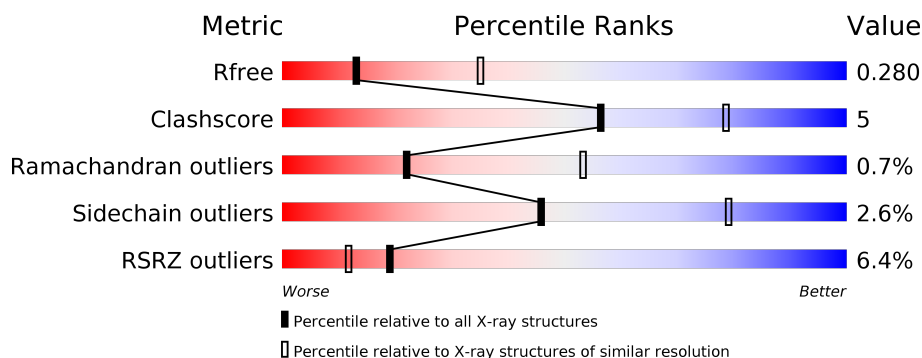
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	525	
1	B	525	

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	SO4	A	597	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8105 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.

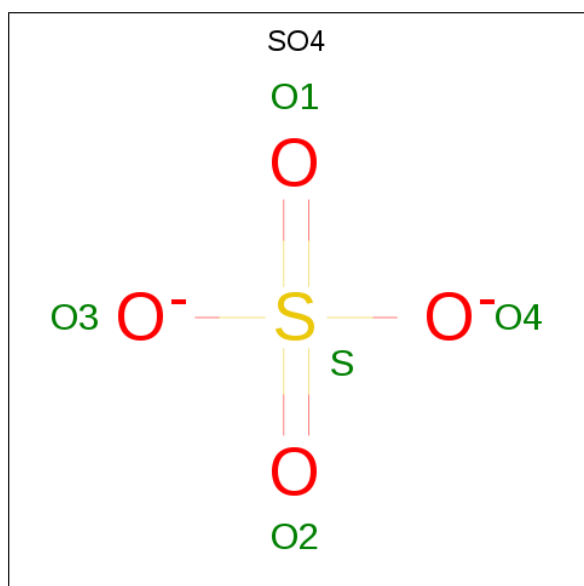
- Molecule 1 is a protein called Putative ketol-acid reductoisomerase (Os05g0573700 protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	1	0
			3861	2446	659	738	18			
1	B	517	Total	C	N	O	S	0	0	0
			3962	2511	674	758	19			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

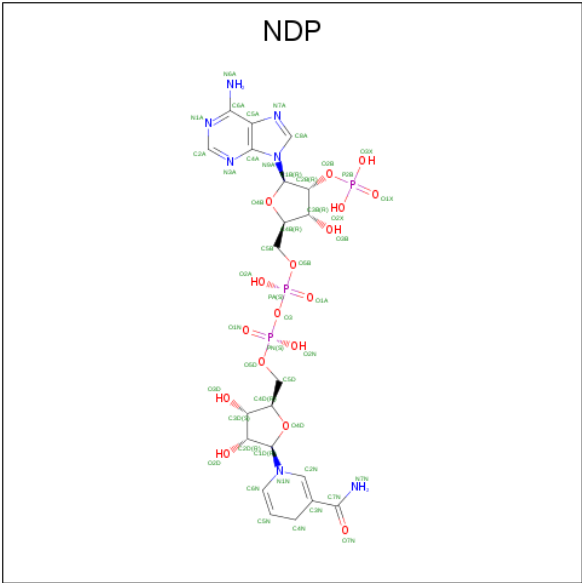
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



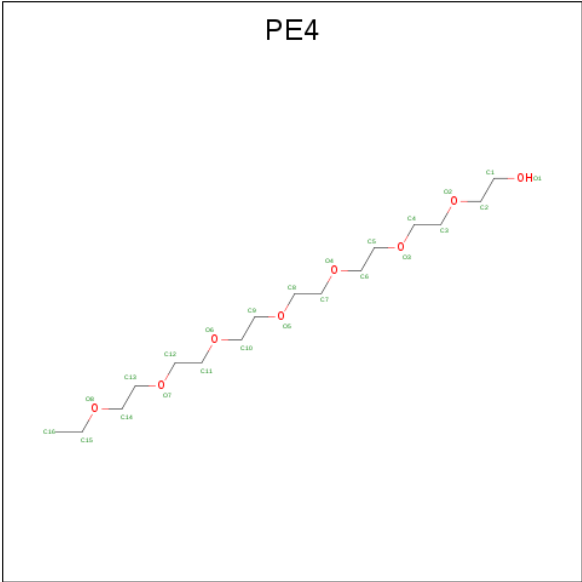
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



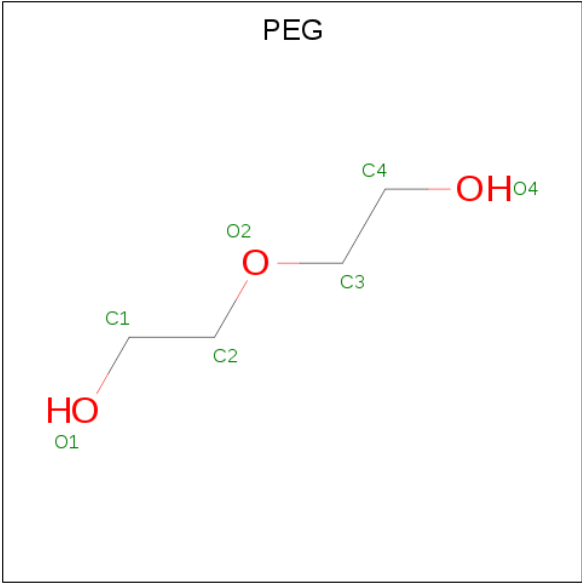
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

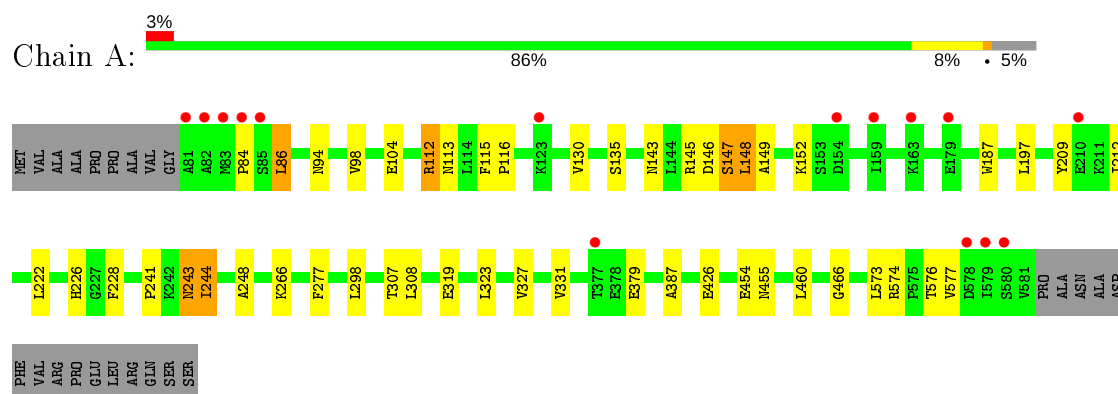
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	103	Total 103	O 103	0	0
7	B	67	Total 67	O 67	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Putative ketol-acid reductoisomerase (Os05g0573700 protein)



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.06 Å 162.06 Å 196.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.22 – 2.80 19.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.22-2.80) 97.7 (19.22-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.79 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.284 0.245 , 0.280	Depositor DCC
R_{free} test set	1598 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8105	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: PE4, NDP, MG, PEG, SO4

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	0.32	0/3941	0.47	1/5325 (0.0%)
1	B	0.33	0/4044	0.48	0/5470
All	All	0.32	0/7985	0.48	1/10795 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	84	PRO	N-CA-CB	5.89	110.37	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	LEU	Peptide
1	B	262	TYR	Peptide

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	3861	0	3821	32	0
1	B	3962	0	3906	47	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
4	A	48	0	26	1	0
4	B	48	0	26	2	0
5	A	4	0	4	0	0
6	B	4	0	4	1	0
7	A	103	0	0	0	0
7	B	67	0	0	0	0
All	All	8105	0	7787	79	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 5.

All (79) 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:148:LEU:H	1:B:149:ALA:HB3	1.03	1.11
1:B:148:LEU:N	1:B:149:ALA:HB3	1.67	1.09
1:B:162:ARG:HH11	1:B:162:ARG:HG3	1.28	0.96
1:A:148:LEU:N	1:A:149:ALA:HB3	2.03	0.73
1:B:262:TYR:O	1:B:262:TYR:HD2	1.72	0.71
1:A:147:SER:H	1:A:149:ALA:HB3	1.55	0.71
1:B:262:TYR:O	1:B:262:TYR:CD2	2.45	0.69
1:A:146:ASP:O	1:A:147:SER:HB2	1.93	0.69
1:B:330:ILE:HG13	1:B:536:LEU:HD11	1.75	0.68
1:A:187:TRP:HZ3	1:A:212:ILE:HA	1.58	0.68
1:B:162:ARG:HG2	1:B:186:ILE:HD13	1.81	0.63
1:A:147:SER:N	1:A:149:ALA:HB3	2.15	0.62
1:B:226:HIS:CD2	1:B:228:PHE:HB2	2.35	0.62
1:A:86:LEU:HD11	1:A:307:THR:HG23	1.83	0.61
1:B:262:TYR:C	1:B:262:TYR:HD2	2.04	0.61
1:A:148:LEU:H	1:A:149:ALA:HB3	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:OE1	1:B:109:ARG:HD2	2.02	0.60
1:A:146:ASP:O	1:A:147:SER:CB	2.49	0.59
1:A:147:SER:H	1:A:149:ALA:CB	2.16	0.59
1:A:243:ASN:H	1:A:243:ASN:HD22	1.52	0.58
1:A:226:HIS:CD2	1:A:228:PHE:HB2	2.37	0.58
1:B:262:TYR:CD2	1:B:262:TYR:C	2.77	0.58
1:B:187:TRP:CZ2	1:B:211:LYS:HE3	2.39	0.57
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.02	0.57
1:B:302:PHE:HE1	1:B:304:PHE:HB3	1.70	0.56
1:A:187:TRP:HH2	1:A:212:ILE:HG13	1.71	0.56
1:A:187:TRP:CZ3	1:A:212:ILE:HA	2.41	0.55
1:B:591:GLU:HG2	1:B:592:LEU:HD12	1.89	0.54
1:A:115:PHE:N	1:A:116:PRO:HD2	2.23	0.53
1:A:454:GLU:O	1:A:455:ASN:HB2	2.10	0.52
1:A:145:ARG:O	1:A:149:ALA:HB2	2.12	0.50
1:B:131:ILE:HG23	1:B:186:ILE:HG22	1.94	0.50
1:A:112[A]:ARG:HE	1:A:266:LYS:HA	1.76	0.50
1:B:241:PRO:HB2	1:B:244:ILE:HG12	1.94	0.49
1:A:243:ASN:N	1:A:243:ASN:HD22	2.10	0.49
1:B:169:ASP:HA	1:B:171:ALA:N	2.28	0.48
1:B:148:LEU:N	1:B:149:ALA:CB	2.59	0.48
4:B:600:NDP:H41N	6:B:6073:PEG:H41	1.96	0.48
1:A:319:GLU:HA	1:A:323:LEU:HB2	1.95	0.47
1:A:209:TYR:HA	1:A:212:ILE:HD12	1.96	0.47
1:B:130:VAL:HG11	1:B:141:ALA:HB2	1.97	0.47
1:B:309:GLU:HG3	1:B:313:LYS:HE2	1.96	0.46
1:B:77:PRO:HA	1:B:78:ALA:HA	1.63	0.46
1:A:98:VAL:HG11	1:A:573:LEU:HD11	1.98	0.46
1:B:167:SER:HA	1:B:170:GLU:HG3	1.97	0.46
1:B:276:SER:HB3	1:B:304:PHE:CZ	2.51	0.46
1:B:589:ARG:HA	1:B:590:PRO:HD3	1.85	0.46
1:B:202:ASP:HB3	1:B:228:PHE:CD1	2.52	0.45
1:B:226:HIS:HD2	1:B:228:PHE:HB2	1.80	0.45
1:B:161:LEU:HD13	1:B:168:PHE:HA	1.99	0.45
1:B:136:GLN:HE21	4:B:600:NDP:H42N	1.83	0.44
1:B:542:VAL:HG12	1:B:546:LYS:HE2	1.99	0.44
1:B:494:VAL:O	1:B:498:VAL:HG22	2.18	0.43
1:B:147:SER:OG	1:B:262:TYR:OH	2.37	0.43
1:B:133:TRP:HD1	1:B:167:SER:HB3	1.83	0.43
1:A:222:LEU:HB2	1:A:244:ILE:HD11	2.00	0.43
1:B:162:ARG:HG2	1:B:186:ILE:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:THR:HG23	1:A:577:VAL:HG13	2.00	0.43
1:B:584:ASN:ND2	1:B:584:ASN:H	2.17	0.43
1:A:327:VAL:O	1:A:331:VAL:HB	2.19	0.43
1:A:248:ALA:O	1:A:277:PHE:HA	2.18	0.42
1:B:187:TRP:HB3	1:B:215:HIS:CD2	2.54	0.42
1:B:294:TRP:O	1:B:298:LEU:HG	2.18	0.42
1:A:226:HIS:HB2	4:A:601:NDP:H1D	2.01	0.42
1:B:211:LYS:O	1:B:215:HIS:ND1	2.45	0.42
1:A:143:ASN:HB3	1:A:298:LEU:HA	2.01	0.42
1:A:130:VAL:HG22	1:A:197:LEU:HD12	2.01	0.42
1:B:226:HIS:HE1	1:B:315:ASP:HB3	1.83	0.42
1:A:426:GLU:HA	1:B:80:GLY:H	1.85	0.42
1:B:169:ASP:N	1:B:170:GLU:HB2	2.36	0.41
1:A:454:GLU:O	1:A:455:ASN:CB	2.68	0.41
1:B:148:LEU:CA	1:B:149:ALA:HB3	2.46	0.41
1:B:274:ASN:OD1	1:B:301:PRO:HG2	2.21	0.41
1:A:241:PRO:HB2	1:A:244:ILE:HG22	2.03	0.41
1:B:202:ASP:HB3	1:B:228:PHE:CG	2.55	0.41
1:B:165:SER:HB3	1:B:168:PHE:HD1	1.85	0.40
1:B:561:ASP:HA	1:B:562:PRO:HD2	1.87	0.40
1:A:387:ALA:HB3	1:A:466:GLY:HA3	2.03	0.40
1:B:491:ASN:HA	1:B:495:ILE:HB	2.04	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	500/525 (95%)	474 (95%)	24 (5%)	2 (0%)	34	66
1	B	515/525 (98%)	489 (95%)	21 (4%)	5 (1%)	15	44
All	All	1015/1050 (97%)	963 (95%)	45 (4%)	7 (1%)	22	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	B	149	ALA
1	B	263	VAL
1	B	271	ALA
1	A	135	SER
1	B	262	TYR
1	B	590	PRO

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	413/432 (96%)	400 (97%)	13 (3%)	40	74
1	B	422/432 (98%)	412 (98%)	10 (2%)	49	81
All	All	835/864 (97%)	812 (97%)	23 (3%)	46	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	94	ASN
1	A	104	GLU
1	A	112[A]	ARG
1	A	112[B]	ARG
1	A	113	ASN
1	A	152	LYS
1	A	243	ASN
1	A	244	ILE
1	A	308	LEU
1	A	379	GLU
1	A	460	LEU
1	A	574	ARG
1	B	123	LYS
1	B	162	ARG
1	B	166	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	ILE
1	B	262	TYR
1	B	302	PHE
1	B	359	ILE
1	B	377	THR
1	B	400	TYR
1	B	584	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	226	HIS
1	A	243	ASN
1	A	341	GLN
1	A	438	GLN
1	B	281	GLN
1	B	461	HIS
1	B	484	HIS
1	B	557	ASN
1	B	584	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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$
4	NDP	B	600	-	45,52,52	1.31	3 (6%)	53,80,80	1.17	2 (3%)
5	PE4	A	6061	2	3,3,23	0.46	0	2,2,22	0.37	0
3	SO4	A	597	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PEG	B	6073	2	3,3,6	0.45	0	2,2,5	0.30	0
4	NDP	A	601	-	45,52,52	1.30	3 (6%)	53,80,80	1.18	2 (3%)

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
4	NDP	B	600	-	-	10/30/77/77	0/5/5/5
5	PE4	A	6061	2	-	0/1/1/21	-
6	PEG	B	6073	2	-	0/1/1/4	-
4	NDP	A	601	-	-	10/30/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	NDP	C4N-C3N	-5.15	1.39	1.49
4	A	601	NDP	C4N-C3N	-5.11	1.39	1.49
4	B	600	NDP	C6N-C5N	3.61	1.39	1.33
4	A	601	NDP	C6N-C5N	3.60	1.39	1.33
4	A	601	NDP	C4N-C5N	-3.58	1.39	1.48
4	B	600	NDP	C4N-C5N	-3.54	1.39	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NDP	N3A-C2A-N1A	-4.93	120.97	128.68
4	B	600	NDP	N3A-C2A-N1A	-4.90	121.02	128.68
4	A	601	NDP	PN-O3-PA	-3.27	121.61	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	NDP	PN-O3-PA	-3.08	122.27	132.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	NDP	C5D-O5D-PN-O1N
4	A	601	NDP	C5B-O5B-PA-O1A
4	A	601	NDP	C5B-O5B-PA-O2A
4	B	600	NDP	C3D-C4D-C5D-O5D
4	B	600	NDP	O4D-C4D-C5D-O5D
4	B	600	NDP	C3B-C2B-O2B-P2B
4	B	600	NDP	C5D-O5D-PN-O3
4	B	600	NDP	C5D-O5D-PN-O2N
4	A	601	NDP	O4D-C1D-N1N-C6N
4	A	601	NDP	PA-O3-PN-O2N
4	A	601	NDP	C2D-C1D-N1N-C6N
4	B	600	NDP	O4D-C1D-N1N-C6N
4	B	600	NDP	C2D-C1D-N1N-C6N
4	A	601	NDP	C3B-C2B-O2B-P2B
4	B	600	NDP	C1B-C2B-O2B-P2B
4	A	601	NDP	C2B-O2B-P2B-O1X
4	A	601	NDP	O4D-C1D-N1N-C2N
4	B	600	NDP	C2B-O2B-P2B-O2X
4	A	601	NDP	C5B-O5B-PA-O3
4	A	601	NDP	PA-O3-PN-O1N

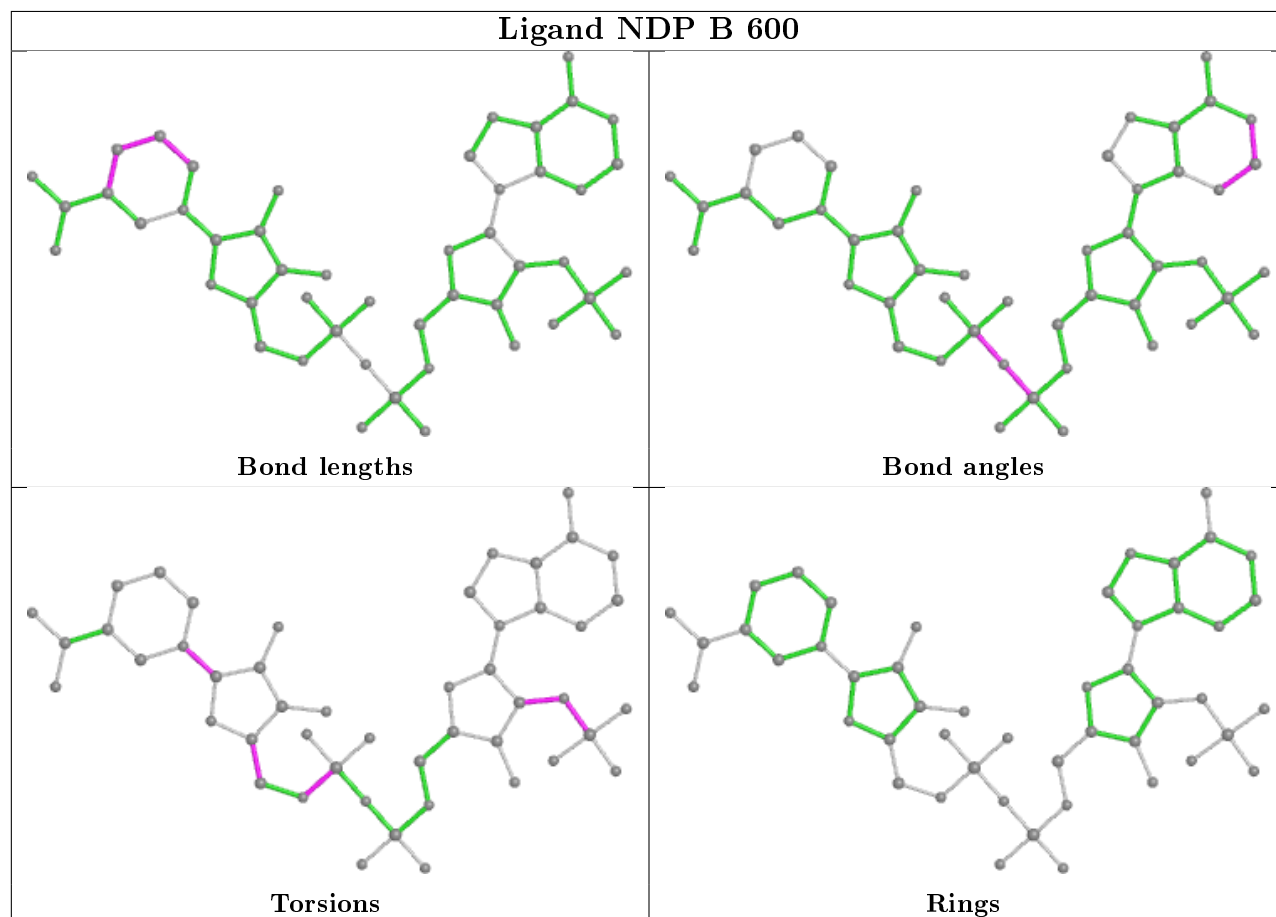
There are no ring outliers.

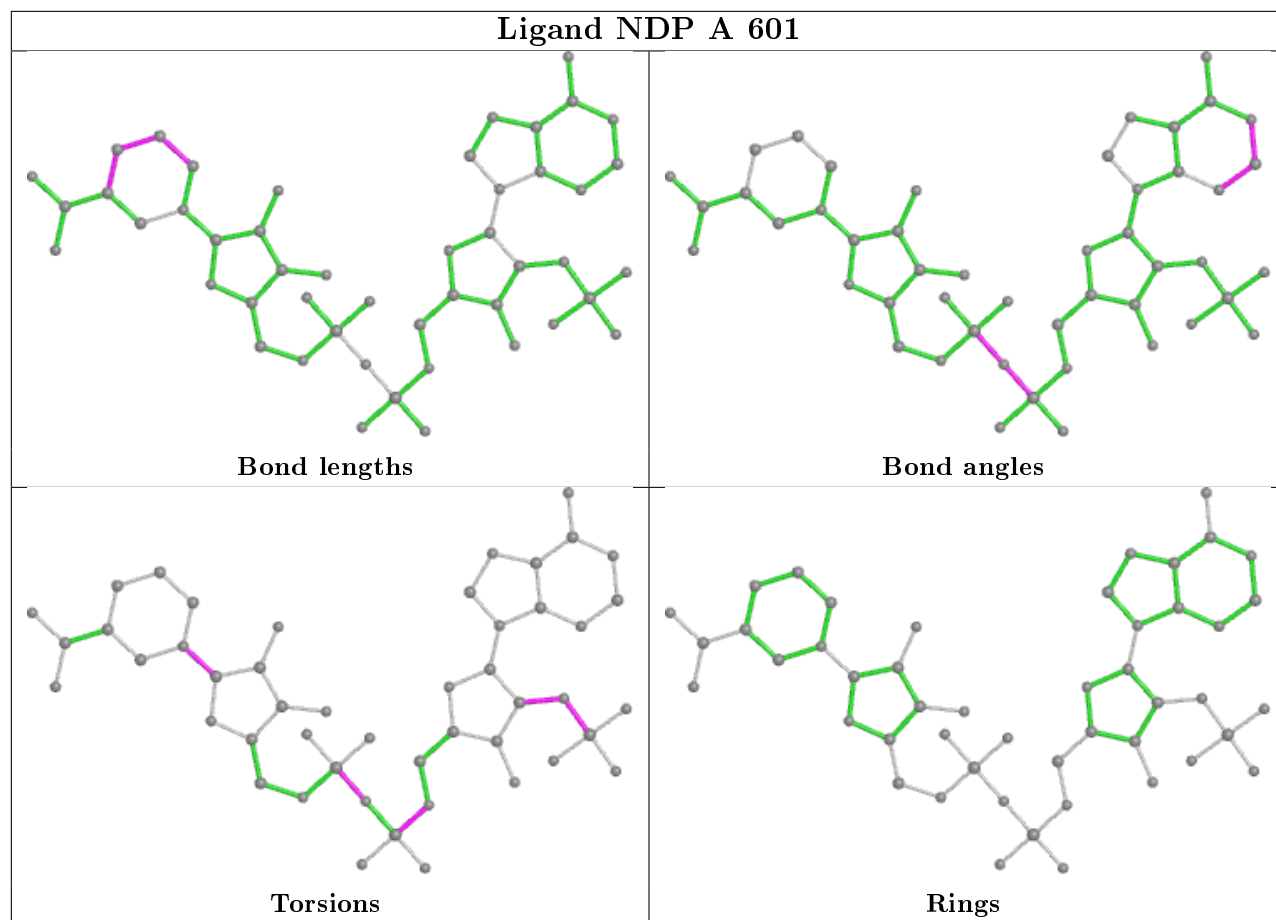
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	NDP	2	0
6	B	6073	PEG	1	0
4	A	601	NDP	1	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	501/525 (95%)	0.18	15 (2%) 50 40	38, 43, 58, 64	0
1	B	517/525 (98%)	0.46	50 (9%) 7 4	41, 46, 57, 72	0
All	All	1018/1050 (96%)	0.32	65 (6%) 19 12	38, 45, 58, 72	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ALA	6.7
1	B	82	ALA	5.2
1	A	580	SER	4.7
1	B	590	PRO	4.4
1	B	77	PRO	4.4
1	B	180	SER	4.3
1	B	584	ASN	4.2
1	B	179	GLU	4.1
1	B	589	ARG	4.0
1	B	166	LYS	4.0
1	A	85	SER	3.9
1	A	81	ALA	3.7
1	B	214	SER	3.7
1	B	79	VAL	3.7
1	B	173	ALA	3.4
1	B	219	ASN	3.3
1	B	267	GLU	3.2
1	B	580	SER	3.2
1	B	592	LEU	3.2
1	B	236	ALA	3.1
1	B	242	LYS	3.0
1	B	177	THR	3.0
1	B	167	SER	2.9
1	B	265	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	GLY	2.9
1	B	583	ALA	2.8
1	A	84	PRO	2.8
1	B	164	GLY	2.8
1	B	378	GLU	2.8
1	A	578	ASP	2.7
1	B	187	TRP	2.7
1	A	163	LYS	2.7
1	B	147	SER	2.7
1	B	450	SER	2.7
1	B	84	PRO	2.6
1	B	577	VAL	2.6
1	B	451	THR	2.6
1	B	591	GLU	2.5
1	B	587	PHE	2.5
1	A	123	LYS	2.5
1	B	552	GLN	2.5
1	B	549	PRO	2.4
1	A	159	ILE	2.4
1	A	210	GLU	2.4
1	B	260	ARG	2.4
1	B	588	VAL	2.3
1	A	579	ILE	2.3
1	B	149	ALA	2.3
1	A	154	ASP	2.3
1	B	586	ASP	2.3
1	B	178	GLU	2.3
1	A	377	THR	2.2
1	B	99	SER	2.2
1	A	179	GLU	2.2
1	B	192	GLY	2.2
1	B	581	VAL	2.1
1	B	553	ASP	2.1
1	B	455	ASN	2.1
1	B	124	GLY	2.1
1	B	174	ALA	2.1
1	B	271	ALA	2.1
1	A	83	MET	2.1
1	B	243	ASN	2.1
1	B	169	ASP	2.0
1	B	379	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

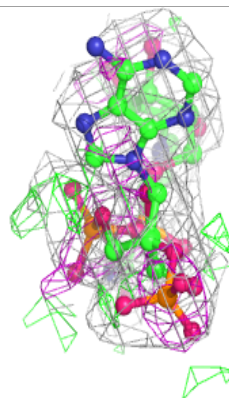
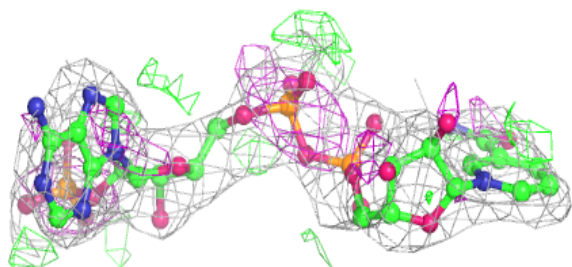
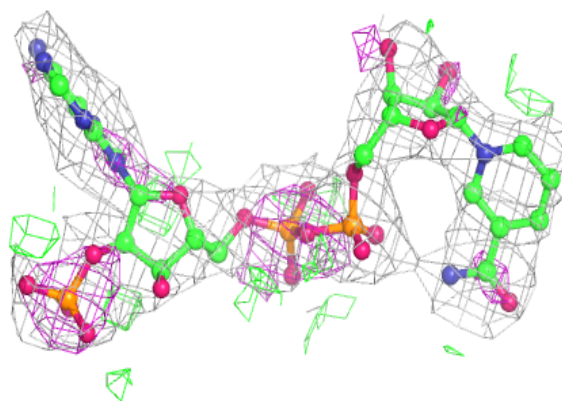
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	597	5/5	0.78	0.44	96,96,97,97	0
5	PE4	A	6061	4/24	0.83	0.28	59,59,59,59	0
6	PEG	B	6073	4/7	0.87	0.23	54,55,55,55	0
2	MG	B	1	1/1	0.87	0.23	77,77,77,77	0
4	NDP	B	600	48/48	0.89	0.26	48,54,59,59	0
2	MG	B	597	1/1	0.91	0.15	43,43,43,43	0
4	NDP	A	601	48/48	0.92	0.30	54,59,62,62	0
2	MG	A	1	1/1	0.94	0.25	63,63,63,63	0

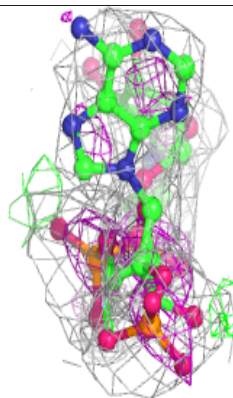
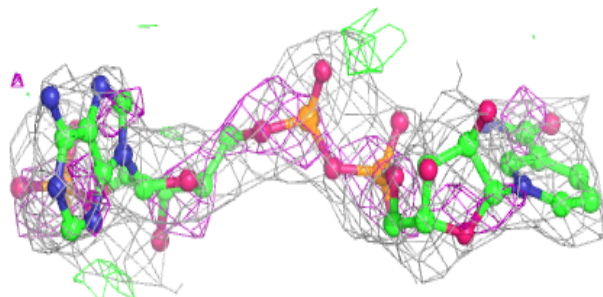
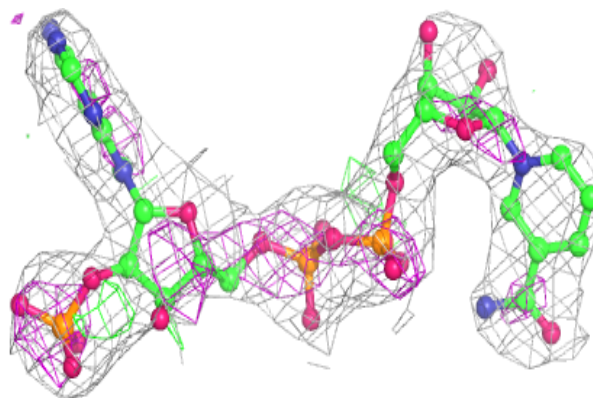
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP B 600:

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

**Electron density around NDP A 601:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.