



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:54 am BST

PDB ID : 5KVU  
Title : Crystal structure of isocitrate dehydrogenase-2 in complex with NADP(+) from *Mycobacterium tuberculosis*  
Authors : Cheng, Y.S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2016-07-15  
Resolution : 2.66 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.

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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 : 2.11  
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

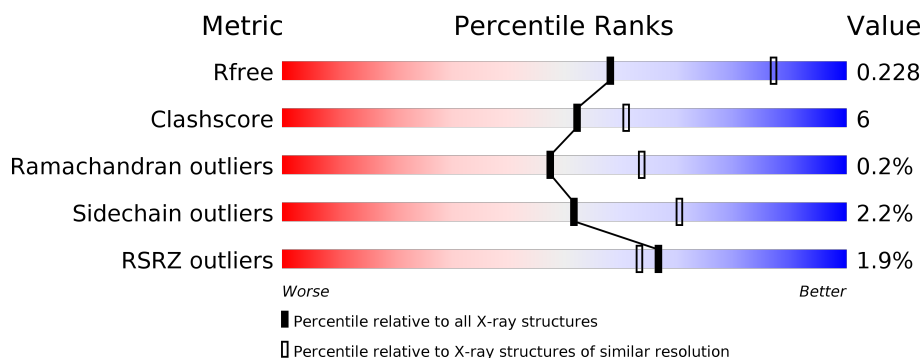
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>14%</span> <span>..</span> </div> </div>
1	B	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>85%</span> <span>13%</span> <span>..</span> </div> </div>
1	C	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>83%</span> <span>15%</span> <span>.</span> </div> </div>
1	D	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	805	-	-	-	X
4	EDO	D	804	-	-	X	-

## 2 Entry composition i

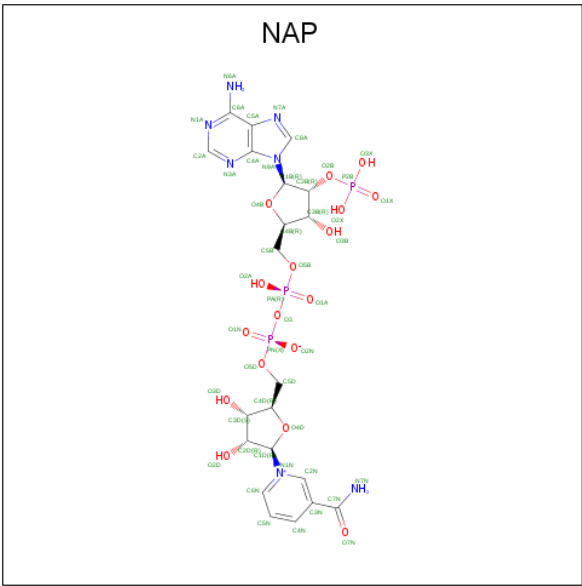
There are 8 unique types of molecules in this entry. The entry contains 23607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	2	0
			5755	3626	989	1106	34			
1	B	738	Total	C	N	O	S	0	0	0
			5725	3609	986	1097	33			
1	C	734	Total	C	N	O	S	0	1	0
			5720	3605	984	1099	32			
1	D	732	Total	C	N	O	S	0	4	0
			5725	3610	986	1097	32			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



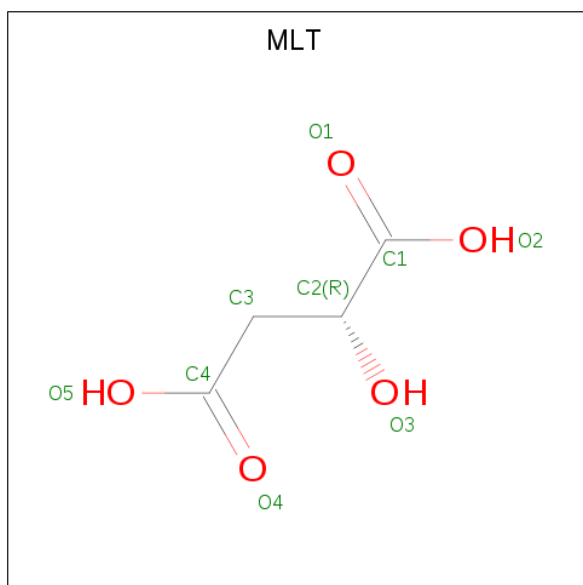
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



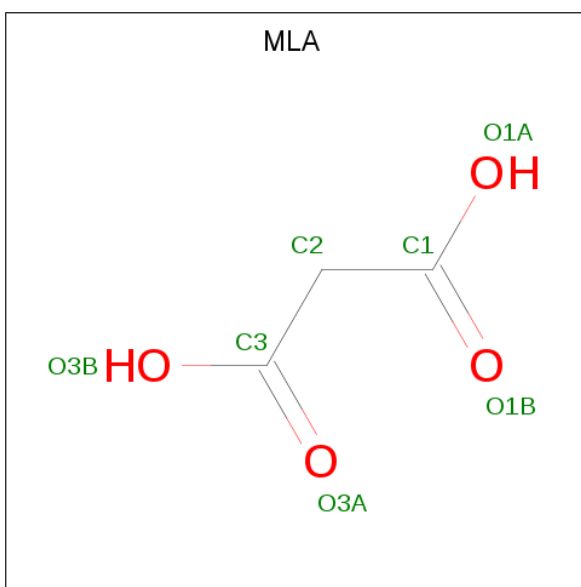
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			9	4	5	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



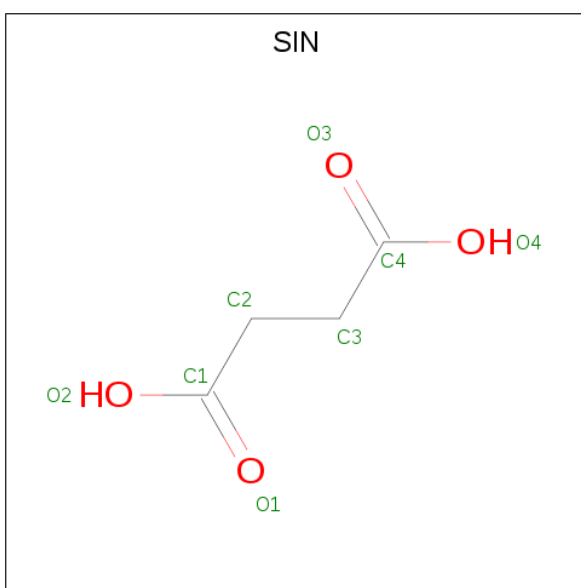
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula:  $C_4H_6O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

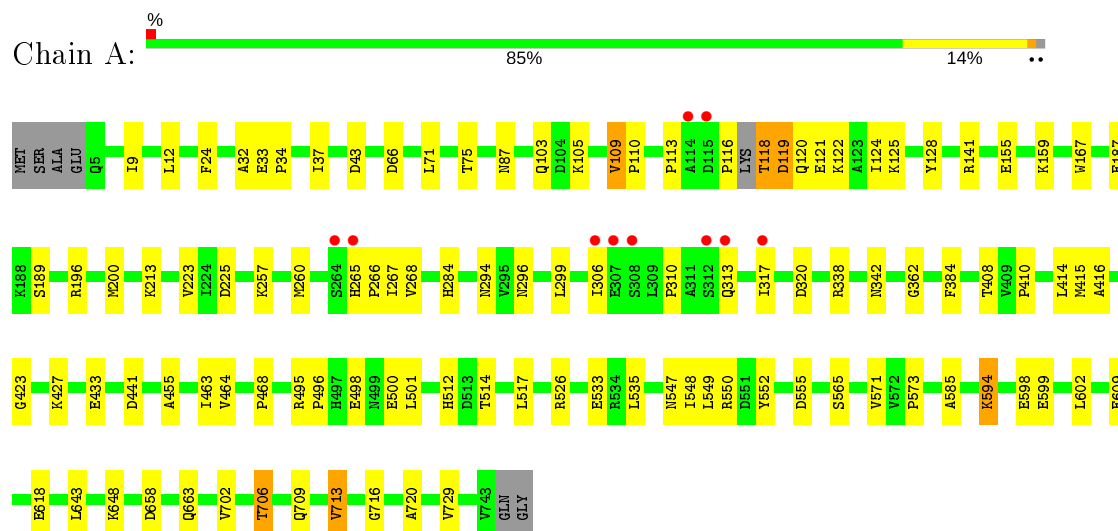
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	145	Total	O	0	0
			145	145		
8	B	92	Total	O	0	0
			92	92		
8	C	109	Total	O	0	0
			109	109		
8	D	77	Total	O	0	0
			77	77		



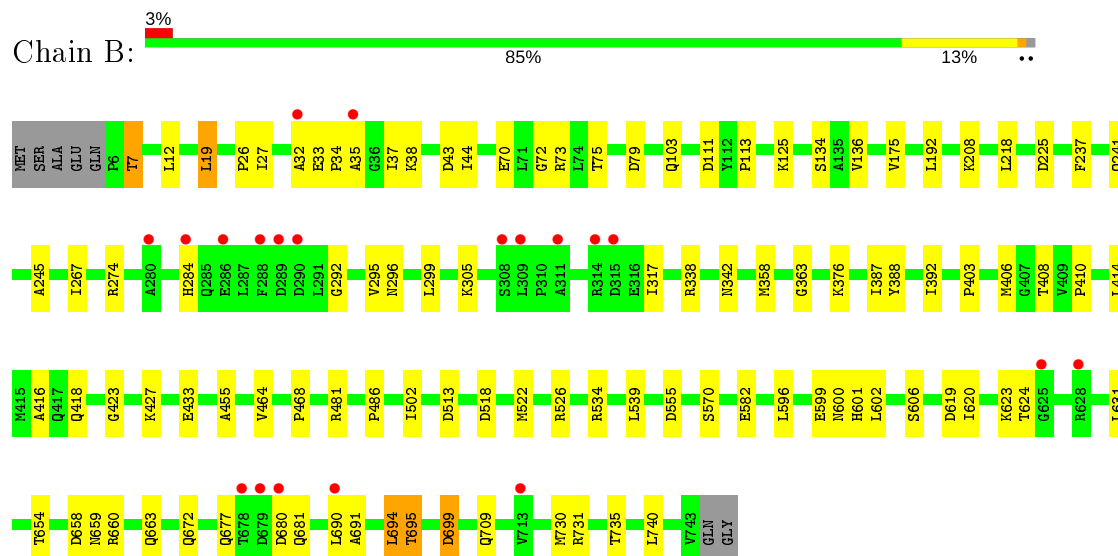
### 3 Residue-property plots [i](#)

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.

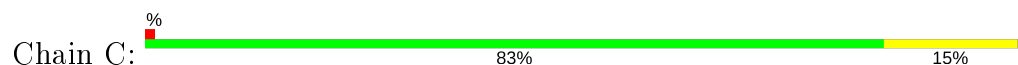
- Molecule 1: Isocitrate dehydrogenase

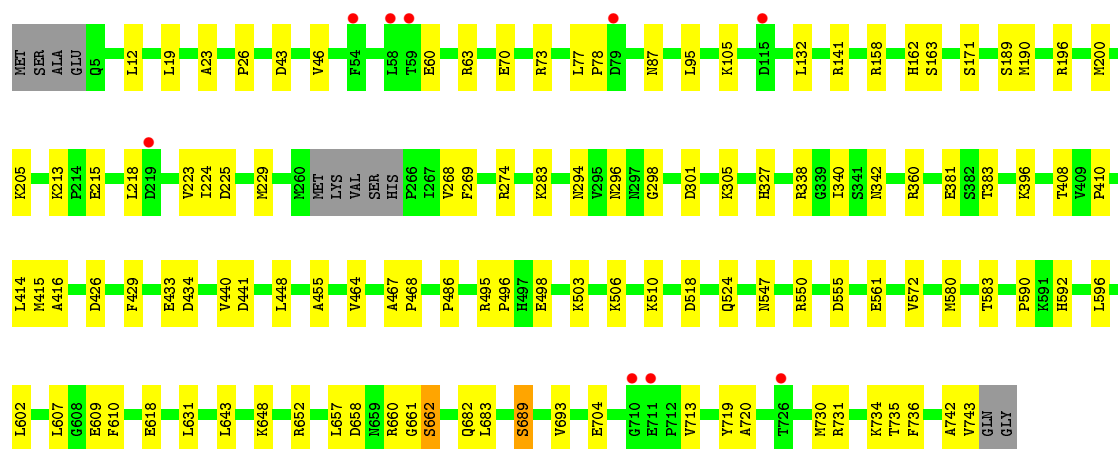


- Molecule 1: Isocitrate dehydrogenase

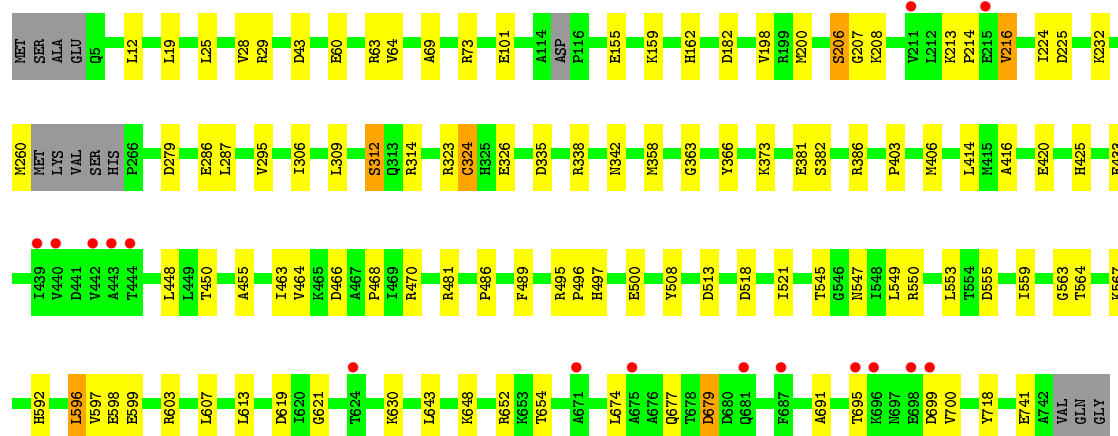
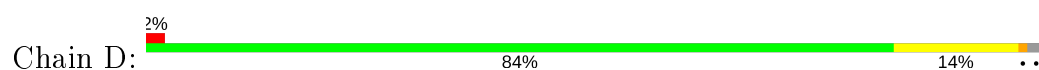


- Molecule 1: Isocitrate dehydrogenase





• Molecule 1: Isocitrate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.83Å 110.86Å 114.91Å 86.01° 78.62° 76.79°	Depositor
Resolution (Å)	48.50 – 2.66 48.92 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.50-2.66) 98.3 (48.92-2.66)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.178 , 0.228 0.178 , 0.228	Depositor DCC
$R_{free}$ test set	4967 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: GOL, MLA, EDO, NAP, MLT, SIN

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	0.31	0/5872	0.46	0/7952
1	B	0.31	0/5839	0.46	0/7909
1	C	0.31	0/5835	0.45	0/7900
1	D	0.31	0/5849	0.45	0/7914
All	All	0.31	0/23395	0.45	0/31675

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	5755	0	5700	68	0
1	B	5725	0	5670	63	0
1	C	5720	0	5677	65	0
1	D	5725	0	5695	59	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	2	0
2	D	48	0	25	5	0
3	A	9	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	3	0
4	B	8	0	12	3	0
4	C	8	0	12	1	0
4	D	4	0	6	4	0
5	B	7	0	2	1	0
5	D	7	0	2	0	0
6	C	8	0	4	0	0
7	C	6	0	8	0	0
7	D	6	0	8	1	0
8	A	145	0	0	1	0
8	B	92	0	0	0	0
8	C	109	0	0	5	0
8	D	77	0	0	1	0
All	All	23607	0	22906	255	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 6.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:HH12	4:A:803:EDO:H12	1.49	0.78
1:B:19:LEU:HD23	1:B:596:LEU:HD23	1.65	0.77
1:D:674:LEU:O	1:D:677:GLN:NE2	2.19	0.75
1:C:105:LYS:NZ	1:C:720:ALA:O	2.21	0.74
1:A:266:PRO:HD2	1:A:296:ASN:HB3	1.71	0.72
1:D:323:ARG:NH1	1:D:326:GLU:OE2	2.24	0.70
1:A:416:ALA:HB3	1:A:468:PRO:HB3	1.75	0.69
1:B:677:GLN:NE2	1:B:680:ASP:O	2.25	0.68
1:C:414:LEU:HD21	1:C:464:VAL:HG21	1.74	0.67
1:C:189:SER:HB3	1:C:496:PRO:HB2	1.75	0.67
1:B:596:LEU:HD22	1:B:602:LEU:HB2	1.77	0.66
1:D:198:VAL:HG23	1:D:216:VAL:HG13	1.78	0.66
1:C:416:ALA:HB3	1:C:468:PRO:HB3	1.78	0.65
1:B:416:ALA:HB3	1:B:468:PRO:HB3	1.77	0.64
1:D:481:ARG:NH2	1:D:513:ASP:O	2.31	0.64
1:C:19:LEU:HD13	1:C:596:LEU:HD22	1.79	0.63
1:D:599:GLU:OE1	1:D:654:THR:OG1	2.16	0.63
1:C:70:GLU:OE2	1:C:73[B]:ARG:NH1	2.32	0.62
2:D:801:NAP:H1B	4:D:804:EDO:H21	1.80	0.62
1:B:408:THR:HG23	1:B:410:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ASN:OD1	1:B:660:ARG:NH2	2.33	0.61
1:D:597:VAL:HG23	1:D:598:GLU:HG3	1.81	0.61
1:A:284:HIS:CE1	1:A:317:ILE:HG12	2.36	0.61
1:A:284:HIS:NE2	1:A:320:ASP:OD2	2.27	0.60
1:C:46:VAL:HG21	1:C:719:TYR:HD1	1.67	0.59
1:D:545:THR:HB	1:D:549:LEU:HB3	1.83	0.59
1:C:338:ARG:HG3	1:C:340:ILE:HG12	1.84	0.59
1:C:294:ASN:OD1	1:C:296:ASN:ND2	2.25	0.59
1:A:257:LYS:NZ	1:A:552:TYR:OH	2.33	0.59
1:D:12:LEU:HB2	1:D:43:ASP:HA	1.85	0.59
1:C:433:GLU:HA	1:C:455:ALA:HB2	1.85	0.58
1:A:414:LEU:HD21	1:A:464:VAL:HG21	1.85	0.58
1:C:596:LEU:HD13	1:C:602:LEU:HB2	1.85	0.57
1:C:360:ARG:HH22	1:C:652:ARG:HH22	1.52	0.57
1:C:196:ARG:NH1	1:C:441:ASP:OD2	2.38	0.57
1:D:559:ILE:HG12	4:D:804:EDO:H11	1.86	0.57
1:A:118:THR:OG1	1:A:119:ASP:N	2.38	0.57
1:D:206:SER:O	1:D:208:LYS:N	2.38	0.56
1:B:27:ILE:HG12	1:B:740:LEU:HD21	1.85	0.56
1:D:155:GLU:O	1:D:159:LYS:HD2	2.04	0.56
1:D:279:ASP:HB2	1:D:324:CYS:SG	2.45	0.56
1:C:503:LYS:HB3	4:C:805:EDO:H11	1.86	0.56
1:A:533:GLU:HG3	4:A:803:EDO:H11	1.87	0.56
1:A:598:GLU:HG3	1:A:599:GLU:HG3	1.87	0.56
1:A:550:ARG:NH2	3:A:802:MLT:O1	2.23	0.56
1:C:225:ASP:OD2	8:C:901:HOH:O	2.18	0.56
1:C:70:GLU:HA	1:C:73[A]:ARG:HE	1.71	0.56
1:B:79:ASP:OD1	1:B:79:ASP:N	2.39	0.55
1:C:506:LYS:O	1:C:510:LYS:NZ	2.38	0.55
1:A:109:VAL:HG12	1:A:110:PRO:HD2	1.89	0.55
1:A:121:GLU:HA	1:A:124:ILE:HG12	1.89	0.55
1:D:101:GLU:OE2	1:D:718:TYR:N	2.37	0.55
1:A:338:ARG:NH1	1:A:594:LYS:HE2	2.22	0.55
1:A:24:PHE:HB2	1:A:663:GLN:NE2	2.22	0.54
1:B:526:ARG:HG2	4:B:804:EDO:H21	1.90	0.54
1:A:408:THR:HG23	1:A:410:PRO:HD3	1.89	0.54
1:D:28:VAL:HG13	1:D:613:LEU:HD21	1.88	0.54
1:C:283:LYS:NZ	8:C:904:HOH:O	2.41	0.54
1:D:414:LEU:HD21	1:D:464:VAL:HG21	1.89	0.54
1:C:327:HIS:O	1:C:327:HIS:ND1	2.41	0.54
1:D:489:PHE:HB2	1:D:521:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:NH1	1:A:498:GLU:OE2	2.37	0.54
1:D:19:LEU:HD13	1:D:596:LEU:HD22	1.89	0.54
1:D:564:THR:HA	4:D:804:EDO:H22	1.90	0.54
1:C:95:LEU:HD22	1:C:132:LEU:HD13	1.90	0.53
1:B:681:GLN:OE1	1:B:681:GLN:N	2.41	0.53
1:B:659:ASN:OD1	1:B:663:GLN:NE2	2.40	0.53
1:D:466:ASP:OD1	1:D:508:TYR:OH	2.20	0.53
1:A:702:VAL:O	1:A:706:THR:HG23	2.10	0.52
1:D:563:GLY:O	4:D:804:EDO:H22	2.10	0.52
1:A:9:ILE:HG21	1:A:71:LEU:HD21	1.90	0.52
1:A:257:LYS:HD2	1:A:260:MET:HG3	1.92	0.52
1:C:205:LYS:HE2	1:C:434:ASP:HB3	1.90	0.52
1:D:420:GLU:OE2	1:D:497:HIS:NE2	2.41	0.52
1:D:652:ARG:HH12	2:D:801:NAP:P2B	2.33	0.51
1:C:301:ASP:OD1	1:C:305:LYS:NZ	2.44	0.51
1:D:679:ASP:N	1:D:679:ASP:OD1	2.42	0.51
1:D:200:MET:HB2	1:D:213:LYS:HB3	1.92	0.51
1:A:594:LYS:NZ	1:A:598:GLU:OE1	2.43	0.51
1:A:105:LYS:NZ	1:A:716:GLY:O	2.28	0.51
1:D:382:SER:OG	1:D:386[A]:ARG:NH2	2.44	0.51
1:B:534:ARG:HB3	1:B:539:LEU:HB2	1.92	0.51
1:B:72:GLY:O	1:B:75:THR:OG1	2.28	0.51
1:A:338:ARG:HH12	1:A:594:LYS:HE2	1.76	0.51
1:C:408:THR:HG23	1:C:410:PRO:HD3	1.91	0.51
1:C:60:GLU:HA	1:C:63:ARG:HH11	1.76	0.51
1:D:621:GLY:HA3	1:D:630:LYS:HG2	1.91	0.51
1:B:103:GLN:NE2	1:B:111:ASP:OD1	2.42	0.50
1:A:141:ARG:HD3	1:A:415:MET:SD	2.51	0.50
1:B:70:GLU:OE1	1:B:73:ARG:NH1	2.45	0.50
1:C:704:GLU:OE2	1:C:735:THR:OG1	2.28	0.50
1:D:691:ALA:O	1:D:695:THR:OG1	2.19	0.50
1:B:32:ALA:HB1	1:B:37:ILE:HB	1.93	0.50
1:B:599:GLU:OE1	1:B:654:THR:OG1	2.20	0.50
1:C:498:GLU:OE2	1:C:524:GLN:NE2	2.45	0.50
1:C:583:THR:HG23	1:C:609:GLU:N	2.27	0.50
1:D:603:ARG:NH1	2:D:801:NAP:O2X	2.45	0.49
1:C:200:MET:HB2	1:C:213:LYS:HB3	1.94	0.49
1:D:545:THR:HG21	1:D:553:LEU:HD12	1.94	0.49
1:A:105:LYS:NZ	1:A:720:ALA:O	2.43	0.49
1:C:26:PRO:HG2	1:C:731:ARG:HD2	1.94	0.49
1:B:601:HIS:NE2	1:B:658:ASP:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:HIS:NE2	2:C:801:NAP:O1X	2.37	0.49
1:C:274:ARG:NH1	8:C:910:HOH:O	2.45	0.48
1:A:433:GLU:HA	1:A:455:ALA:HB2	1.95	0.48
1:A:196:ARG:NH1	1:A:441:ASP:OD2	2.47	0.48
1:B:486:PRO:HB3	1:B:518:ASP:HB3	1.95	0.48
1:C:269:PHE:HE2	1:C:298:GLY:HA2	1.78	0.48
1:D:358:MET:SD	1:D:363:GLY:HA2	2.54	0.48
1:C:158:ARG:NH1	8:C:903:HOH:O	2.40	0.48
1:B:113:PRO:HG2	1:B:125:LYS:HB2	1.95	0.48
1:B:596:LEU:HD12	1:B:600:ASN:HA	1.96	0.48
1:D:306:ILE:HG13	1:D:314:ARG:NH1	2.28	0.47
1:A:113:PRO:HG2	1:A:125:LYS:HB2	1.95	0.47
1:A:155:GLU:OE2	1:A:159:LYS:HD3	2.13	0.47
1:B:481:ARG:NH2	1:B:513:ASP:O	2.42	0.47
1:B:245:ALA:HB2	1:B:376:LYS:HD2	1.96	0.47
1:A:294:ASN:OD1	1:A:296:ASN:ND2	2.47	0.47
1:A:526:ARG:NH1	4:A:803:EDO:H12	2.26	0.47
1:D:433:GLU:HA	1:D:455:ALA:HB2	1.97	0.47
1:B:691:ALA:O	1:B:695:THR:OG1	2.26	0.47
1:C:218:LEU:HD13	1:C:224:ILE:HG21	1.97	0.47
1:C:658:ASP:OD2	1:C:660:ARG:NH2	2.47	0.47
1:B:44:ILE:HD12	1:B:136:VAL:HG11	1.97	0.46
1:B:418:GLN:HB3	1:B:423:GLY:HA3	1.96	0.46
1:A:313:GLN:O	1:A:317:ILE:HG13	2.14	0.46
1:A:32:ALA:HB1	1:A:37:ILE:HB	1.98	0.46
1:D:592:HIS:HE2	2:D:801:NAP:H2B	1.80	0.46
1:B:423:GLY:O	1:B:427:LYS:NZ	2.48	0.46
1:B:134:SER:OG	5:B:802:MLA:O3A	2.23	0.46
1:A:167:TRP:CD1	1:A:362:GLY:HA2	2.50	0.46
1:B:358:MET:SD	1:B:363:GLY:HA2	2.55	0.46
1:A:71:LEU:O	1:A:75:THR:HG23	2.16	0.46
1:B:596:LEU:HD21	1:B:730:MET:CE	2.46	0.46
1:D:182:ASP:HB2	1:D:381:GLU:OE1	2.16	0.46
1:C:381:GLU:OE2	1:C:383:THR:OG1	2.22	0.45
1:D:403:PRO:HA	1:D:406:MET:HG2	1.97	0.45
1:A:423:GLY:O	1:A:427:LYS:NZ	2.49	0.45
1:B:38:LYS:N	1:B:38:LYS:HD2	2.32	0.45
1:B:433:GLU:HA	1:B:455:ALA:HB2	1.99	0.45
1:B:12:LEU:HB2	1:B:43:ASP:HA	1.98	0.45
1:C:223:VAL:HB	1:C:464:VAL:HG13	1.98	0.45
1:A:159:LYS:HD2	1:A:159:LYS:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:PRO:HB3	1:C:518:ASP:HB3	1.99	0.45
1:A:189:SER:HB3	1:A:496:PRO:HB2	1.99	0.44
1:B:33:GLU:CD	1:B:34:PRO:HD3	2.38	0.44
1:C:12:LEU:HB2	1:C:43:ASP:HA	1.99	0.44
1:D:60:GLU:HA	1:D:63:ARG:HD3	1.99	0.44
1:D:101:GLU:CD	1:D:718:TYR:H	2.21	0.44
1:B:284:HIS:CE1	1:B:317:ILE:HG12	2.52	0.44
1:B:502:ILE:HG21	4:B:803:EDO:H22	1.99	0.44
1:B:690:LEU:O	1:B:694:LEU:HB2	2.17	0.44
1:A:706:THR:HA	1:A:709:GLN:HE21	1.82	0.44
1:B:387:ILE:HG13	1:B:388:TYR:N	2.33	0.44
1:C:141:ARG:HD3	1:C:415:MET:SD	2.58	0.44
1:C:213:LYS:HB2	1:C:429:PHE:CZ	2.53	0.44
1:A:200:MET:HB2	1:A:213:LYS:HB3	1.99	0.44
1:B:601:HIS:CD2	1:B:658:ASP:HB3	2.53	0.44
1:B:241:GLN:OE1	1:B:376:LYS:HE3	2.18	0.44
1:C:23:ALA:HB2	1:C:730:MET:HB3	2.00	0.44
1:A:103:GLN:NE2	1:A:109:VAL:O	2.36	0.44
1:A:12:LEU:HB2	1:A:43:ASP:HA	2.00	0.44
1:A:643:LEU:HD12	1:A:648:LYS:HB2	1.99	0.44
1:C:607:LEU:HA	1:C:610:PHE:CD2	2.53	0.44
1:D:366:TYR:CD2	7:D:803:GOL:H2	2.53	0.44
1:A:713:VAL:HG11	1:A:729:VAL:HG11	2.00	0.43
1:B:208:LYS:HA	1:B:208:LYS:HD2	1.80	0.43
1:A:427:LYS:HE2	1:A:463:ILE:HD12	2.00	0.43
1:B:192:LEU:HD11	1:B:218:LEU:HD13	2.00	0.43
1:B:620:ILE:O	1:B:624:THR:OG1	2.33	0.43
1:B:403:PRO:HA	1:B:406:MET:HG2	1.99	0.43
1:B:601:HIS:HD2	1:B:709:GLN:OE1	2.01	0.43
1:A:284:HIS:ND1	1:A:317:ILE:HG12	2.33	0.43
1:B:35:ALA:HB3	1:B:37:ILE:HG12	1.98	0.43
1:B:7:THR:HB	1:B:38:LYS:HB2	2.01	0.43
1:C:618:GLU:OE2	1:D:312:SER:OG	2.36	0.43
1:A:116:PRO:HG2	1:A:122:LYS:HD3	2.01	0.43
1:B:175:VAL:HG23	1:B:392:ILE:HD12	2.00	0.43
1:D:466:ASP:OD2	1:D:470:ARG:NE	2.47	0.43
1:A:547:ASN:O	1:A:550:ARG:HB3	2.19	0.43
1:C:467:ALA:HB3	1:C:468:PRO:HD3	2.01	0.43
1:A:384:PHE:CD2	1:A:548:ILE:HG21	2.54	0.43
1:C:648:LYS:O	1:C:662:SER:OG	2.24	0.43
1:D:416:ALA:HB3	1:D:468:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:PRO:HB3	1:D:518:ASP:HB3	2.01	0.43
1:D:592:HIS:NE2	2:D:801:NAP:H2B	2.34	0.43
1:A:187:GLU:OE2	1:A:495:ARG:NE	2.39	0.43
1:B:660:ARG:HD3	1:B:730:MET:O	2.19	0.43
1:B:274:ARG:HG3	1:B:295:VAL:HG21	2.00	0.42
1:C:657:LEU:HD11	1:C:661:GLY:HA3	2.01	0.42
1:D:496:PRO:O	1:D:500:GLU:HG2	2.19	0.42
1:A:565:SER:HB2	1:A:585:ALA:HB3	2.01	0.42
1:B:299:LEU:HD12	1:B:299:LEU:HA	1.92	0.42
1:A:223:VAL:HB	1:A:464:VAL:HG13	2.02	0.42
1:D:547:ASN:O	1:D:550:ARG:HB3	2.19	0.42
1:B:672:GLN:HE21	1:B:695:THR:HG23	1.83	0.42
1:D:25:LEU:O	1:D:29:ARG:HG3	2.18	0.42
1:D:643:LEU:HD12	1:D:648:LYS:HB2	2.01	0.42
1:C:213:LYS:HE3	1:C:426:ASP:O	2.20	0.42
1:C:547:ASN:O	1:C:550:ARG:HB3	2.20	0.42
1:B:619:ASP:HB3	1:B:623:LYS:HE2	2.01	0.42
1:B:267:ILE:HD13	1:B:296:ASN:HD21	1.85	0.42
1:B:570:SER:HB3	1:B:582:GLU:HB2	2.01	0.42
1:B:606:SER:OG	1:B:659:ASN:ND2	2.40	0.42
1:D:335:ASP:OD2	1:D:338:ARG:NH1	2.46	0.42
1:D:621:GLY:HA3	1:D:630:LYS:CG	2.49	0.42
1:A:571:VAL:O	1:A:573:PRO:HD3	2.19	0.42
1:A:602:LEU:O	1:A:658:ASP:HB2	2.20	0.42
1:B:694:LEU:HD12	1:B:694:LEU:HA	1.84	0.42
1:C:87:ASN:HB2	8:C:911:HOH:O	2.20	0.42
1:D:699:ASP:N	1:D:699:ASP:OD1	2.53	0.42
1:D:741:GLU:N	1:D:741:GLU:OE1	2.53	0.42
1:A:512:HIS:HE1	8:A:1014:HOH:O	2.02	0.42
1:C:171:SER:HB3	1:C:396:LYS:HE2	2.02	0.42
1:A:267:ILE:HD13	1:A:267:ILE:HA	1.87	0.41
1:C:190:MET:SD	1:C:448:LEU:HB3	2.60	0.41
1:C:229:MET:HE1	1:C:268:VAL:HG12	2.02	0.41
1:D:495:ARG:HA	1:D:496:PRO:HD3	1.88	0.41
1:A:284:HIS:N	1:A:284:HIS:CD2	2.88	0.41
1:B:237:PHE:O	1:B:241:GLN:HG2	2.19	0.41
1:C:77:LEU:HA	1:C:78:PRO:HD3	1.81	0.41
1:D:162:HIS:H	1:D:162:HIS:CD2	2.36	0.41
1:D:373:LYS:HE2	1:D:373:LYS:HB3	1.89	0.41
1:A:257:LYS:HB2	1:A:257:LYS:HE2	1.91	0.41
1:C:631:LEU:HA	1:C:631:LEU:HD12	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:LYS:HG2	1:D:607:LEU:HD23	2.02	0.41
1:A:120:GLN:O	1:A:124:ILE:HG23	2.20	0.41
1:A:496:PRO:O	1:A:500:GLU:HG2	2.20	0.41
1:C:590:PRO:HD3	2:C:801:NAP:H51N	2.03	0.41
1:D:287:LEU:HD21	1:D:309:LEU:HD11	2.02	0.41
1:A:514:THR:HA	1:A:517:LEU:HD12	2.03	0.41
1:A:87:ASN:O	2:A:801:NAP:H2N	2.21	0.41
1:C:162:HIS:HE1	1:C:561:GLU:O	2.04	0.41
1:C:631:LEU:HD23	1:C:683:LEU:HD23	2.03	0.41
1:D:63:ARG:NH1	8:D:912:HOH:O	2.54	0.41
1:B:26:PRO:HG2	1:B:731:ARG:HD3	2.03	0.41
1:C:495:ARG:HA	1:C:496:PRO:HD2	1.88	0.41
1:A:299:LEU:HA	1:A:299:LEU:HD12	1.89	0.41
1:A:33:GLU:HB3	1:A:34:PRO:HD3	2.02	0.41
1:C:583:THR:HG21	1:C:609:GLU:HG3	2.03	0.41
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.90	0.41
1:B:418:GLN:HB3	1:B:423:GLY:CA	2.51	0.41
1:B:414:LEU:HD21	1:B:464:VAL:HG21	2.03	0.41
1:C:596:LEU:HD11	1:C:730:MET:HE3	2.03	0.41
1:C:643:LEU:HD12	1:C:648:LYS:HB2	2.03	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.78	0.40
1:C:572:VAL:HB	1:C:580:MET:HB3	2.02	0.40
1:D:224:ILE:HG22	1:D:463:ILE:HG12	2.03	0.40
1:D:69:ALA:O	1:D:73:ARG:HG3	2.21	0.40
1:B:292:GLY:O	1:B:305:LYS:HE2	2.22	0.40
1:A:118:THR:HG21	1:A:121:GLU:CD	2.41	0.40
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.95	0.40
1:B:522:MET:HG2	4:B:804:EDO:H12	2.04	0.40
1:C:682:GLN:OE1	1:C:682:GLN:N	2.37	0.40
1:C:689:SER:O	1:C:693:VAL:HG12	2.21	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	736/745 (99%)	708 (96%)	26 (4%)	2 (0%)	41	56
1	B	736/745 (99%)	711 (97%)	23 (3%)	2 (0%)	41	56
1	C	731/745 (98%)	711 (97%)	19 (3%)	1 (0%)	51	69
1	D	730/745 (98%)	702 (96%)	26 (4%)	2 (0%)	41	56
All	All	2933/2980 (98%)	2832 (97%)	94 (3%)	7 (0%)	47	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	PRO
1	C	742	ALA
1	D	207	GLY
1	B	338	ARG
1	A	66	ASP
1	B	699	ASP
1	D	214	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	618/622 (99%)	603 (98%)	15 (2%)	49	67
1	B	611/622 (98%)	601 (98%)	10 (2%)	62	78
1	C	613/622 (99%)	602 (98%)	11 (2%)	59	75
1	D	615/622 (99%)	594 (97%)	21 (3%)	37	53
All	All	2457/2488 (99%)	2400 (98%)	57 (2%)	52	68

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	118	THR
1	A	119	ASP
1	A	128	TYR
1	A	225	ASP
1	A	265	HIS
1	A	268	VAL
1	A	306	ILE
1	A	342	ASN
1	A	555	ASP
1	A	594	LYS
1	A	609	GLU
1	A	618	GLU
1	A	706	THR
1	A	713	VAL
1	B	7	THR
1	B	19	LEU
1	B	225	ASP
1	B	342	ASN
1	B	555	ASP
1	B	631	LEU
1	B	694	LEU
1	B	695	THR
1	B	699	ASP
1	B	735	THR
1	C	163	SER
1	C	215	GLU
1	C	342	ASN
1	C	440	VAL
1	C	555	ASP
1	C	662	SER
1	C	689	SER
1	C	713	VAL
1	C	734	LYS
1	C	736	PHE
1	C	743	VAL
1	D	64	VAL
1	D	206	SER
1	D	216	VAL
1	D	225	ASP
1	D	232[A]	LYS
1	D	232[B]	LYS
1	D	260	MET

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Mol	Chain	Res	Type
1	D	286	GLU
1	D	295	VAL
1	D	312	SER
1	D	324	CYS
1	D	342	ASN
1	D	425[A]	HIS
1	D	425[B]	HIS
1	D	448	LEU
1	D	450	THR
1	D	555	ASP
1	D	596	LEU
1	D	619	ASP
1	D	679	ASP
1	D	700	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	601	HIS
1	D	294	ASN
1	D	296	ASN
1	D	672	GLN

### 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 ⓘ

16 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
4	EDO	B	804	-	3,3,3	0.52	0	2,2,2	0.20	0
4	EDO	D	804	-	3,3,3	0.47	0	2,2,2	0.13	0
7	GOL	D	803	-	5,5,5	0.33	0	5,5,5	0.34	0
2	NAP	C	801	-	45,52,52	0.88	3 (6%)	56,80,80	1.04	2 (3%)
4	EDO	C	805	-	3,3,3	0.58	0	2,2,2	0.17	0
2	NAP	A	801	-	45,52,52	0.86	1 (2%)	56,80,80	1.06	3 (5%)
2	NAP	D	801	-	45,52,52	0.88	3 (6%)	56,80,80	1.13	4 (7%)
4	EDO	C	804	-	3,3,3	0.57	0	2,2,2	0.12	0
2	NAP	B	801	-	45,52,52	0.88	2 (4%)	56,80,80	1.05	2 (3%)
7	GOL	C	803	-	5,5,5	0.30	0	5,5,5	0.38	0
3	MLT	A	802	-	2,8,8	0.31	0	3,10,10	1.60	0
5	MLA	B	802	-	0,6,6	0.00	-	0,7,7	0.00	-
6	SIN	C	802	-	1,7,7	0.08	0	2,8,8	1.34	0
5	MLA	D	802	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	A	803	-	3,3,3	0.53	0	2,2,2	0.29	0
4	EDO	B	803	-	3,3,3	0.51	0	2,2,2	0.28	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
4	EDO	B	804	-	-	0/1/1/1	-
4	EDO	D	804	-	-	0/1/1/1	-
7	GOL	D	803	-	-	2/4/4/4	-
2	NAP	C	801	-	-	14/31/67/67	0/5/5/5
4	EDO	C	805	-	-	1/1/1/1	-
2	NAP	A	801	-	-	9/31/67/67	0/5/5/5
2	NAP	D	801	-	-	12/31/67/67	0/5/5/5
4	EDO	C	804	-	-	0/1/1/1	-
2	NAP	B	801	-	-	9/31/67/67	0/5/5/5
7	GOL	C	803	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLT	A	802	-	-	2/2/8/8	-
5	MLA	B	802	-	-	0/0/4/4	-
6	SIN	C	802	-	-	1/1/5/5	-
5	MLA	D	802	-	-	0/0/4/4	-
4	EDO	A	803	-	-	0/1/1/1	-
4	EDO	B	803	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	NAP	C5A-C4A	2.69	1.48	1.40
2	A	801	NAP	C5A-C4A	2.66	1.48	1.40
2	D	801	NAP	C5A-C4A	2.64	1.47	1.40
2	B	801	NAP	C5A-C4A	2.63	1.47	1.40
2	C	801	NAP	O4B-C1B	2.22	1.44	1.41
2	D	801	NAP	O4D-C1D	2.16	1.44	1.41
2	D	801	NAP	O4B-C1B	2.15	1.44	1.41
2	C	801	NAP	O4D-C1D	2.03	1.43	1.41
2	B	801	NAP	O4B-C1B	2.02	1.43	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	N3A-C2A-N1A	-3.40	123.36	128.68
2	D	801	NAP	N3A-C2A-N1A	-3.39	123.38	128.68
2	B	801	NAP	C4A-C5A-N7A	-3.23	106.03	109.40
2	B	801	NAP	N3A-C2A-N1A	-3.17	123.72	128.68
2	C	801	NAP	C4A-C5A-N7A	-3.13	106.14	109.40
2	C	801	NAP	N3A-C2A-N1A	-3.05	123.92	128.68
2	D	801	NAP	C4A-C5A-N7A	-2.82	106.46	109.40
2	A	801	NAP	C4A-C5A-N7A	-2.69	106.60	109.40
2	A	801	NAP	C2A-N1A-C6A	2.16	122.45	118.75
2	D	801	NAP	C6N-N1N-C2N	-2.07	120.08	121.97
2	D	801	NAP	C2A-N1A-C6A	2.06	122.27	118.75

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	803	GOL	O1-C1-C2-C3
2	C	801	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	801	NAP	C5B-O5B-PA-O3
2	C	801	NAP	C5D-O5D-PN-O1N
2	C	801	NAP	C5D-O5D-PN-O2N
2	C	801	NAP	O4D-C1D-N1N-C2N
2	C	801	NAP	O4D-C1D-N1N-C6N
2	A	801	NAP	C2B-O2B-P2B-O2X
2	A	801	NAP	C5D-O5D-PN-O1N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	A	801	NAP	O4D-C1D-N1N-C6N
2	A	801	NAP	C2D-C1D-N1N-C2N
2	D	801	NAP	C5B-O5B-PA-O2A
2	D	801	NAP	C5B-O5B-PA-O3
2	D	801	NAP	C5D-O5D-PN-O1N
2	D	801	NAP	O4D-C1D-N1N-C2N
2	D	801	NAP	O4D-C1D-N1N-C6N
2	B	801	NAP	C5B-O5B-PA-O1A
2	B	801	NAP	C5B-O5B-PA-O3
2	B	801	NAP	PA-O3-PN-O5D
2	B	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	O4D-C1D-N1N-C6N
7	C	803	GOL	O1-C1-C2-C3
3	A	802	MLT	C1-C2-C3-C4
7	D	803	GOL	O1-C1-C2-O2
7	C	803	GOL	O1-C1-C2-O2
4	C	805	EDO	O1-C1-C2-O2
2	C	801	NAP	PA-O3-PN-O5D
2	A	801	NAP	PA-O3-PN-O5D
2	D	801	NAP	PA-O3-PN-O5D
2	A	801	NAP	C5D-O5D-PN-O3
2	D	801	NAP	C2B-O2B-P2B-O2X
2	C	801	NAP	PN-O3-PA-O2A
2	C	801	NAP	C5B-O5B-PA-O2A
2	A	801	NAP	C5D-O5D-PN-O2N
2	D	801	NAP	C5B-O5B-PA-O1A
2	D	801	NAP	C5D-O5D-PN-O2N
2	B	801	NAP	C5D-O5D-PN-O2N
2	D	801	NAP	PN-O3-PA-O2A
2	B	801	NAP	PN-O3-PA-O1A
6	C	802	SIN	C1-C2-C3-C4
3	A	802	MLT	O3-C2-C3-C4
2	C	801	NAP	O4D-C4D-C5D-O5D
4	B	803	EDO	O1-C1-C2-O2

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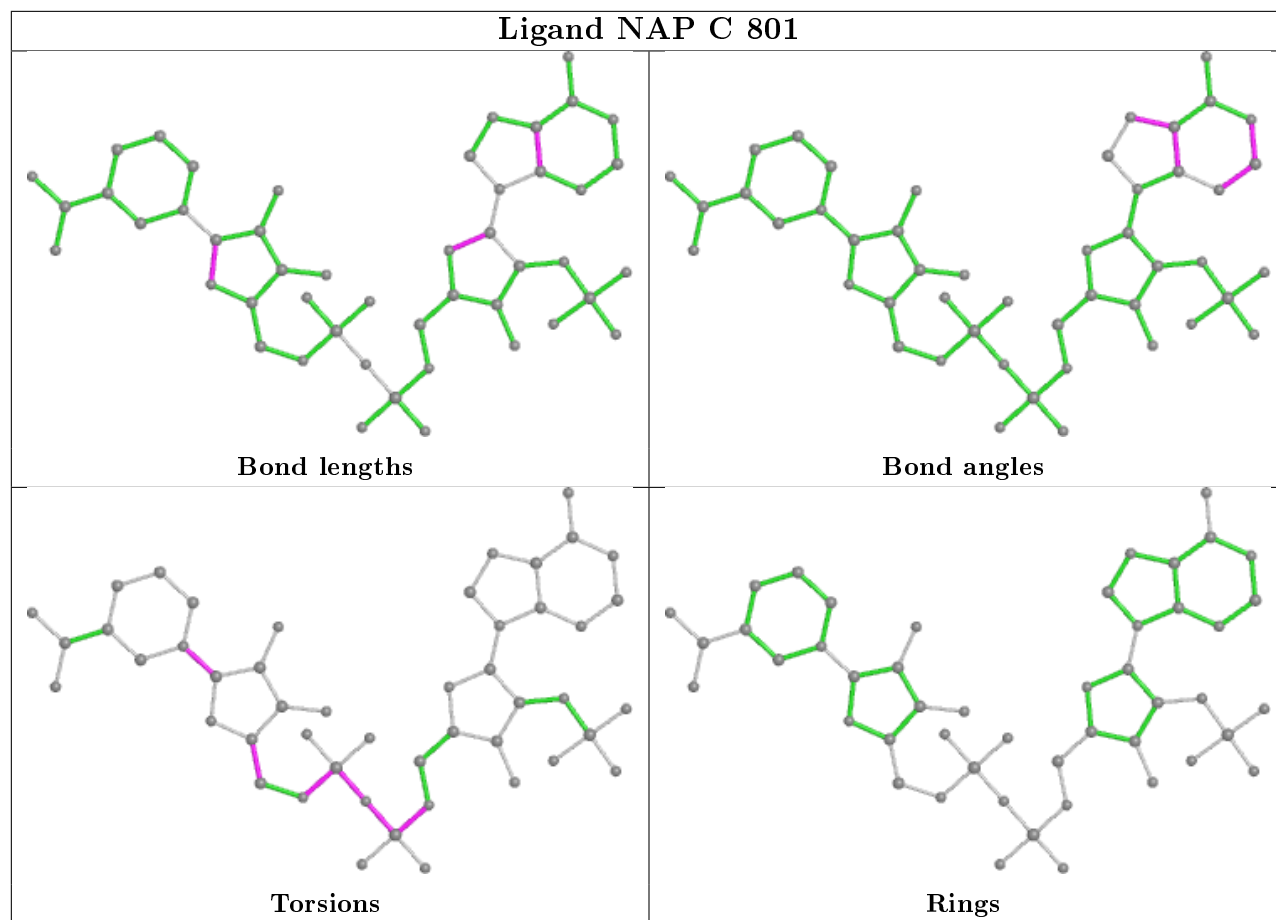
Mol	Chain	Res	Type	Atoms
2	C	801	NAP	C5D-O5D-PN-O3
2	C	801	NAP	C2D-C1D-N1N-C2N
2	A	801	NAP	C2D-C1D-N1N-C6N
2	D	801	NAP	C5D-O5D-PN-O3
2	B	801	NAP	C5D-O5D-PN-O3
2	C	801	NAP	PN-O3-PA-O1A
2	D	801	NAP	PN-O3-PA-O1A
2	B	801	NAP	PN-O3-PA-O2A
2	C	801	NAP	C3D-C4D-C5D-O5D
7	C	803	GOL	O2-C2-C3-O3

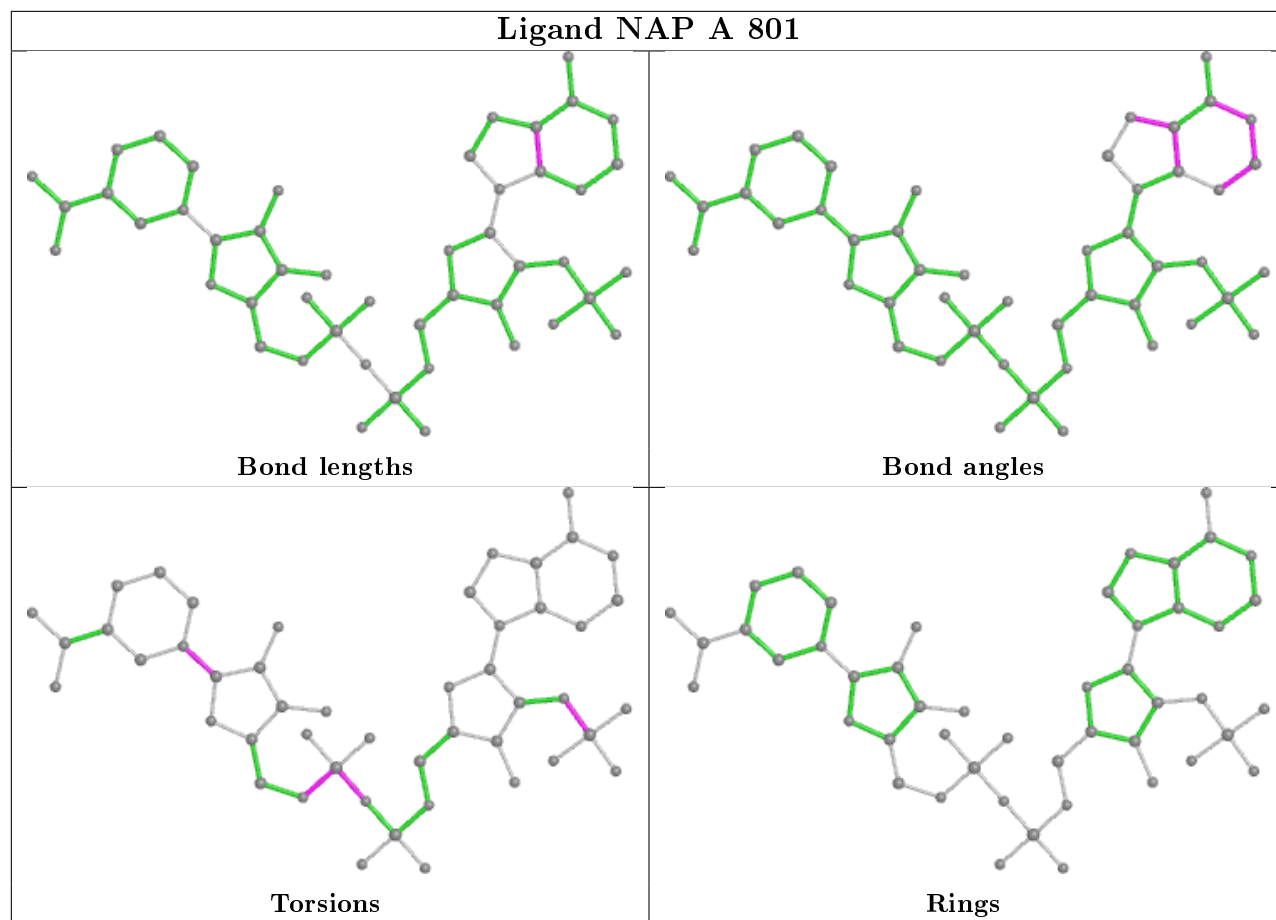
There are no ring outliers.

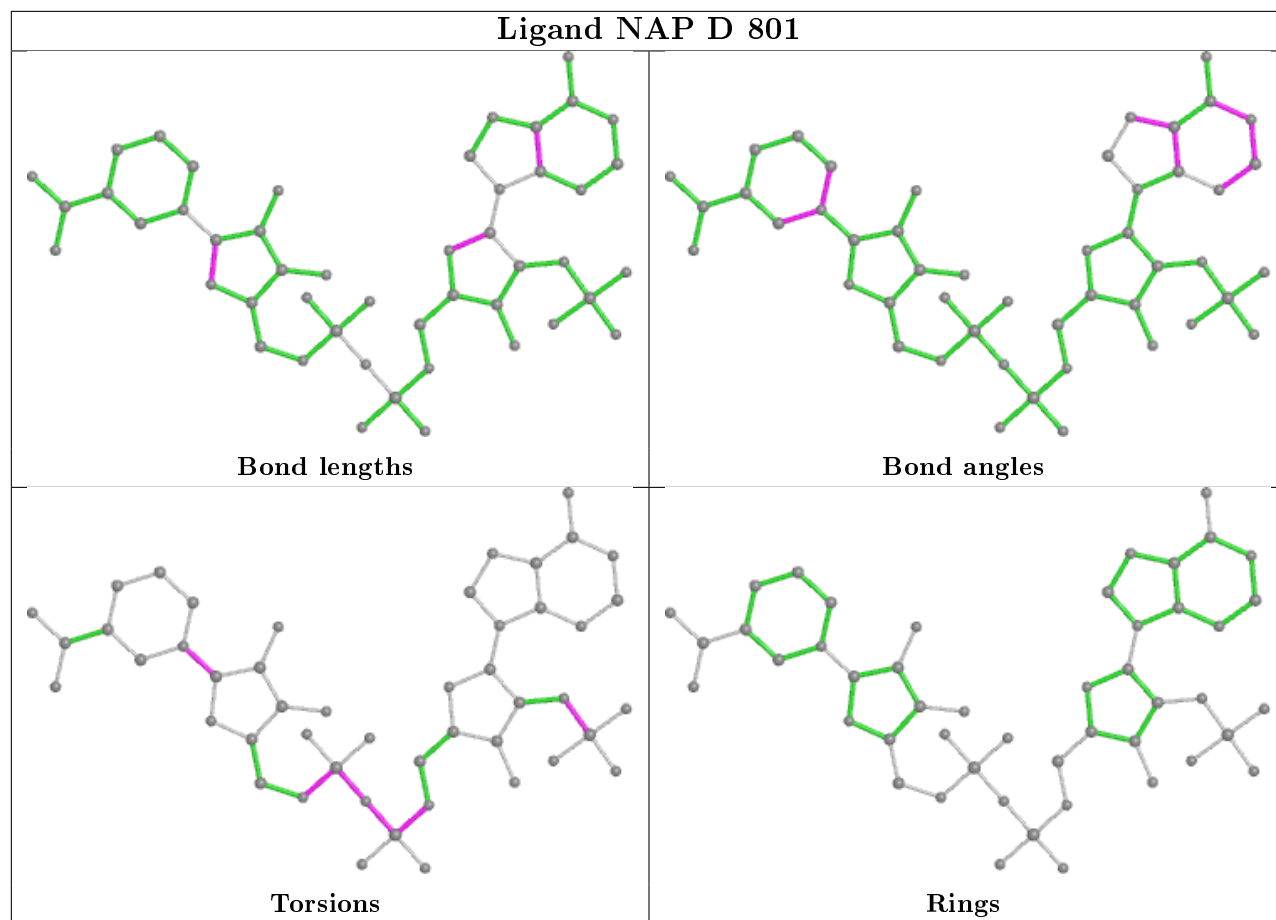
11 monomers are involved in 21 short contacts:

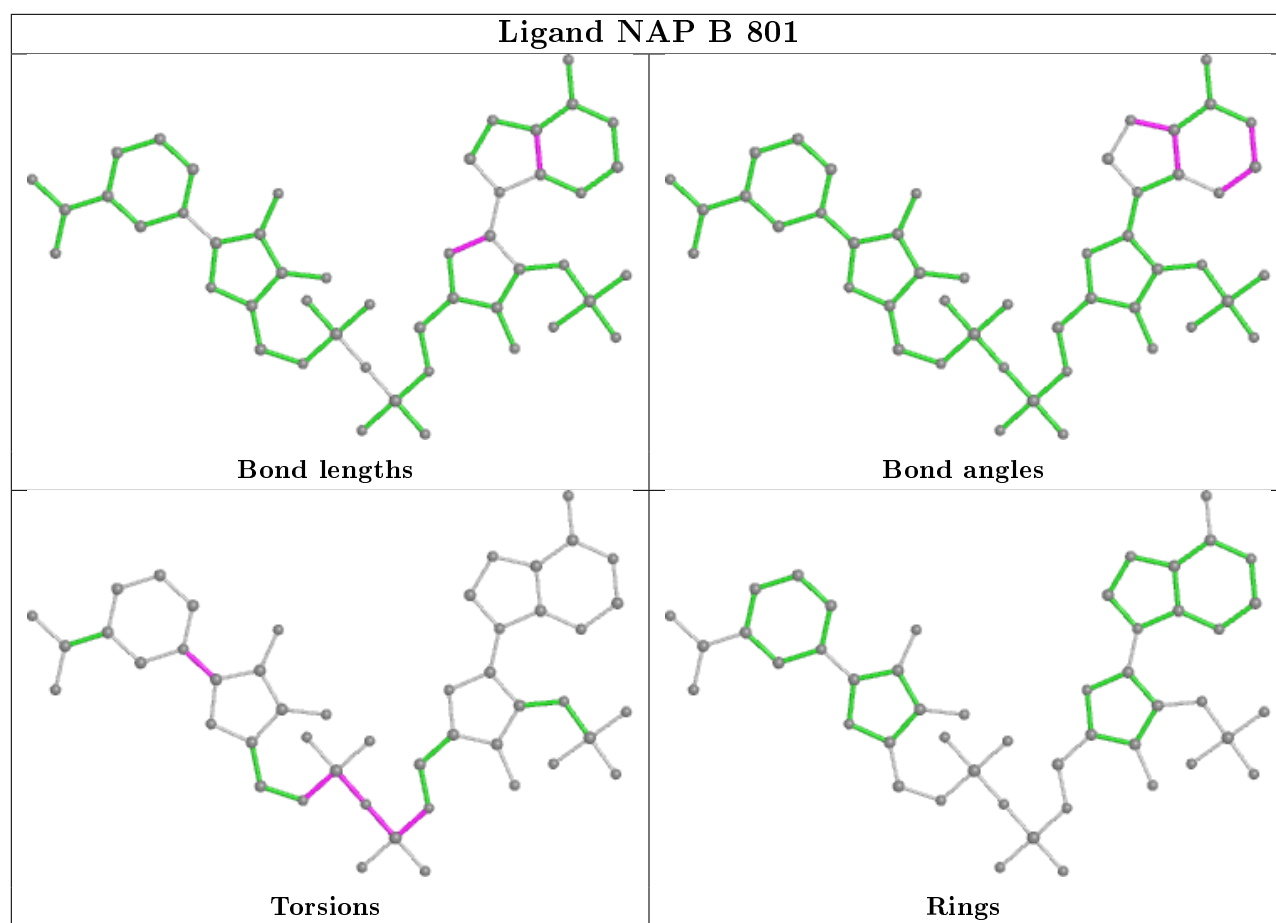
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	804	EDO	2	0
4	D	804	EDO	4	0
7	D	803	GOL	1	0
2	C	801	NAP	2	0
4	C	805	EDO	1	0
2	A	801	NAP	1	0
2	D	801	NAP	5	0
3	A	802	MLT	1	0
5	B	802	MLA	1	0
4	A	803	EDO	3	0
4	B	803	EDO	1	0

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, 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	738/745 (99%)	-0.04	10 (1%) 75 73	31, 47, 75, 103	0
1	B	738/745 (99%)	0.06	20 (2%) 54 50	34, 51, 80, 95	0
1	C	734/745 (98%)	-0.03	9 (1%) 79 77	33, 51, 74, 95	0
1	D	732/745 (98%)	0.07	16 (2%) 62 57	29, 55, 79, 92	0
All	All	2942/2980 (98%)	0.01	55 (1%) 66 63	29, 51, 78, 103	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	3.7
1	D	440	VAL	3.7
1	C	59	THR	3.6
1	D	675	ALA	3.6
1	B	308	SER	3.3
1	C	115	ASP	3.3
1	D	695	THR	3.3
1	A	307	GLU	3.3
1	A	265	HIS	3.2
1	B	286	GLU	3.2
1	B	309	LEU	3.1
1	A	308	SER	3.1
1	B	679	ASP	2.9
1	D	442	VAL	2.9
1	D	671	ALA	2.9
1	C	711	GLU	2.9
1	C	710	GLY	2.8
1	B	713	VAL	2.8
1	D	681	GLN	2.8
1	B	288	PHE	2.7
1	A	313	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	306	ILE	2.7
1	C	79	ASP	2.7
1	B	625	GLY	2.6
1	B	289	ASP	2.6
1	D	624	THR	2.6
1	C	726	THR	2.6
1	D	443	ALA	2.5
1	D	215	GLU	2.5
1	A	115	ASP	2.5
1	B	280	ALA	2.4
1	B	290	ASP	2.4
1	A	264	SER	2.4
1	A	317	ILE	2.4
1	D	687	PHE	2.3
1	B	680	ASP	2.3
1	B	315	ASP	2.3
1	B	678	THR	2.3
1	B	314	ARG	2.2
1	D	444	THR	2.2
1	D	696	LYS	2.2
1	D	698	GLU	2.2
1	C	58	LEU	2.1
1	D	699	ASP	2.1
1	C	219	ASP	2.1
1	A	114	ALA	2.1
1	B	628	ARG	2.1
1	A	312	SER	2.1
1	B	35	ALA	2.0
1	D	439	ILE	2.0
1	C	54	PHE	2.0
1	B	690	LEU	2.0
1	B	284	HIS	2.0
1	B	32	ALA	2.0
1	B	311	ALA	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 ⓘ

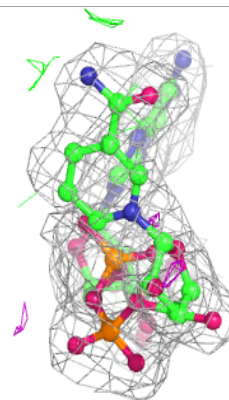
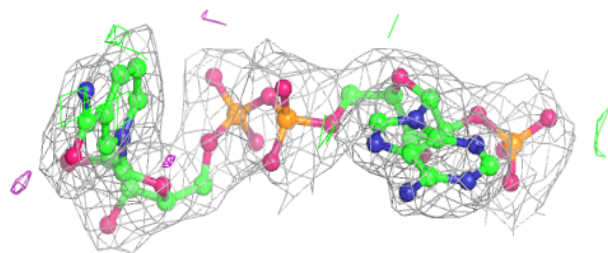
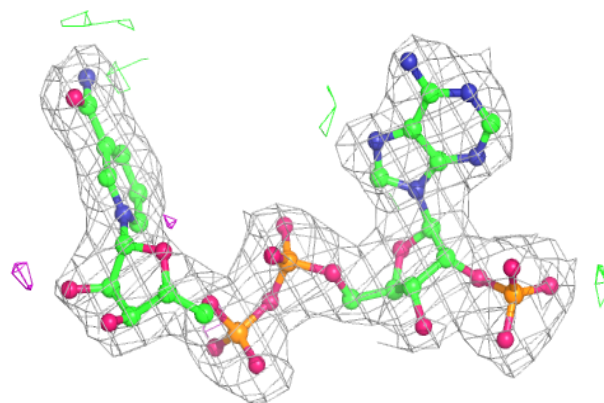
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	EDO	A	803	4/4	0.75	0.31	50,57,61,63	0
4	EDO	C	805	4/4	0.79	0.53	49,53,53,55	0
5	MLA	D	802	7/7	0.86	0.22	59,62,65,67	0
4	EDO	B	804	4/4	0.86	0.25	46,47,49,49	0
3	MLT	A	802	9/9	0.87	0.21	54,60,62,64	0
4	EDO	C	804	4/4	0.88	0.24	49,52,56,58	0
4	EDO	B	803	4/4	0.89	0.33	54,54,58,61	0
6	SIN	C	802	8/8	0.93	0.30	57,67,69,69	0
7	GOL	C	803	6/6	0.93	0.18	44,50,55,55	0
5	MLA	B	802	7/7	0.94	0.14	58,61,63,66	0
4	EDO	D	804	4/4	0.95	0.25	42,44,45,51	0
7	GOL	D	803	6/6	0.96	0.14	58,60,63,67	0
2	NAP	C	801	48/48	0.97	0.18	37,47,51,62	0
2	NAP	B	801	48/48	0.97	0.18	41,48,56,68	0
2	NAP	A	801	48/48	0.97	0.18	34,41,46,50	0
2	NAP	D	801	48/48	0.98	0.16	34,41,48,52	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.

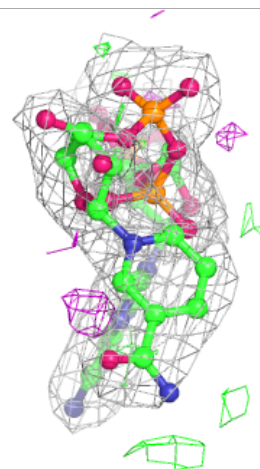
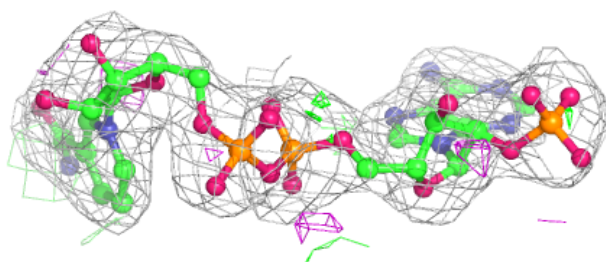
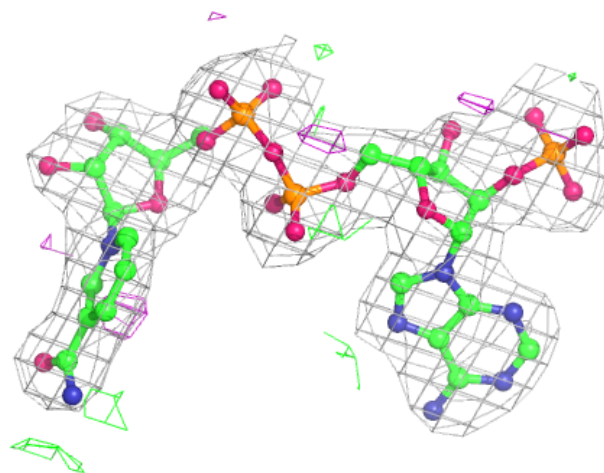
**Electron density around NAP C 801:**

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



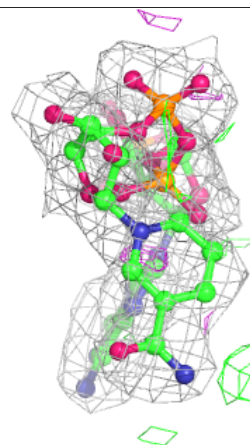
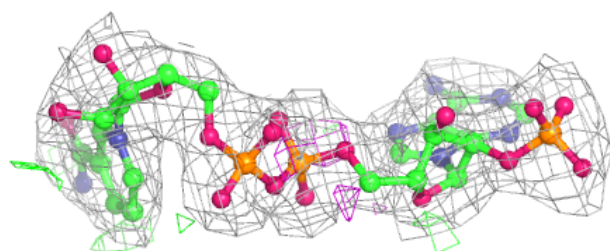
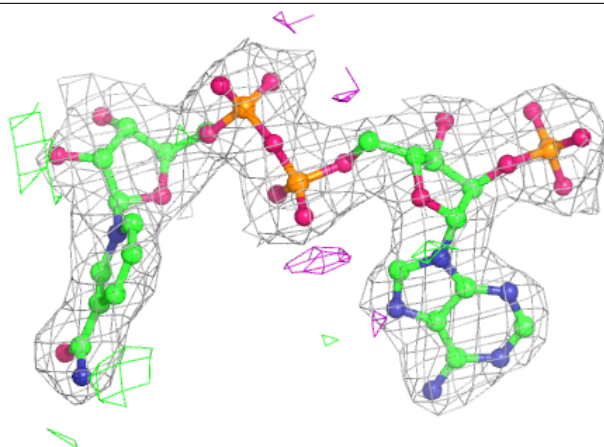
**Electron density around NAP B 801:**

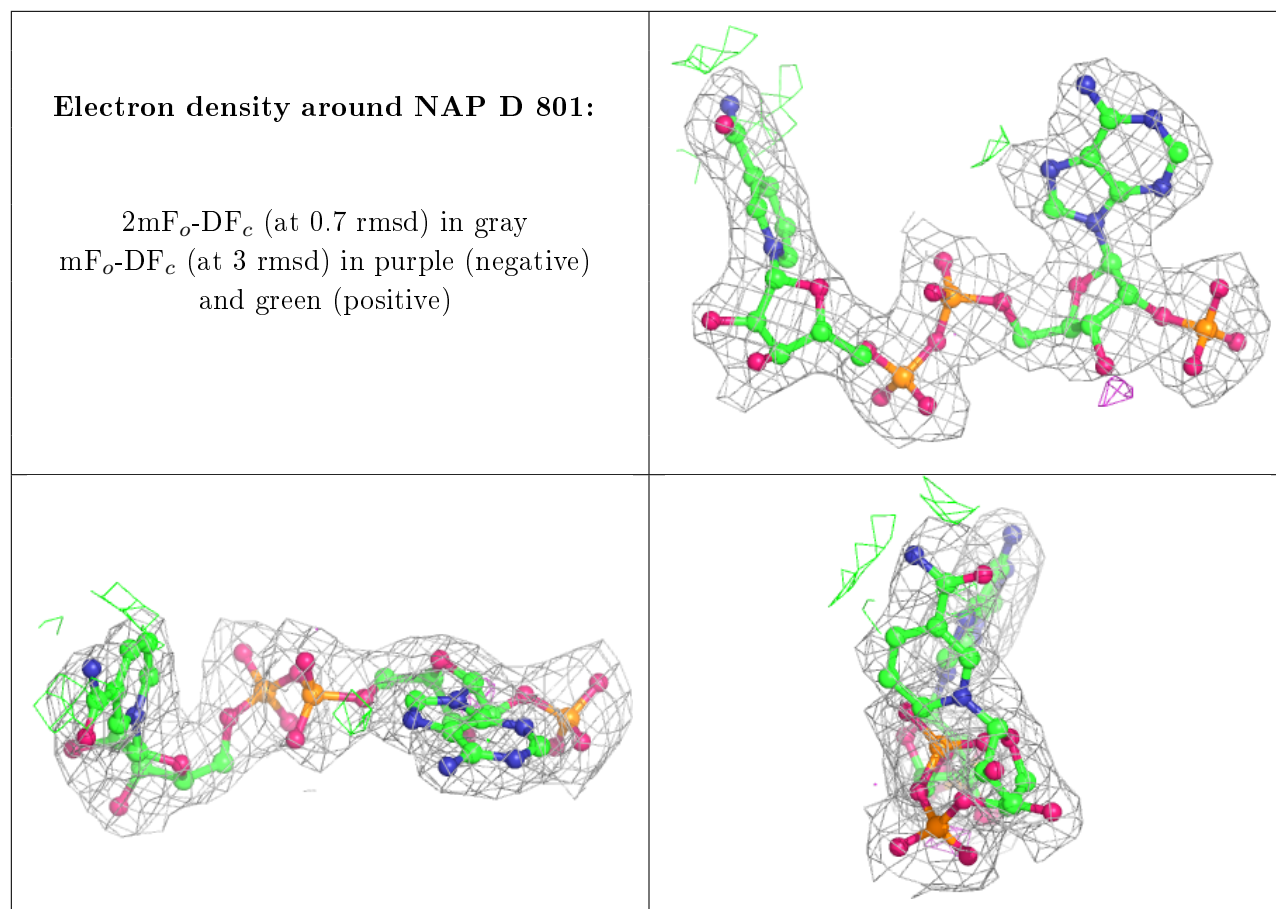
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAP A 801:**

$2mF_o-DF_c$  (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.