



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 02:25 AM EDT

PDB ID : 3ANN  
Title : Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase (DXR) complexed with quinolin-2-ylmethylphosphonic acid  
Authors : Endo, K.; Kato, M.; Deng, L.; Song, Y.; Yajima, S.  
Deposited on : 2010-09-03  
Resolution : 2.00 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](mailto: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>.

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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 : 2.36  
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

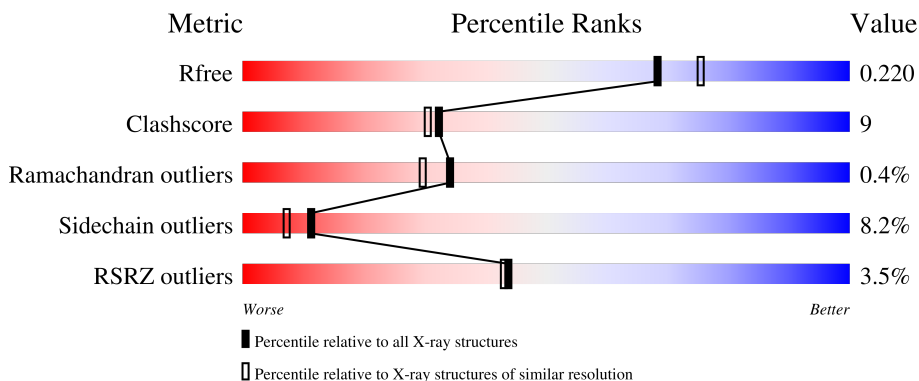
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


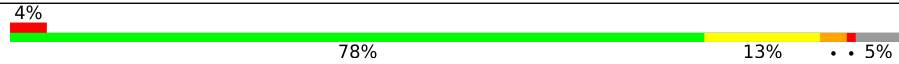
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	420	
1	B	420	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6598 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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	Total 3036	C 1895	N 536	O 579	S 26	0	0	0
1	B	398	Total 3025	C 1889	N 534	O 576	S 26	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

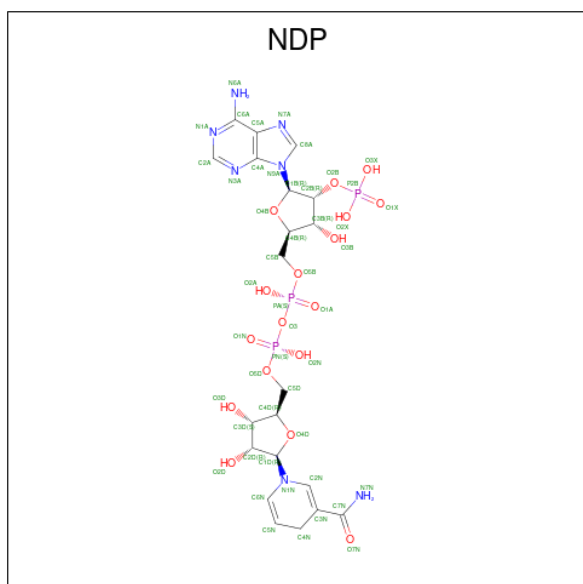
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P45568
A	-9	ARG	-	expression tag	UNP P45568
A	-8	GLY	-	expression tag	UNP P45568
A	-7	SER	-	expression tag	UNP P45568
A	-6	HIS	-	expression tag	UNP P45568
A	-5	HIS	-	expression tag	UNP P45568
A	-4	HIS	-	expression tag	UNP P45568
A	-3	HIS	-	expression tag	UNP P45568
A	-2	HIS	-	expression tag	UNP P45568
A	-1	HIS	-	expression tag	UNP P45568
A	0	GLY	-	expression tag	UNP P45568
A	398	SER	-	expression tag	UNP P45568
A	399	ALA	-	expression tag	UNP P45568
A	400	CYS	-	expression tag	UNP P45568
A	401	ASP	-	expression tag	UNP P45568
A	402	LEU	-	expression tag	UNP P45568
A	403	GLY	-	expression tag	UNP P45568
A	404	THR	-	expression tag	UNP P45568
A	405	PRO	-	expression tag	UNP P45568
A	406	GLY	-	expression tag	UNP P45568
A	407	ARG	-	expression tag	UNP P45568
A	408	PRO	-	expression tag	UNP P45568
A	409	ALA	-	expression tag	UNP P45568
B	-10	MET	-	expression tag	UNP P45568
B	-9	ARG	-	expression tag	UNP P45568

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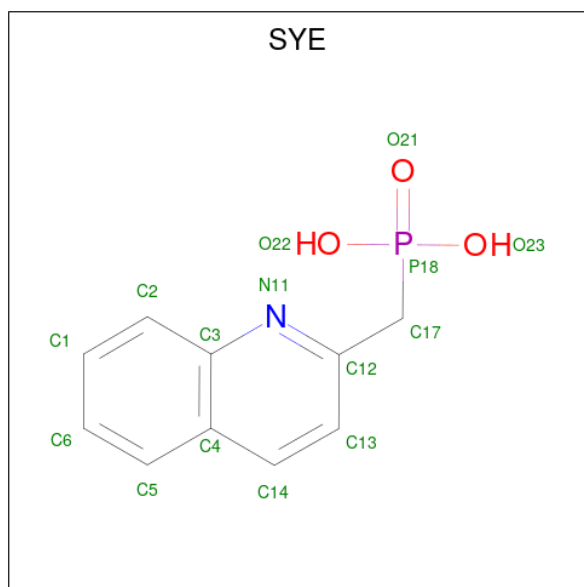
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP P45568
B	-7	SER	-	expression tag	UNP P45568
B	-6	HIS	-	expression tag	UNP P45568
B	-5	HIS	-	expression tag	UNP P45568
B	-4	HIS	-	expression tag	UNP P45568
B	-3	HIS	-	expression tag	UNP P45568
B	-2	HIS	-	expression tag	UNP P45568
B	-1	HIS	-	expression tag	UNP P45568
B	0	GLY	-	expression tag	UNP P45568
B	398	SER	-	expression tag	UNP P45568
B	399	ALA	-	expression tag	UNP P45568
B	400	CYS	-	expression tag	UNP P45568
B	401	ASP	-	expression tag	UNP P45568
B	402	LEU	-	expression tag	UNP P45568
B	403	GLY	-	expression tag	UNP P45568
B	404	THR	-	expression tag	UNP P45568
B	405	PRO	-	expression tag	UNP P45568
B	406	GLY	-	expression tag	UNP P45568
B	407	ARG	-	expression tag	UNP P45568
B	408	PRO	-	expression tag	UNP P45568
B	409	ALA	-	expression tag	UNP P45568

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

- Molecule 3 is (quinolin-2-ylmethyl)phosphonic acid (three-letter code: SYE) (formula: C<sub>10</sub>H<sub>10</sub>NO<sub>3</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	10	1	3	1	0	0
3	B	1	15	10	1	3	1	0	0

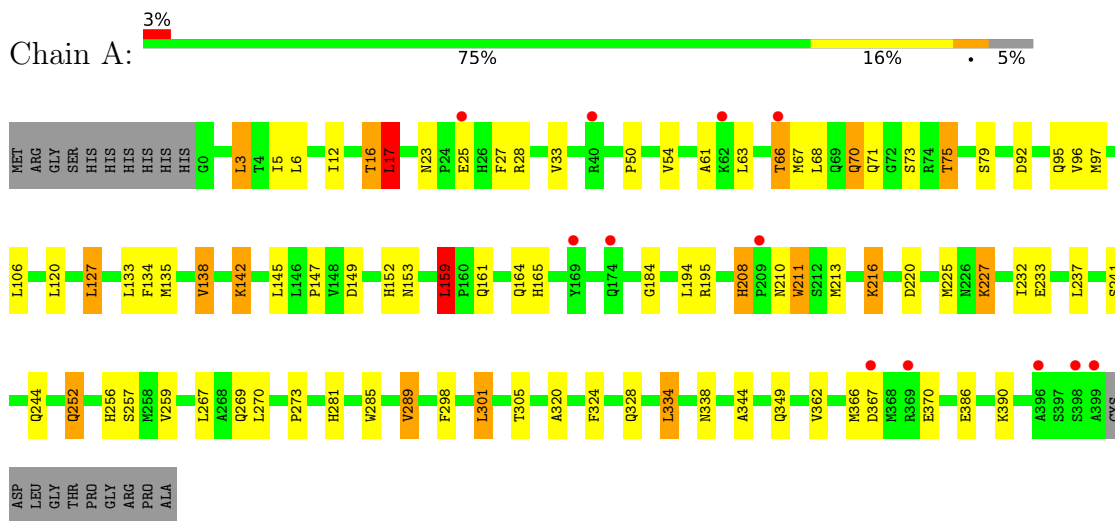
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	207	Total	O	0	0
			207	207		

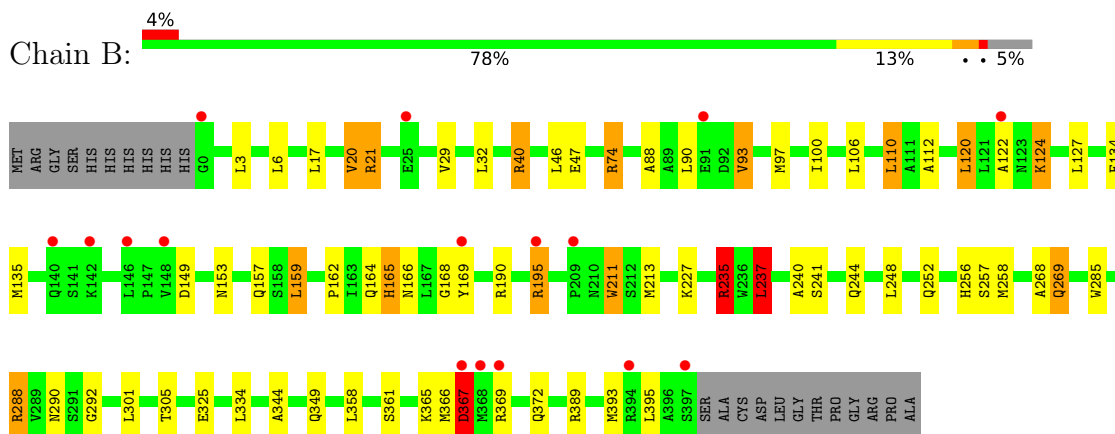
### 3 Residue-property plots [i](#)

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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.63Å 59.28Å 87.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.40 – 2.00 33.41 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.40-2.00) 99.8 (33.41-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.184 , 0.218 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	3321 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, SYE

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	0.74	0/3084	0.80	5/4181 (0.1%)
1	B	0.74	1/3073 (0.0%)	0.91	12/4166 (0.3%)
All	All	0.74	1/6157 (0.0%)	0.86	17/8347 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	ARG	CZ-NH1	6.48	1.41	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ARG	NE-CZ-NH2	-13.43	113.59	120.30
1	B	235	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	B	21	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	B	21	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	235	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	288	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	237	LEU	CA-CB-CG	6.72	130.76	115.30
1	A	159	LEU	CB-CG-CD1	6.32	121.74	111.00
1	B	3	LEU	CA-CB-CG	6.01	129.12	115.30
1	B	159	LEU	CB-CG-CD1	5.90	121.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LEU	CA-CB-CG	5.72	128.47	115.30
1	B	40	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	B	74	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	334	LEU	CB-CG-CD2	5.34	120.08	111.00
1	A	96	VAL	CG1-CB-CG2	5.14	119.12	110.90
1	A	17	LEU	CB-CG-CD1	5.06	119.60	111.00
1	B	165	HIS	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	3059	63	0
1	B	3025	0	3049	48	0
2	A	48	0	26	1	0
2	B	48	0	26	4	0
3	A	15	0	8	1	0
3	B	15	0	8	0	0
4	A	204	0	0	1	0
4	B	207	0	0	5	0
All	All	6598	0	6176	109	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 9.

All (109) 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:256:HIS:HD2	1:B:269:GLN:HE22	1.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:MET:HE2	1:B:268:ALA:HB2	1.48	0.93
1:B:256:HIS:CD2	1:B:269:GLN:HE22	1.91	0.89
1:B:124:LYS:HE2	4:B:484:HOH:O	1.77	0.83
1:B:21:ARG:HD3	1:B:47:GLU:OE2	1.79	0.81
1:B:211:TRP:O	4:B:486:HOH:O	1.98	0.81
1:B:122:ALA:O	2:B:702:NDP:O4D	2.01	0.79
1:B:258:MET:CE	1:B:268:ALA:HB2	2.12	0.79
1:B:241:SER:H	1:B:244:GLN:HE21	1.27	0.79
1:B:235:ARG:NH2	1:B:325:GLU:OE2	2.15	0.77
1:A:5:ILE:CD1	1:A:17:LEU:HD13	2.16	0.76
1:A:12:ILE:O	1:A:16:THR:HG23	1.86	0.76
1:A:127:LEU:HD11	1:A:135:MET:CE	2.16	0.75
1:A:241:SER:H	1:A:244:GLN:HE21	1.34	0.74
1:A:208:HIS:HD2	1:A:210:ASN:H	1.33	0.73
1:A:153:ASN:HD21	1:A:281:HIS:CD2	2.07	0.72
1:A:135:MET:CE	1:A:145:LEU:HD11	2.20	0.70
1:A:127:LEU:HD11	1:A:135:MET:HE3	1.73	0.70
1:B:288:ARG:NE	4:B:412:HOH:O	2.01	0.70
1:A:16:THR:HG21	1:A:97:MET:HG2	1.74	0.69
1:B:366:MET:O	1:B:367:ASP:C	2.31	0.68
1:A:73:SER:OG	1:A:75:THR:HG23	1.95	0.67
1:B:235:ARG:CD	1:B:240:ALA:O	2.43	0.67
1:B:252:GLN:HE22	1:B:305:THR:H	1.44	0.65
1:B:100:ILE:HD12	2:B:702:NDP:N3A	2.12	0.64
1:B:235:ARG:HD3	1:B:240:ALA:O	1.98	0.64
1:B:195:ARG:HD3	1:B:195:ARG:H	1.63	0.64
1:B:135:MET:CE	1:B:168:GLY:HA3	2.29	0.62
1:B:252:GLN:NE2	1:B:305:THR:H	1.97	0.62
1:A:50:PRO:O	1:A:75:THR:HB	1.99	0.62
1:A:164:GLN:NE2	1:A:285:TRP:HE1	1.98	0.62
1:B:288:ARG:NH2	4:B:412:HOH:O	2.19	0.61
1:B:164:GLN:NE2	1:B:285:TRP:HE1	1.99	0.61
1:A:216:LYS:CE	1:A:220:ASP:OD2	2.49	0.61
1:A:135:MET:HE1	1:A:145:LEU:HD11	1.83	0.60
1:B:241:SER:H	1:B:244:GLN:NE2	1.99	0.60
1:A:134:PHE:O	1:A:138:VAL:HG13	2.04	0.58
1:A:142:LYS:HD2	1:A:142:LYS:N	2.19	0.58
1:B:122:ALA:O	2:B:702:NDP:C4D	2.51	0.57
1:A:127:LEU:HD11	1:A:135:MET:HE2	1.85	0.57
1:B:235:ARG:HD2	1:B:240:ALA:O	2.05	0.57
1:B:17:LEU:HA	1:B:20:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:HIS:HE1	4:A:466:HOH:O	1.89	0.56
1:B:90:LEU:HB2	1:B:93:VAL:HG13	1.87	0.56
1:A:252:GLN:HE22	1:A:305:THR:H	1.55	0.55
1:A:208:HIS:CD2	1:A:210:ASN:H	2.21	0.54
1:B:21:ARG:CD	1:B:47:GLU:OE2	2.54	0.54
1:A:232:ILE:HD12	1:A:324:PHE:HB2	1.89	0.54
1:A:232:ILE:HD11	1:A:320:ALA:O	2.06	0.54
1:B:127:LEU:HD11	1:B:237:LEU:HD13	1.91	0.53
1:A:344:ALA:HA	1:A:349:GLN:HE21	1.74	0.53
1:B:153:ASN:ND2	1:B:157:GLN:HE21	2.07	0.53
1:A:273:PRO:HB3	3:A:800:SYE:H1	1.90	0.52
1:A:153:ASN:HD21	1:A:281:HIS:HD2	1.52	0.52
1:A:211:TRP:CE2	1:A:213:MET:HG3	2.45	0.52
1:A:67:MET:O	1:A:71:GLN:HG2	2.09	0.52
1:A:23:ASN:ND2	1:A:289:VAL:HG22	2.26	0.51
1:A:241:SER:H	1:A:244:GLN:NE2	2.07	0.51
1:A:252:GLN:NE2	1:A:305:THR:H	2.09	0.51
1:A:133:LEU:HG	1:A:328:GLN:HE22	1.76	0.51
1:A:127:LEU:HD21	1:A:237:LEU:HD13	1.93	0.50
1:B:165:HIS:O	1:B:166:ASN:HB2	2.12	0.50
1:A:135:MET:HE3	1:A:145:LEU:HD11	1.92	0.49
1:B:256:HIS:CD2	1:B:269:GLN:NE2	2.73	0.49
1:B:149:ASP:HA	2:B:702:NDP:H5N	1.93	0.49
1:A:216:LYS:HE2	1:A:220:ASP:OD2	2.13	0.48
1:A:68:LEU:HB3	1:A:73:SER:HB3	1.95	0.48
1:A:161:GLN:HG3	1:A:165:HIS:CD2	2.47	0.48
1:B:135:MET:HE1	1:B:168:GLY:HA3	1.95	0.48
1:A:362:VAL:O	1:A:366:MET:HG2	2.12	0.48
1:A:66:THR:O	1:A:70:GLN:CG	2.61	0.48
1:A:298:PHE:HA	1:A:301:LEU:HD22	1.96	0.48
1:A:161:GLN:HG3	1:A:165:HIS:HD2	1.79	0.48
1:A:5:ILE:CD1	1:A:17:LEU:CD1	2.89	0.47
1:B:190:ARG:NH2	4:B:536:HOH:O	2.47	0.47
1:A:147:PRO:HB3	1:A:237:LEU:HD21	1.95	0.47
1:A:270:LEU:HD22	1:B:258:MET:HE1	1.97	0.47
1:A:66:THR:O	1:A:70:GLN:HG2	2.14	0.47
1:B:344:ALA:HA	1:B:349:GLN:HE21	1.80	0.46
1:A:61:ALA:CB	1:A:79:SER:HB3	2.45	0.46
1:A:184:GLY:HA3	1:A:227:LYS:HE3	1.98	0.46
1:A:386:GLU:HG3	1:A:390:LYS:HE3	1.98	0.46
1:B:97:MET:HA	1:B:120:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:HIS:HE1	1:A:233:GLU:OE2	1.98	0.45
1:B:127:LEU:CD1	1:B:237:LEU:HD13	2.46	0.45
1:A:33:VAL:HG22	1:A:54:VAL:HG13	1.99	0.45
1:A:216:LYS:HE3	1:A:220:ASP:OD2	2.16	0.45
1:B:110:LEU:HG	1:B:134:PHE:CE2	2.52	0.44
1:A:67:MET:HA	1:A:70:GLN:HG3	2.00	0.43
1:B:211:TRP:CE2	1:B:213:MET:HG3	2.54	0.43
1:A:208:HIS:HD2	1:A:210:ASN:N	2.08	0.42
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.89	0.42
1:B:165:HIS:O	1:B:166:ASN:CB	2.66	0.42
1:A:149:ASP:HA	2:A:701:NDP:H5N	2.00	0.42
1:A:3:LEU:HD21	1:A:27:PHE:HB3	2.00	0.42
1:A:159:LEU:HD13	1:A:259:VAL:HG21	2.01	0.42
1:A:256:HIS:HD2	1:A:269:GLN:OE1	2.04	0.41
1:A:270:LEU:HD12	1:A:270:LEU:N	2.35	0.41
1:A:5:ILE:HD12	1:A:17:LEU:CD1	2.51	0.41
1:B:162:PRO:O	1:B:165:HIS:O	2.38	0.41
1:B:361:SER:O	1:B:365:LYS:HG3	2.21	0.41
1:B:389:ARG:O	1:B:393:MET:HG3	2.21	0.41
1:A:225:MET:HG2	1:A:338:ASN:ND2	2.34	0.41
1:B:29:VAL:HG11	1:B:32:LEU:HD21	2.03	0.41
1:B:88:ALA:HB1	1:B:112:ALA:HB2	2.02	0.40
1:B:290:ASN:ND2	1:B:292:GLY:H	2.19	0.40
1:A:5:ILE:HD13	1:A:17:LEU:HD13	2.00	0.40
1:A:298:PHE:CB	1:B:248:LEU:HD21	2.52	0.40
1:A:135:MET:HE3	1:A:145:LEU:CD1	2.51	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	398/420 (95%)	388 (98%)	9 (2%)	1 (0%)	41	37
1	B	396/420 (94%)	387 (98%)	7 (2%)	2 (0%)	29	23
All	All	794/840 (94%)	775 (98%)	16 (2%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	SER
1	B	367	ASP
1	B	257	SER

### 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	328/344 (95%)	299 (91%)	29 (9%)	10	6
1	B	327/344 (95%)	302 (92%)	25 (8%)	13	8
All	All	655/688 (95%)	601 (92%)	54 (8%)	11	7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	16	THR
1	A	17	LEU
1	A	25	GLU
1	A	28	ARG
1	A	63	LEU
1	A	66	THR
1	A	70	GLN
1	A	75	THR
1	A	92	ASP
1	A	95	GLN
1	A	106	LEU
1	A	120	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	127	LEU
1	A	138	VAL
1	A	142	LYS
1	A	159	LEU
1	A	194	LEU
1	A	195	ARG
1	A	211	TRP
1	A	216	LYS
1	A	227	LYS
1	A	252	GLN
1	A	267	LEU
1	A	289	VAL
1	A	301	LEU
1	A	334	LEU
1	A	367	ASP
1	A	370	GLU
1	B	6	LEU
1	B	20	VAL
1	B	40	ARG
1	B	46	LEU
1	B	74	ARG
1	B	93	VAL
1	B	106	LEU
1	B	110	LEU
1	B	120	LEU
1	B	124	LYS
1	B	159	LEU
1	B	169	TYR
1	B	195	ARG
1	B	211	TRP
1	B	227	LYS
1	B	235	ARG
1	B	237	LEU
1	B	269	GLN
1	B	301	LEU
1	B	334	LEU
1	B	358	LEU
1	B	367	ASP
1	B	369	ARG
1	B	372	GLN
1	B	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	HIS
1	A	69	GLN
1	A	144	GLN
1	A	152	HIS
1	A	164	GLN
1	A	175	ASN
1	A	208	HIS
1	A	226	ASN
1	A	239	ASN
1	A	244	GLN
1	A	252	GLN
1	A	256	HIS
1	A	281	HIS
1	A	290	ASN
1	A	328	GLN
1	A	349	GLN
1	B	69	GLN
1	B	70	GLN
1	B	82	GLN
1	B	123	ASN
1	B	144	GLN
1	B	153	ASN
1	B	164	GLN
1	B	175	ASN
1	B	244	GLN
1	B	252	GLN
1	B	256	HIS
1	B	269	GLN
1	B	281	HIS
1	B	290	ASN
1	B	349	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](#)

4 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	NDP	A	701	-	45,52,52	1.51	4 (8%)	53,80,80	1.43	7 (13%)
3	SYE	A	800	-	16,16,16	1.65	5 (31%)	22,23,23	1.30	2 (9%)
3	SYE	B	801	-	16,16,16	2.12	4 (25%)	22,23,23	1.24	2 (9%)
2	NDP	B	702	-	45,52,52	1.53	4 (8%)	53,80,80	1.24	3 (5%)

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	NDP	A	701	-	-	6/30/77/77	0/5/5/5
3	SYE	A	800	-	-	0/5/5/5	0/2/2/2
3	SYE	B	801	-	-	0/5/5/5	0/2/2/2
2	NDP	B	702	-	-	4/30/77/77	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NDP	O7N-C7N	6.55	1.40	1.24
2	B	702	NDP	O7N-C7N	5.97	1.38	1.24
3	B	801	SYE	C17-C12	5.01	1.56	1.51
2	A	701	NDP	C2A-N3A	4.30	1.39	1.32
3	B	801	SYE	P18-O23	3.95	1.64	1.54
2	B	702	NDP	C2A-N3A	3.87	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	NDP	C6N-C5N	3.76	1.40	1.33
3	A	800	SYE	P18-O22	3.66	1.63	1.54
3	B	801	SYE	P18-C17	3.34	1.85	1.79
2	A	701	NDP	C6N-C5N	3.03	1.38	1.33
3	A	800	SYE	P18-O23	2.99	1.61	1.54
2	B	702	NDP	C2A-N1A	2.50	1.38	1.33
2	A	701	NDP	C2A-N1A	2.44	1.38	1.33
3	A	800	SYE	C14-C13	2.31	1.41	1.36
3	A	800	SYE	C6-C5	2.15	1.41	1.36
3	A	800	SYE	C12-N11	2.04	1.36	1.32
3	B	801	SYE	C12-N11	2.04	1.36	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NDP	N3A-C2A-N1A	-6.69	118.22	128.68
2	B	702	NDP	N3A-C2A-N1A	-5.24	120.49	128.68
3	A	800	SYE	C17-C12-N11	3.76	118.80	116.08
2	A	701	NDP	PN-O3-PA	-2.61	123.88	132.83
2	A	701	NDP	C1B-N9A-C4A	-2.52	122.21	126.64
2	B	702	NDP	C3N-C7N-N7N	2.50	122.10	117.67
3	A	800	SYE	C17-C12-C13	-2.42	119.68	121.42
3	B	801	SYE	C12-N11-C3	2.35	121.95	118.00
3	B	801	SYE	C13-C12-N11	-2.30	119.96	123.12
2	A	701	NDP	C3N-C7N-N7N	2.26	121.67	117.67
2	A	701	NDP	O7N-C7N-C3N	-2.22	116.71	120.90
2	A	701	NDP	C2A-N1A-C6A	2.17	122.46	118.75
2	A	701	NDP	O2A-PA-O1A	2.08	122.54	112.24
2	B	702	NDP	C2D-C1D-N1N	2.01	118.35	113.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	702	NDP	C2D-C1D-N1N-C6N
2	A	701	NDP	C2D-C1D-N1N-C6N
2	A	701	NDP	O4D-C1D-N1N-C6N
2	A	701	NDP	C2B-O2B-P2B-O3X
2	B	702	NDP	O4D-C1D-N1N-C6N
2	B	702	NDP	O4B-C4B-C5B-O5B
2	A	701	NDP	C2B-O2B-P2B-O2X
2	B	702	NDP	C2B-O2B-P2B-O2X

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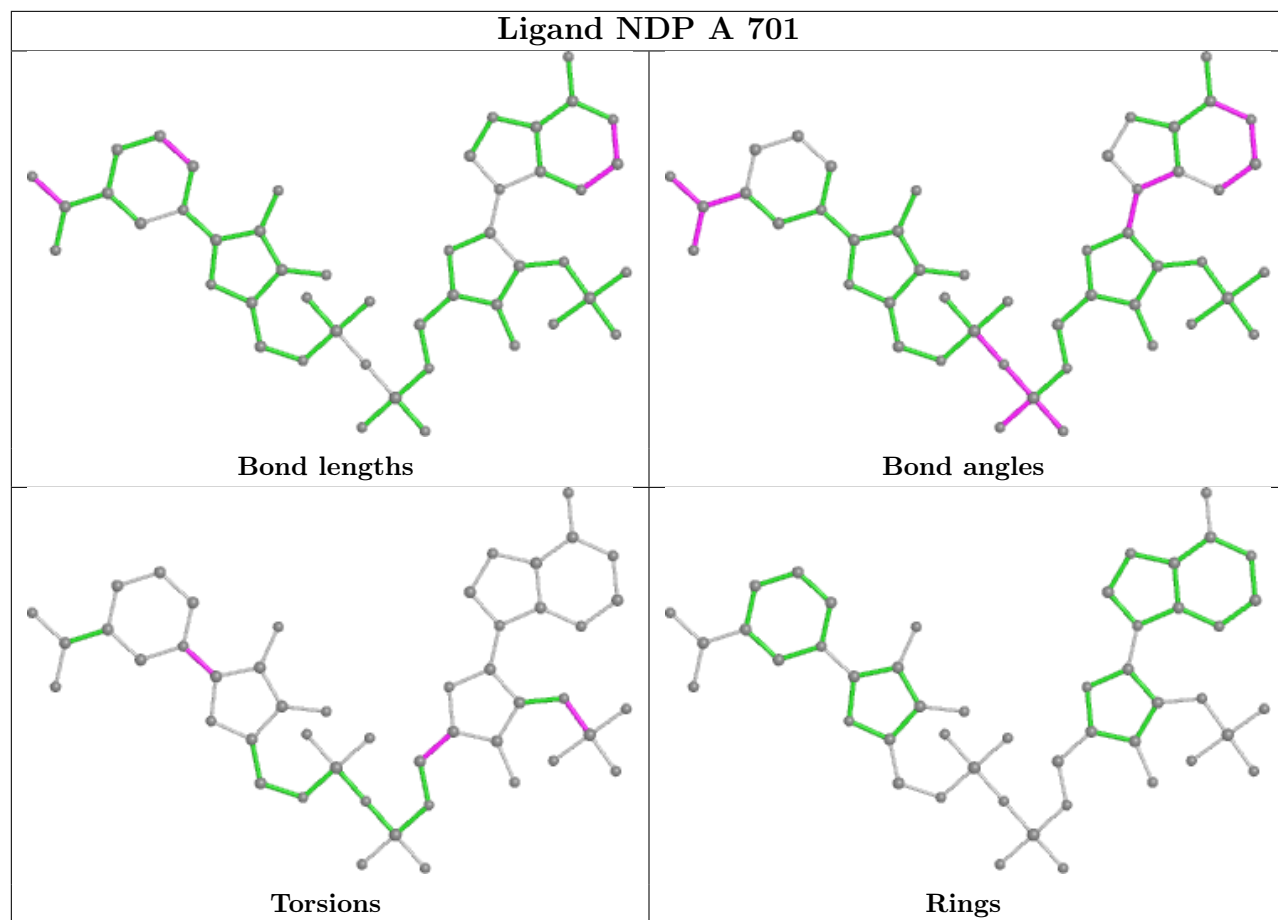
Mol	Chain	Res	Type	Atoms
2	A	701	NDP	O4B-C4B-C5B-O5B
2	A	701	NDP	O4D-C1D-N1N-C2N

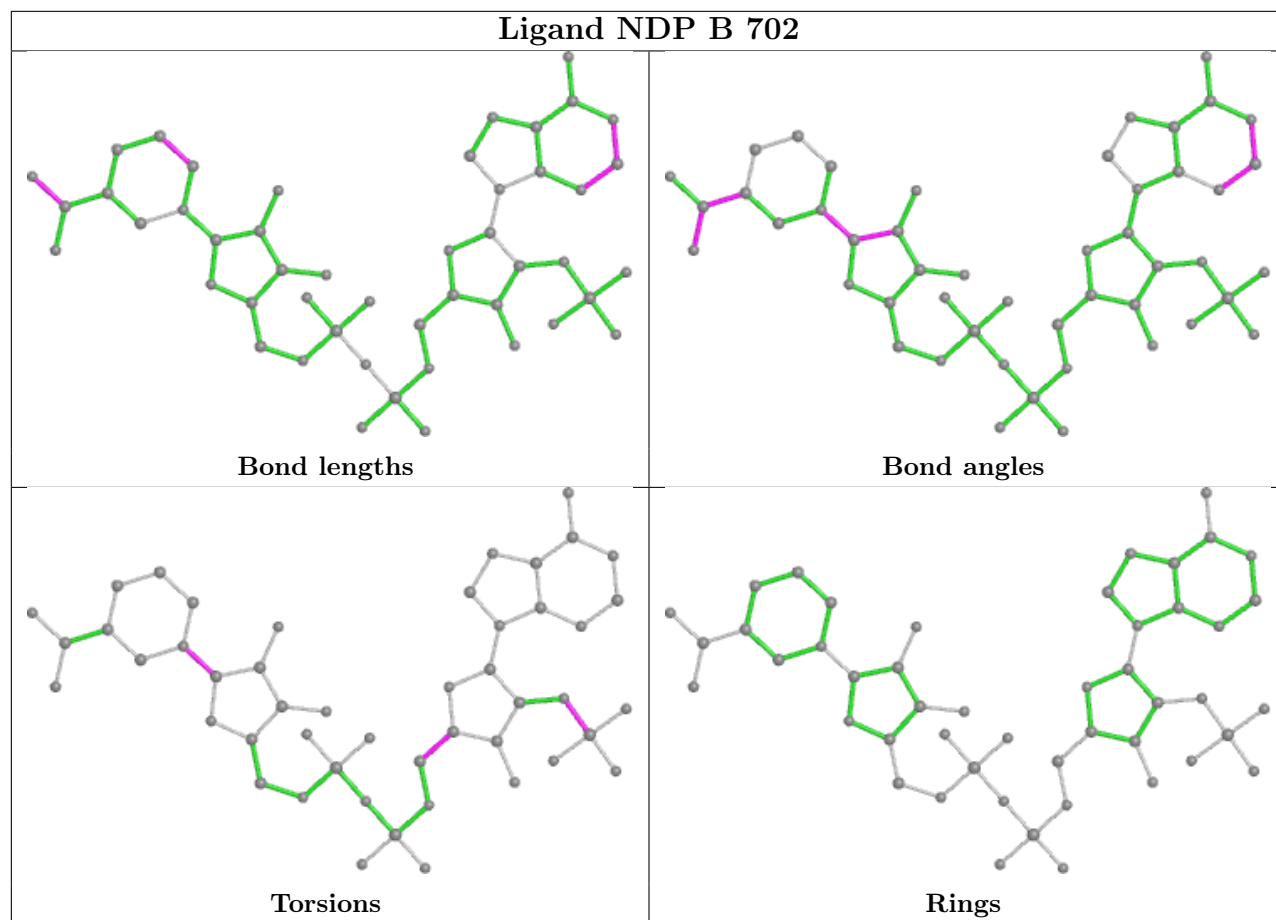
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NDP	1	0
3	A	800	SYE	1	0
2	B	702	NDP	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/420 (95%)	0.13	12 (3%) 50 49	13, 21, 42, 67	0
1	B	398/420 (94%)	0.05	16 (4%) 38 37	14, 22, 37, 54	0
All	All	798/840 (95%)	0.09	28 (3%) 44 43	13, 22, 39, 67	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	ALA	8.1
1	A	169	TYR	7.0
1	B	367	ASP	5.5
1	A	398	SER	5.2
1	A	209	PRO	4.7
1	A	367	ASP	4.6
1	B	169	TYR	4.4
1	B	369	ARG	4.0
1	B	195	ARG	3.9
1	A	369	ARG	3.8
1	B	368	MET	3.6
1	A	25	GLU	3.3
1	B	394	ARG	3.1
1	B	25	GLU	2.8
1	A	62	LYS	2.6
1	B	397	SER	2.4
1	B	140	GLN	2.3
1	B	122	ALA	2.2
1	B	0	GLY	2.2
1	B	148	VAL	2.2
1	A	66	THR	2.2
1	B	91	GLU	2.2
1	B	209	PRO	2.1
1	B	142	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	146	LEU	2.1
1	A	174	GLN	2.0
1	A	396	ALA	2.0
1	A	40	ARG	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

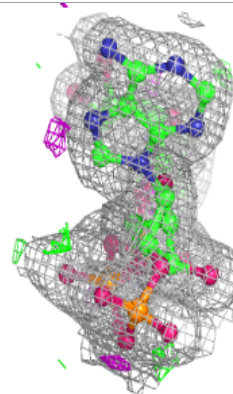
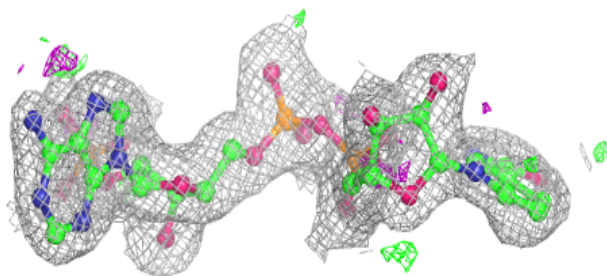
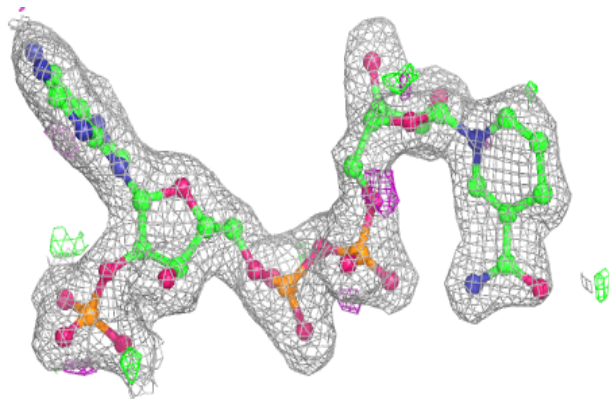
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	A	701	48/48	0.95	0.10	21,27,37,40	0
2	NDP	B	702	48/48	0.96	0.10	17,21,28,31	0
3	SYE	A	800	15/15	0.98	0.09	13,17,20,20	0
3	SYE	B	801	15/15	0.98	0.10	16,18,20,20	0

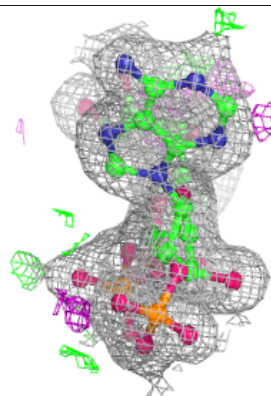
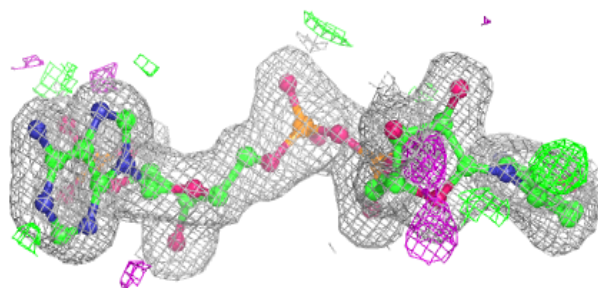
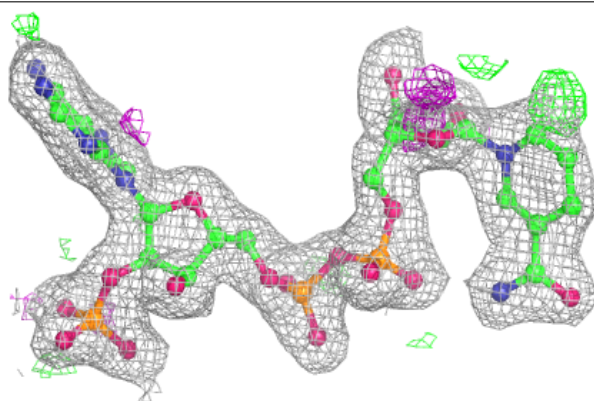
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NDP A 701:**

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

**Electron density around NDP B 702:**

$2mF_o-DF_c$  (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.