



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:40 AM UTC

PDB ID : 6PAY / pdb_00006pay
Title : Structure of HsICDH1:Mg(II):ICT:NADPH(50%) complex reveals structural basis for observation of half-sites reactivity
Authors : Silvaggi, N.R.; Melkonian, T.R.; Roman, J.V.; Moran, G.R.
Deposited on : 2019-06-12
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

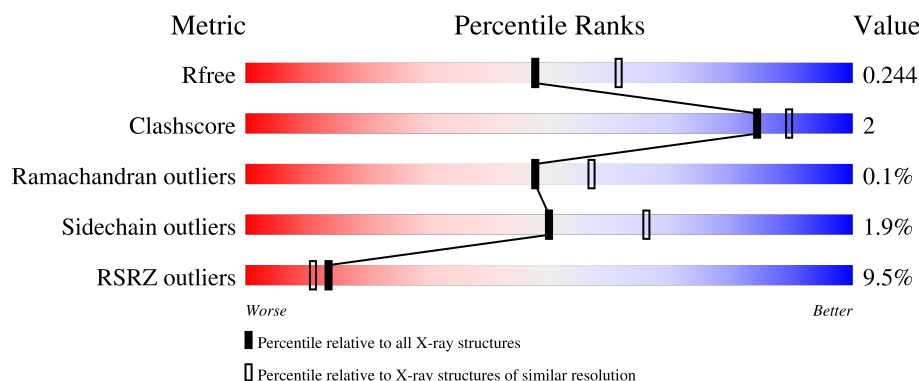
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	414	7% 93% 6% ..
1	B	414	5% 94% 5%
1	C	414	13% 91% 7% .
1	D	414	14% 90% 8% .

2 Entry composition [i](#)

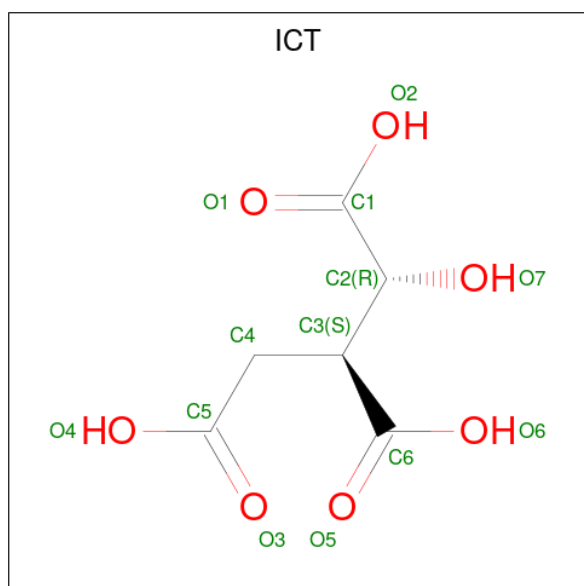
There are 6 unique types of molecules in this entry. The entry contains 25350 atoms, of which 12115 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	H	N	O	S	0	0	0
			6278	2044	3061	544	611	18			
1	B	412	Total	C	H	N	O	S	0	0	0
			6302	2057	3070	545	612	18			
1	C	408	Total	C	H	N	O	S	0	0	0
			6125	2011	2967	528	602	17			
1	D	406	Total	C	H	N	O	S	0	0	0
			6127	2005	2977	531	596	18			

- Molecule 2 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	6	4	7		
2	B	1	Total	C	H	O	0	0
			17	6	4	7		

Continued on next page...

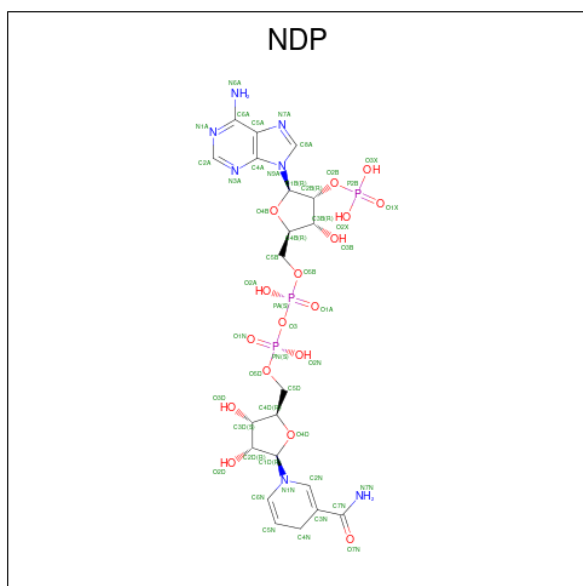
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			17	6	4	7		
2	D	1	Total	C	H	O	0	0
			17	6	4	7		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

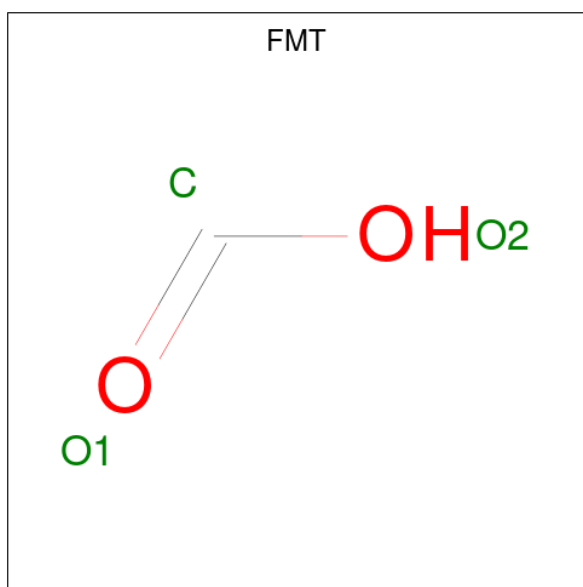
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			56	15	16	6	16		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

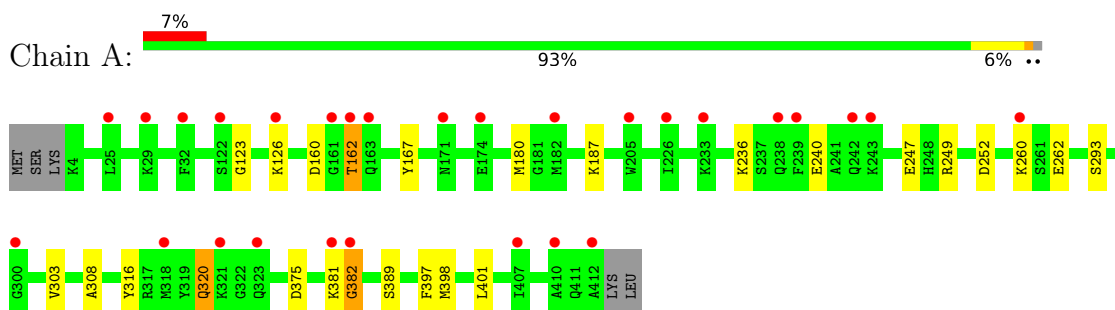
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total	O	0	0
			113	113		
6	B	106	Total	O	0	0
			106	106		
6	C	76	Total	O	0	0
			76	76		
6	D	66	Total	O	0	0
			66	66		

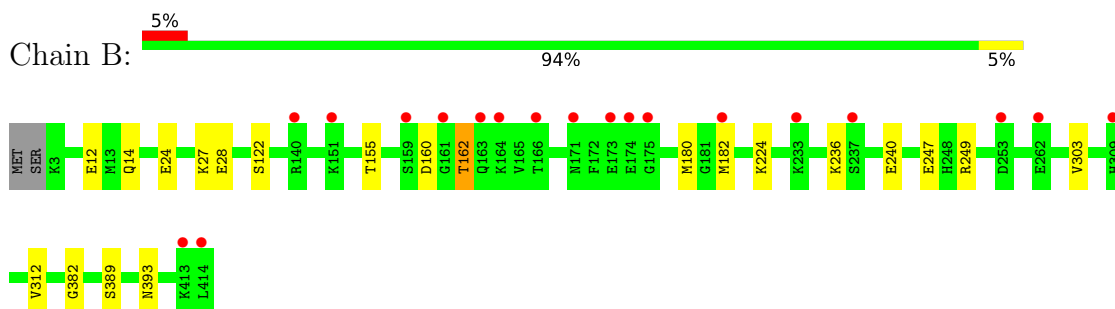
3 Residue-property plots [i](#)

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.

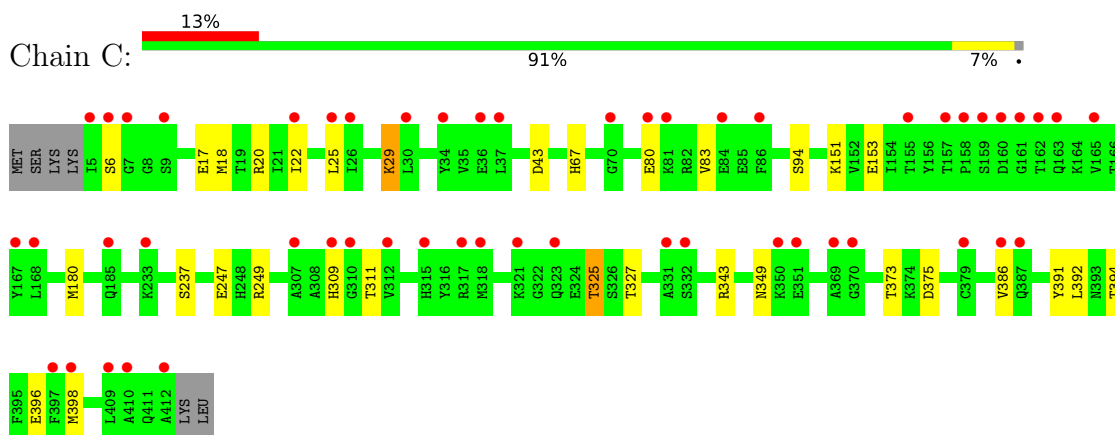
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



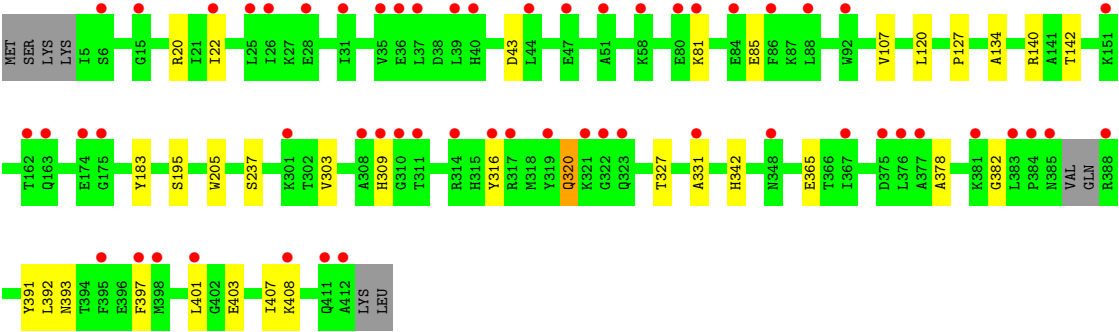
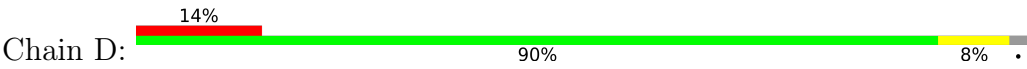
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.60Å 74.60Å 142.90Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	47.10 – 2.20 47.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.5 (47.10-2.20) 85.2 (47.10-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (dev_3525: ???)	Depositor
R, R_{free}	0.224 , 0.242 0.227 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25350	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1451e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NDP, MG, FMT, ICT

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	0.12	0/3285	0.34	0/4438
1	B	0.13	0/3300	0.32	0/4456
1	C	0.12	0/3226	0.34	0/4368
1	D	0.14	0/3217	0.33	0/4350
All	All	0.13	0/13028	0.33	0/17612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3217	3061	3144	14	0
1	B	3232	3070	3164	8	0
1	C	3158	2967	3046	17	0
1	D	3150	2977	3053	21	0
2	A	13	4	4	0	0
2	B	13	4	4	0	0
2	C	13	4	5	1	0
2	D	13	4	4	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	40	16	19	1	0
5	A	12	5	4	1	0
5	B	6	2	2	0	0
5	D	3	1	1	0	0
6	A	113	0	0	0	0
6	B	106	0	0	0	0
6	C	76	0	0	0	0
6	D	66	0	0	2	0
All	All	13235	12115	12450	58	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 2.

All (58) 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:D:365:GLU:O	6:D:601:HOH:O	1.84	0.94
1:D:81:LYS:NZ	1:D:85:GLU:OE1	2.09	0.85
1:D:309:HIS:HE1	1:D:331:ALA:HB3	1.52	0.74
1:C:67:HIS:O	1:C:343:ARG:NH2	2.22	0.72
1:A:160:ASP:OD1	1:A:162:THR:OG1	2.11	0.69
1:C:6:SER:O	1:C:349:ASN:ND2	2.33	0.60
1:C:247:GLU:OE1	1:C:249:ARG:NH2	2.34	0.60
1:B:12:GLU:OE2	1:B:27:LYS:NZ	2.28	0.56
4:A:503:NDP:H8A	4:A:503:NDP:H51A	1.87	0.56
1:B:247:GLU:OE1	1:B:249:ARG:NH2	2.38	0.55
1:D:81:LYS:HD3	1:D:81:LYS:C	2.31	0.55
1:D:20:ARG:NH2	1:D:43:ASP:OD1	2.40	0.54
1:D:342:HIS:HB2	6:D:612:HOH:O	2.07	0.54
1:D:403:GLU:O	1:D:407:ILE:HD13	2.07	0.54
1:C:392:LEU:HB3	1:C:396:GLU:HG3	1.89	0.53
1:C:325:THR:HG23	1:C:394:THR:OG1	2.09	0.53
1:C:25:LEU:HD11	1:C:29:LYS:HD2	1.92	0.51
1:C:17:GLU:HB2	1:C:311:THR:HB	1.93	0.50
1:B:160:ASP:OD1	1:B:162:THR:OG1	2.27	0.50
1:A:247:GLU:OE1	1:A:249:ARG:NH2	2.44	0.50
1:C:80:GLU:O	1:C:83:VAL:HG22	2.11	0.50
1:C:20:ARG:NH2	1:C:43:ASP:OD1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLN:NE2	1:B:24:GLU:OE2	2.46	0.49
1:D:309:HIS:CE1	1:D:331:ALA:HB3	2.41	0.49
1:A:167:TYR:HB3	1:D:142:THR:HG21	1.95	0.48
1:D:378:ALA:O	1:D:382:GLY:N	2.46	0.47
1:A:375:ASP:HB3	5:A:507:FMT:C	2.45	0.47
1:A:260:LYS:HA	1:D:120:LEU:HD13	1.97	0.47
1:D:397:PHE:CE2	1:D:401:LEU:HD11	2.50	0.47
1:A:397:PHE:CE2	1:A:401:LEU:HD11	2.50	0.46
1:A:316:TYR:O	1:A:320:GLN:HG2	2.15	0.46
1:B:182:MET:HE2	1:C:180:MET:CE	2.46	0.45
1:D:140:ARG:HD3	1:D:183:TYR:OH	2.16	0.45
1:C:151:LYS:HE3	1:C:153:GLU:CD	2.42	0.45
1:A:126:LYS:CE	1:A:262:GLU:HG3	2.46	0.44
1:A:247:GLU:OE1	1:A:249:ARG:NH1	2.49	0.44
1:C:373:THR:OG1	1:C:375:ASP:OD1	2.24	0.44
1:D:316:TYR:O	1:D:320:GLN:HG2	2.16	0.44
1:A:381:LYS:O	1:A:382:GLY:C	2.61	0.44
1:C:391:TYR:C	1:C:392:LEU:HD12	2.44	0.43
1:D:22:ILE:HD11	1:D:327:THR:HB	2.00	0.43
1:C:94:SER:OG	2:C:501:ICT:O3	2.27	0.43
1:D:127:PRO:HG2	1:D:205:TRP:HH2	1.83	0.43
1:B:393:ASN:C	1:B:393:ASN:OD1	2.62	0.42
1:C:22:ILE:HD11	1:C:327:THR:HB	2.00	0.42
1:A:252:ASP:N	1:A:252:ASP:OD1	2.53	0.41
1:C:22:ILE:HD11	1:C:327:THR:CG2	2.50	0.41
1:A:123:GLY:O	1:A:262:GLU:HA	2.21	0.41
1:D:365:GLU:CD	1:D:408:LYS:HZ1	2.27	0.41
1:C:18:MET:HE2	1:C:325:THR:HG21	2.01	0.41
1:D:309:HIS:HE1	1:D:331:ALA:CB	2.29	0.41
1:A:236:LYS:NZ	1:A:240:GLU:OE2	2.50	0.41
1:D:391:TYR:C	1:D:392:LEU:HD12	2.46	0.41
1:D:393:ASN:OD1	1:D:393:ASN:C	2.65	0.40
1:B:236:LYS:NZ	1:B:240:GLU:OE1	2.54	0.40
1:D:107:VAL:HG23	1:D:134:ALA:HB2	2.02	0.40
1:A:293:SER:HB2	1:A:308:ALA:HB2	2.04	0.40
1:B:24:GLU:O	1:B:28:GLU:HG2	2.20	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	407/414 (98%)	391 (96%)	15 (4%)	1 (0%)	43	51
1	B	410/414 (99%)	397 (97%)	12 (3%)	1 (0%)	43	51
1	C	406/414 (98%)	392 (97%)	14 (3%)	0	100	100
1	D	402/414 (97%)	386 (96%)	16 (4%)	0	100	100
All	All	1625/1656 (98%)	1566 (96%)	57 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	GLY
1	B	382	GLY

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	338/350 (97%)	331 (98%)	7 (2%)	47	63
1	B	338/350 (97%)	330 (98%)	8 (2%)	43	58
1	C	326/350 (93%)	320 (98%)	6 (2%)	51	68
1	D	326/350 (93%)	322 (99%)	4 (1%)	63	78
All	All	1328/1400 (95%)	1303 (98%)	25 (2%)	50	66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	180	MET
1	A	187	LYS
1	A	303	VAL
1	A	320	GLN
1	A	389	SER
1	A	398	MET
1	B	122	SER
1	B	155	THR
1	B	162	THR
1	B	180	MET
1	B	224	LYS
1	B	303	VAL
1	B	312	VAL
1	B	389	SER
1	C	29	LYS
1	C	237	SER
1	C	309	HIS
1	C	325	THR
1	C	386	VAL
1	C	398	MET
1	D	195	SER
1	D	237	SER
1	D	303	VAL
1	D	320	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	171	ASN
1	A	194	HIS
1	A	213	ASN
1	A	277	GLN
1	A	357	ASN
1	B	53	ASN
1	B	194	HIS
1	B	213	ASN
1	B	277	GLN
1	B	283	GLN
1	B	309	HIS
1	B	315	HIS
1	C	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	68	ASN
1	C	101	ASN
1	C	170	HIS
1	C	171	ASN
1	C	194	HIS
1	C	213	ASN
1	C	228	GLN
1	C	277	GLN
1	C	342	HIS
1	D	40	HIS
1	D	48	ASN
1	D	67	HIS
1	D	228	GLN
1	D	277	GLN
1	D	309	HIS

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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
5	FMT	A	504	-	2,2,2	0.71	0	1,1,1	0.43	0
5	FMT	A	505	-	2,2,2	0.70	0	1,1,1	0.43	0
5	FMT	D	503	-	2,2,2	0.70	0	1,1,1	0.42	0
2	ICT	A	501	3	12,12,12	1.17	0	13,16,16	1.59	5 (38%)
4	NDP	A	503	-	42,43,52	2.64	9 (21%)	62,67,80	1.59	15 (24%)
5	FMT	A	506	-	2,2,2	0.68	0	1,1,1	0.43	0
2	ICT	B	501	3	12,12,12	1.23	1 (8%)	13,16,16	1.59	4 (30%)
2	ICT	C	501	3	12,12,12	1.19	0	13,16,16	1.67	6 (46%)
5	FMT	B	503	-	2,2,2	0.71	0	1,1,1	0.44	0
5	FMT	B	504	-	2,2,2	0.72	0	1,1,1	0.44	0
2	ICT	D	501	3	12,12,12	1.14	0	13,16,16	1.65	5 (38%)
5	FMT	A	507	-	2,2,2	0.69	0	1,1,1	0.22	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
2	ICT	A	501	3	-	2/16/16/16	-
4	NDP	A	503	-	-	6/27/59/77	0/4/4/5
2	ICT	B	501	3	-	2/16/16/16	-
2	ICT	C	501	3	-	6/16/16/16	-
2	ICT	D	501	3	-	2/16/16/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	NDP	P2B-O2B	12.88	1.82	1.59
4	A	503	NDP	PA-O3	5.52	1.65	1.59
4	A	503	NDP	PN-O5D	4.61	1.77	1.59
4	A	503	NDP	O2B-C2B	-2.78	1.34	1.44
4	A	503	NDP	C5A-C4A	2.75	1.44	1.39
4	A	503	NDP	C2A-N1A	2.52	1.38	1.33
4	A	503	NDP	C4A-N3A	2.14	1.38	1.34
4	A	503	NDP	O4B-C1B	2.11	1.46	1.42
4	A	503	NDP	C8A-N9A	2.10	1.41	1.37
2	B	501	ICT	C2-C1	-2.00	1.49	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NDP	O3-PA-O1A	-3.97	98.76	110.70
4	A	503	NDP	O2B-P2B-O1X	-3.64	96.35	109.33
4	A	503	NDP	O2N-PN-O3	3.60	117.01	107.27
4	A	503	NDP	P2B-O2B-C2B	-3.20	114.87	123.43
4	A	503	NDP	PA-O5B-C5B	-3.05	103.85	121.35
4	A	503	NDP	O5D-PN-O1N	-2.65	98.42	108.94
4	A	503	NDP	O3X-P2B-O2X	2.64	117.69	107.80
2	C	501	ICT	O6-C6-C3	2.58	120.61	113.93
2	C	501	ICT	O2-C1-C2	2.50	120.26	113.31
2	D	501	ICT	O6-C6-C3	2.46	120.32	113.93
2	A	501	ICT	O2-C1-C2	2.41	120.01	113.31
2	A	501	ICT	O6-C6-C3	2.40	120.15	113.93
2	B	501	ICT	O6-C6-O5	-2.39	118.65	124.08
2	D	501	ICT	O6-C6-O5	-2.39	118.65	124.08
4	A	503	NDP	C5D-C4D-C3D	-2.38	106.64	115.21
2	D	501	ICT	O2-C1-C2	2.34	119.83	113.31
2	B	501	ICT	O6-C6-C3	2.32	119.96	113.93
2	A	501	ICT	O2-C1-O1	-2.30	118.85	124.08
2	D	501	ICT	O4-C5-C4	2.30	121.14	114.00
2	B	501	ICT	O2-C1-C2	2.28	119.65	113.31
2	C	501	ICT	O6-C6-O5	-2.27	118.93	124.08
4	A	503	NDP	O3X-P2B-O2B	-2.22	97.20	105.85
4	A	503	NDP	N3A-C4A-N9A	2.18	130.88	127.17
4	A	503	NDP	C2A-N1A-C6A	-2.18	115.15	118.73
2	C	501	ICT	C3-C4-C5	-2.17	109.89	113.95
4	A	503	NDP	O2N-PN-O1N	2.16	122.50	112.44
2	A	501	ICT	O6-C6-O5	-2.15	119.19	124.08
2	B	501	ICT	O4-C5-C4	2.11	120.56	114.00
2	C	501	ICT	O2-C1-O1	-2.04	119.45	124.08
4	A	503	NDP	C5A-C4A-N3A	-2.02	123.94	126.72
4	A	503	NDP	O4B-C1B-C2B	-2.02	103.11	106.59
4	A	503	NDP	PN-O5D-C5D	-2.02	109.80	121.35
2	A	501	ICT	O4-C5-C4	2.01	120.26	114.00
2	D	501	ICT	O2-C1-O1	-2.01	119.52	124.08
2	C	501	ICT	O4-C5-C4	2.00	120.23	114.00

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	NDP	C5D-O5D-PN-O3
4	A	503	NDP	C5D-O5D-PN-O2N
4	A	503	NDP	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

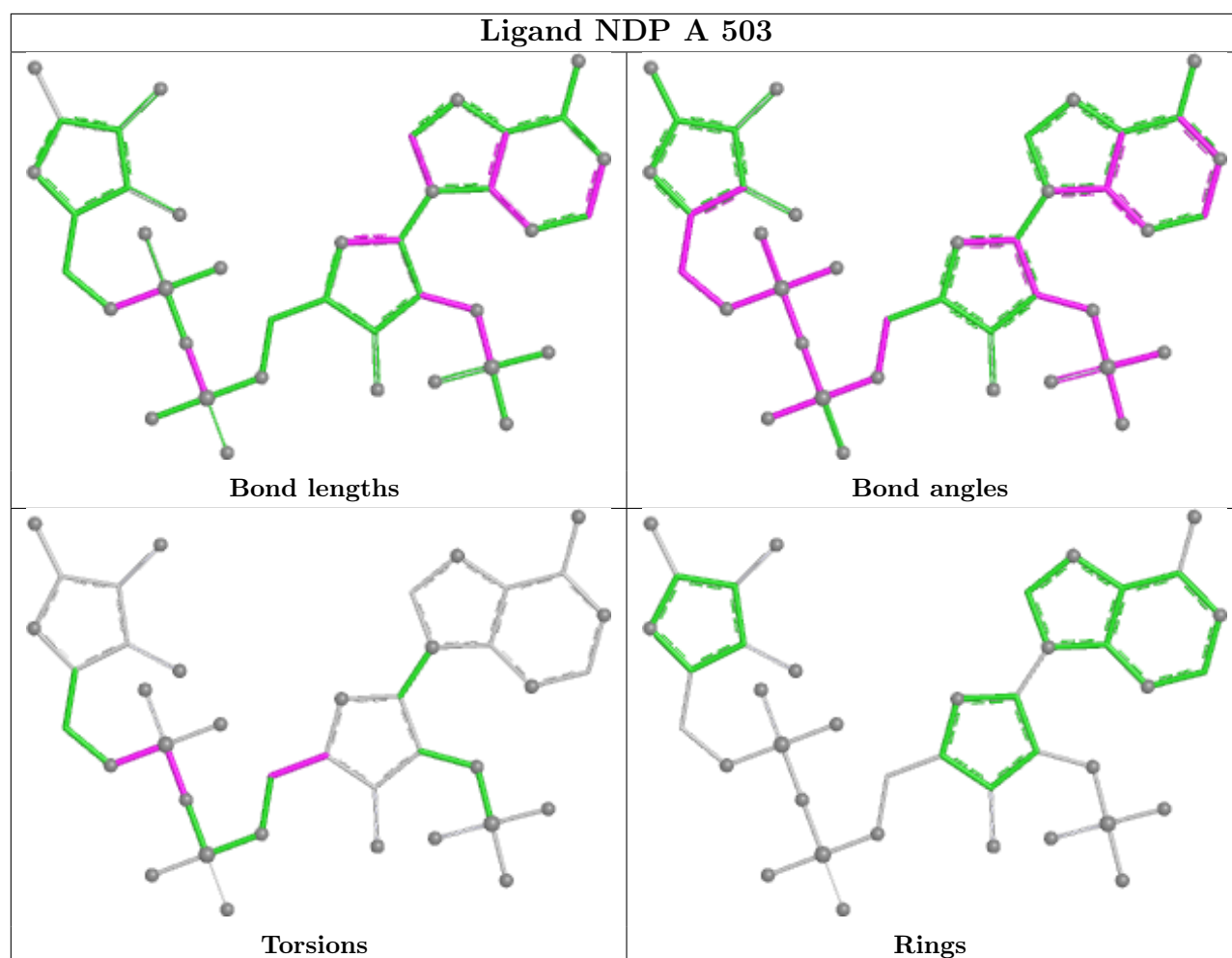
Mol	Chain	Res	Type	Atoms
4	A	503	NDP	C3B-C4B-C5B-O5B
2	C	501	ICT	O2-C1-C2-C3
2	C	501	ICT	O1-C1-C2-C3
2	A	501	ICT	C4-C3-C6-O6
2	B	501	ICT	C4-C3-C6-O5
2	B	501	ICT	C4-C3-C6-O6
2	C	501	ICT	C4-C3-C6-O5
2	C	501	ICT	C4-C3-C6-O6
2	C	501	ICT	O2-C1-C2-O7
4	A	503	NDP	C5D-O5D-PN-O1N
2	C	501	ICT	O1-C1-C2-O7
2	A	501	ICT	C4-C3-C6-O5
2	D	501	ICT	C3-C4-C5-O3
2	D	501	ICT	C3-C4-C5-O4
4	A	503	NDP	PA-O3-PN-O2N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	NDP	1	0
2	C	501	ICT	1	0
5	A	507	FMT	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	409/414 (98%)	0.65	28 (6%)	23 20	20, 41, 62, 78	0
1	B	412/414 (99%)	0.52	19 (4%)	37 34	24, 38, 52, 65	0
1	C	408/414 (98%)	0.91	52 (12%)	8 6	25, 48, 70, 85	0
1	D	406/414 (98%)	0.91	57 (14%)	6 4	22, 44, 75, 89	0
All	All	1635/1656 (98%)	0.75	156 (9%)	14 11	20, 41, 71, 89	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	THR	6.9
1	A	381	LYS	6.5
1	D	385	ASN	5.8
1	D	412	ALA	5.8
1	D	309	HIS	5.6
1	D	310	GLY	5.3
1	C	159	SER	4.9
1	A	122	SER	4.9
1	C	412	ALA	4.8
1	C	309	HIS	4.7
1	C	163	GLN	4.6
1	C	5	ILE	4.5
1	D	383	LEU	4.5
1	C	7	GLY	4.4
1	C	161	GLY	4.3
1	D	47	GLU	4.2
1	C	323	GLN	4.1
1	D	84	GLU	4.0
1	C	25	LEU	3.7
1	D	317	ARG	3.7
1	B	309	HIS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	384	PRO	3.6
1	D	388	ARG	3.6
1	D	36	GLU	3.6
1	C	310	GLY	3.5
1	B	414	LEU	3.5
1	B	173	GLU	3.5
1	C	317	ARG	3.4
1	A	412	ALA	3.3
1	D	321	LYS	3.3
1	D	51	ALA	3.3
1	D	80	GLU	3.3
1	D	319	TYR	3.2
1	C	397	PHE	3.2
1	D	323	GLN	3.2
1	C	398	MET	3.2
1	C	36	GLU	3.1
1	A	382	GLY	3.0
1	A	242	GLN	2.9
1	D	26	ILE	2.9
1	C	410	ALA	2.9
1	A	126	LYS	2.9
1	A	300	GLY	2.9
1	B	151	LYS	2.9
1	B	413	LYS	2.9
1	A	161	GLY	2.9
1	C	350	LYS	2.9
1	A	163	GLN	2.8
1	C	332	SER	2.8
1	C	22	ILE	2.8
1	C	158	PRO	2.8
1	C	34	TYR	2.8
1	A	162	THR	2.8
1	D	31	ILE	2.8
1	C	318	MET	2.8
1	D	39	LEU	2.8
1	D	35	VAL	2.8
1	C	80	GLU	2.7
1	D	322	GLY	2.7
1	C	312	VAL	2.7
1	D	367	ILE	2.7
1	B	262	GLU	2.7
1	C	84	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	301	LYS	2.7
1	D	331	ALA	2.7
1	D	377	ALA	2.7
1	A	407	ILE	2.7
1	A	323	GLN	2.7
1	D	314	ARG	2.7
1	C	160	ASP	2.6
1	A	260	LYS	2.6
1	B	161	GLY	2.6
1	D	28	GLU	2.6
1	C	351	GLU	2.6
1	A	243	LYS	2.6
1	C	81	LYS	2.6
1	A	32	PHE	2.6
1	D	22	ILE	2.6
1	D	316	TYR	2.6
1	D	58	LYS	2.6
1	C	369	ALA	2.6
1	B	174	GLU	2.5
1	D	375	ASP	2.5
1	B	237	SER	2.5
1	D	395	PHE	2.5
1	D	397	PHE	2.5
1	D	81	LYS	2.5
1	D	162	THR	2.5
1	D	44	LEU	2.5
1	A	171	ASN	2.5
1	D	398	MET	2.5
1	D	174	GLU	2.4
1	C	233	LYS	2.4
1	D	408	LYS	2.4
1	C	387	GLN	2.4
1	D	86	PHE	2.4
1	D	6	SER	2.4
1	D	92	TRP	2.4
1	C	321	LYS	2.4
1	C	168	LEU	2.4
1	C	409	LEU	2.4
1	D	381	LYS	2.4
1	D	37	LEU	2.3
1	D	151	LYS	2.3
1	D	40	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	307	ALA	2.3
1	C	331	ALA	2.3
1	D	401	LEU	2.3
1	C	167	TYR	2.3
1	C	6	SER	2.2
1	A	239	PHE	2.2
1	C	26	ILE	2.2
1	C	386	VAL	2.2
1	A	29	LYS	2.2
1	B	175	GLY	2.2
1	D	376	LEU	2.2
1	C	185	GLN	2.2
1	D	25	LEU	2.2
1	D	163	GLN	2.2
1	C	86	PHE	2.2
1	B	253	ASP	2.2
1	C	70	GLY	2.2
1	C	37	LEU	2.2
1	C	379	CYS	2.2
1	C	157	THR	2.2
1	B	163	GLN	2.1
1	D	15	GLY	2.1
1	B	164	LYS	2.1
1	A	318	MET	2.1
1	D	348	ASN	2.1
1	A	174	GLU	2.1
1	D	411	GLN	2.1
1	D	175	GLY	2.1
1	A	233	LYS	2.1
1	D	88	LEU	2.1
1	A	182	MET	2.1
1	D	311	THR	2.1
1	C	165	VAL	2.1
1	A	410	ALA	2.1
1	A	25	LEU	2.1
1	B	182	MET	2.1
1	C	315	HIS	2.1
1	C	370	GLY	2.1
1	A	321	LYS	2.1
1	B	233	LYS	2.1
1	C	9	SER	2.1
1	C	30	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	155	THR	2.0
1	A	226	ILE	2.0
1	B	159	SER	2.0
1	A	205	TRP	2.0
1	D	308	ALA	2.0
1	B	171	ASN	2.0
1	A	238	GLN	2.0
1	B	140	ARG	2.0
1	B	166	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

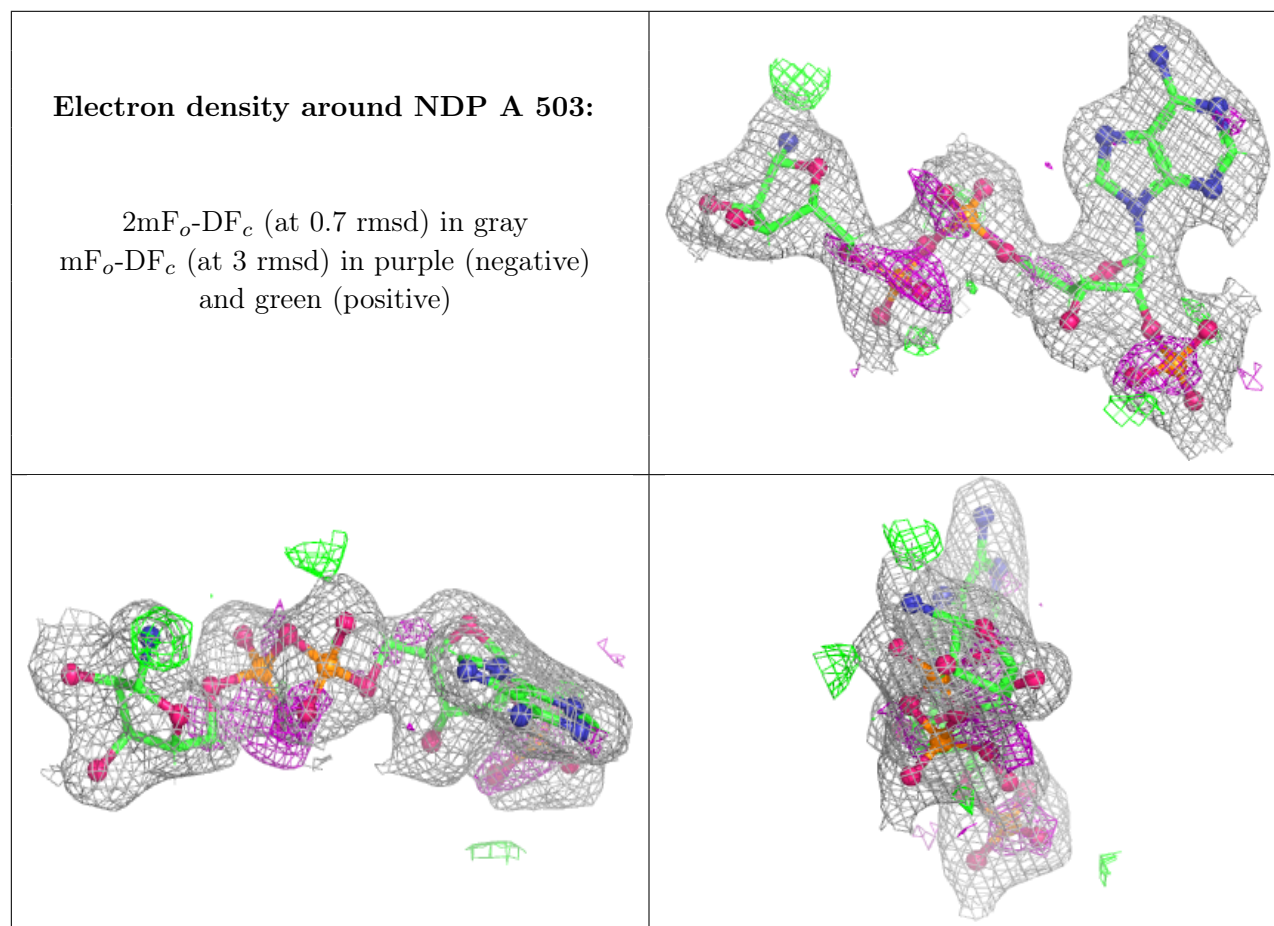
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FMT	D	503	3/3	0.76	0.30	17,17,17,21	0
5	FMT	A	507	3/3	0.82	0.32	19,19,23,23	0
5	FMT	B	504	3/3	0.83	0.23	17,17,17,21	0
5	FMT	B	503	3/3	0.83	0.25	17,17,17,21	0
3	MG	D	502	1/1	0.84	0.09	29,29,29,29	0
5	FMT	A	505	3/3	0.85	0.31	17,17,17,21	0
3	MG	C	502	1/1	0.87	0.10	19,19,19,19	0
2	ICT	D	501	13/13	0.89	0.12	17,37,57,58	0
2	ICT	C	501	13/13	0.90	0.10	21,31,47,47	0
5	FMT	A	506	3/3	0.90	0.27	17,17,17,21	0
3	MG	B	502	1/1	0.91	0.10	8,8,8,8	0
3	MG	A	502	1/1	0.93	0.07	6,6,6,6	0
5	FMT	A	504	3/3	0.93	0.24	17,17,17,21	0
2	ICT	B	501	13/13	0.94	0.07	4,12,28,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ICT	A	501	13/13	0.95	0.09	2,10,18,27	0
4	NDP	A	503	40/48	0.96	0.07	11,11,13,13	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.