



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:11 PM JST

PDB ID : 7X12  
Title : Crystal structure of ME1 in complex with NADPH  
Authors : Amano, Y.  
Deposited on : 2022-02-22  
Resolution : 2.07 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

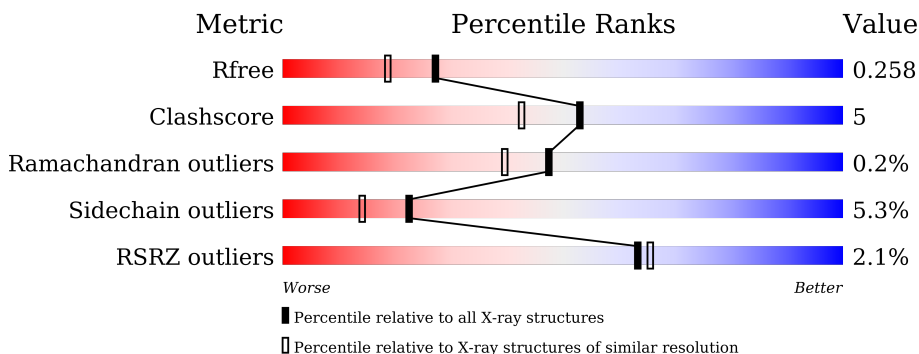
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	572	 % 81% 17% .
1	B	572	 % 84% 13% ..
1	C	572	 5% 81% 16% ..
1	D	572	 % 84% 14% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18485 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.

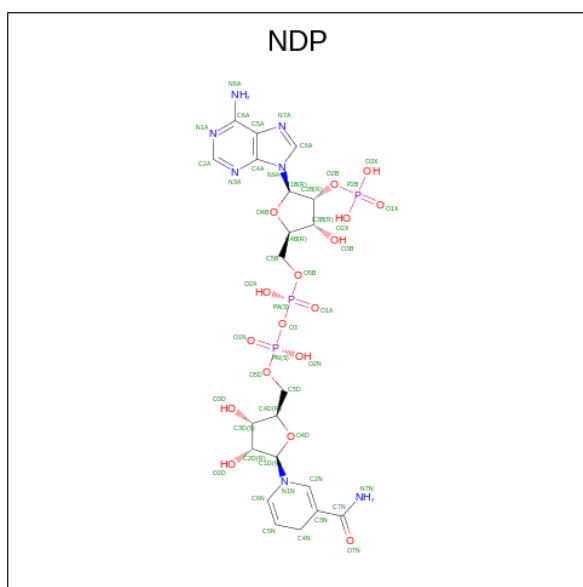
- Molecule 1 is a protein called NADP-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	564	4451	2834	765	832	20	0	0	0
1	B	564	4451	2834	765	832	20	0	0	0
1	C	564	4451	2834	765	832	20	0	0	0
1	D	564	4451	2834	765	832	20	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

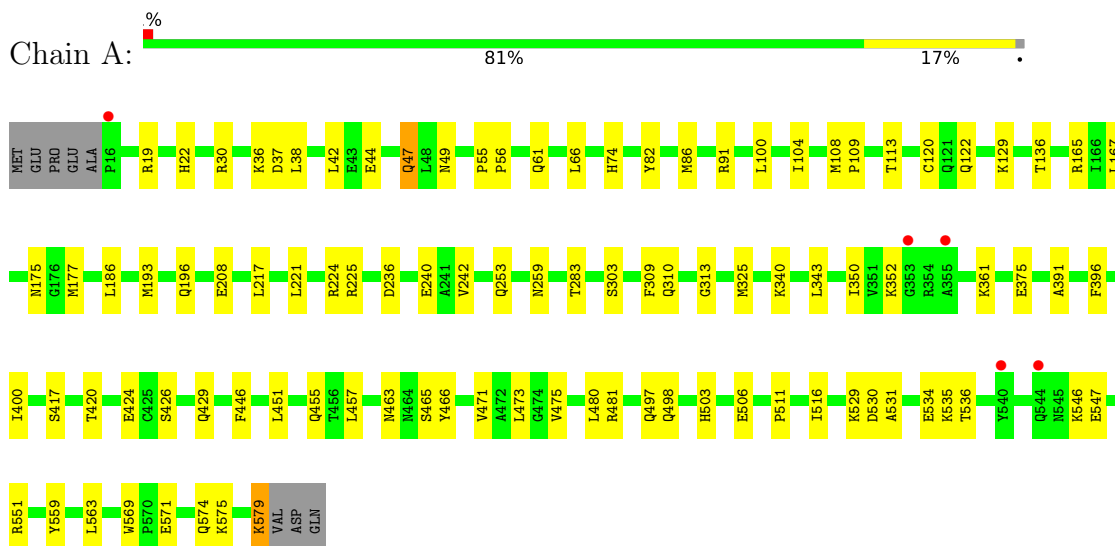
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	154	Total	O	0	0
			154	154		
4	C	130	Total	O	0	0
			130	130		
4	D	149	Total	O	0	0
			149	149		

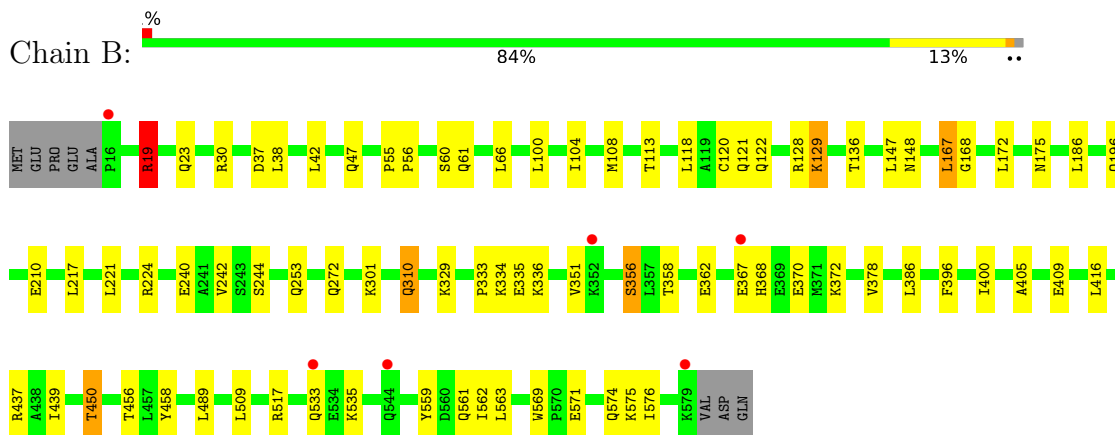
### 3 Residue-property plots i

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.

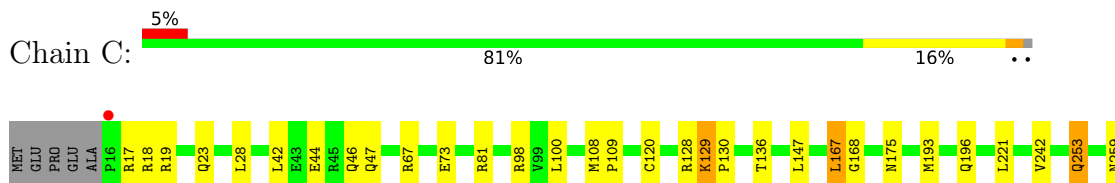
- Molecule 1: NADP-dependent malic enzyme

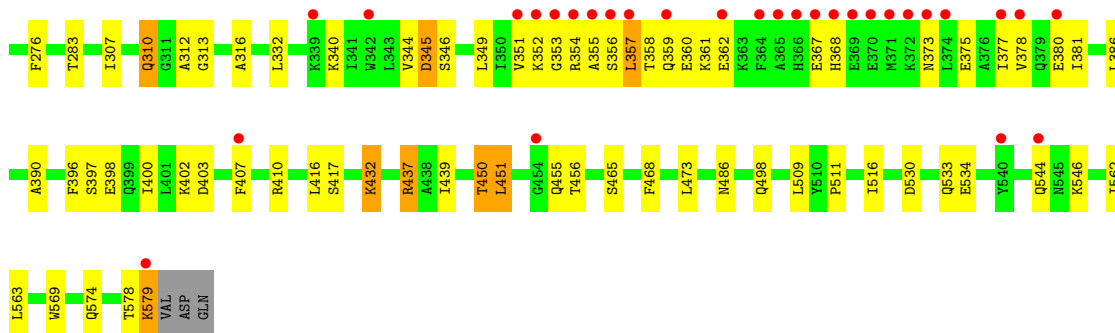


- Molecule 1: NADP-dependent malic enzyme

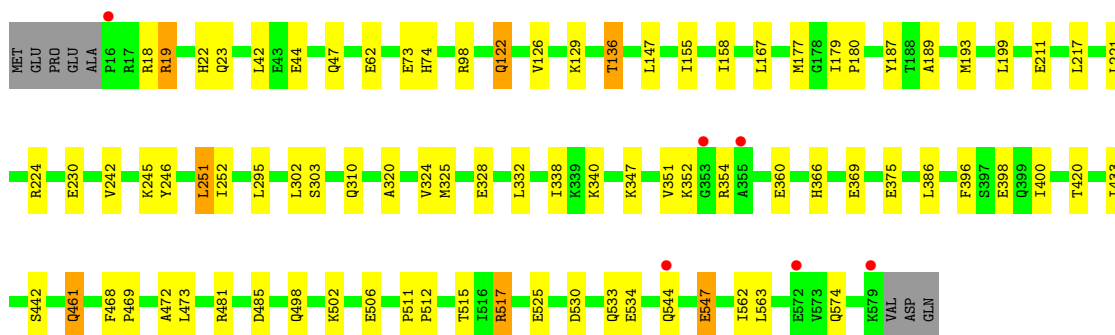
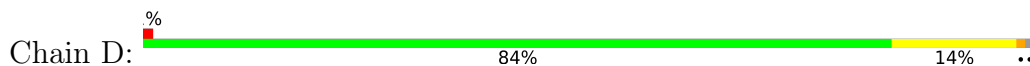


- Molecule 1: NADP-dependent malic enzyme





● Molecule 1: NADP-dependent malic enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.28Å 181.59Å 116.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 2.07 45.14 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.2 (45.18-2.07) 95.2 (45.14-2.07)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.216 , 0.258 0.216 , 0.258	Depositor DCC
$R_{free}$ test set	8760 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.392	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: MN, NDP

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	0.36	0/4538	0.72	1/6142 (0.0%)
1	B	0.38	0/4538	0.75	0/6142
1	C	0.35	0/4538	0.74	3/6142 (0.0%)
1	D	0.35	0/4538	0.74	1/6142 (0.0%)
All	All	0.36	0/18152	0.74	5/24568 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ARG	CG-CD-NE	-6.16	98.86	111.80
1	C	81	ARG	CG-CD-NE	-5.96	99.28	111.80
1	C	129	LYS	CB-CA-C	5.46	121.31	110.40
1	D	224	ARG	CG-CD-NE	-5.35	100.56	111.80
1	A	129	LYS	CB-CA-C	5.12	120.65	110.40

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	4451	0	4483	52	0
1	B	4451	0	4483	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4451	0	4483	64	0
1	D	4451	0	4483	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	26	3	0
3	B	48	0	26	1	0
3	C	48	0	26	6	0
3	D	48	0	26	0	0
4	A	52	0	0	0	0
4	B	154	0	0	8	0
4	C	130	0	0	4	0
4	D	149	0	0	3	0
All	All	18485	0	18036	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:HB2	4:B:834:HOH:O	1.48	1.13
1:C:129:LYS:HB2	4:C:798:HOH:O	1.51	1.09
1:B:37:ASP:HB2	4:B:764:HOH:O	1.58	1.02
1:A:375:GLU:HA	1:A:400:ILE:HD11	1.43	1.00
1:A:375:GLU:HA	1:A:400:ILE:CD1	2.02	0.89
1:A:42:LEU:HD23	1:D:574:GLN:HE21	1.38	0.88
1:C:310:GLN:O	1:C:390:ALA:HB2	1.75	0.85
1:C:310:GLN:O	1:C:310:GLN:HG3	1.77	0.85
1:D:19:ARG:HG2	1:D:562:ILE:HG22	1.55	0.85
1:B:19:ARG:HH21	1:B:19:ARG:HB2	1.47	0.79
1:B:333:PRO:HG2	1:B:336:LYS:HG3	1.66	0.78
1:D:19:ARG:HB2	1:D:19:ARG:HH21	1.49	0.77
1:B:19:ARG:HG2	1:B:562:ILE:HG22	1.69	0.74
1:C:378:VAL:HG21	1:C:400:ILE:HG23	1.68	0.74
1:D:129:LYS:HB2	4:D:738:HOH:O	1.86	0.74
1:B:19:ARG:NH1	1:B:196:GLN:HE22	1.87	0.73
1:A:569:TRP:H	1:A:574:GLN:NE2	1.89	0.70
1:C:313:GLY:HA3	3:C:602:NDP:O5B	1.91	0.69
1:C:451:LEU:HD12	1:C:455:GLN:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:HE21	1:D:42:LEU:HD23	1.59	0.68
1:C:193:MET:HE1	1:C:473:LEU:HA	1.78	0.66
1:B:37:ASP:CB	4:B:764:HOH:O	2.31	0.65
1:D:44:GLU:HA	1:D:563:LEU:HD21	1.77	0.65
1:C:19:ARG:NH2	1:C:196:GLN:HE22	1.97	0.62
1:A:375:GLU:CA	1:A:400:ILE:HD11	2.25	0.62
1:D:502:LYS:NZ	1:D:506:GLU:OE2	2.33	0.62
1:C:373:ASN:O	1:C:377:ILE:HG13	2.00	0.61
1:C:546:LYS:HE2	4:C:823:HOH:O	1.99	0.61
1:B:129:LYS:HB2	4:B:840:HOH:O	2.01	0.61
1:D:19:ARG:HB2	1:D:19:ARG:NH2	2.14	0.60
1:D:193:MET:HE1	1:D:473:LEU:HA	1.82	0.60
1:B:136:THR:HB	1:B:221:LEU:HD11	1.82	0.60
1:D:187:TYR:HE2	1:D:472:ALA:HB2	1.67	0.60
1:B:333:PRO:HG2	1:B:336:LYS:CG	2.30	0.60
1:A:120:CYS:O	1:A:175:ASN:HB3	2.02	0.59
1:C:359:GLN:HA	1:C:362:GLU:HG2	1.83	0.59
1:C:349:LEU:O	1:C:354:ARG:NH1	2.36	0.58
1:C:569:TRP:H	1:C:574:GLN:NE2	2.02	0.58
1:A:530:ASP:O	1:A:534:GLU:HG2	2.03	0.58
1:A:498:GLN:HB2	1:A:511:PRO:HG3	1.86	0.57
1:C:44:GLU:HA	1:C:563:LEU:HD21	1.86	0.57
1:B:405:ALA:O	1:B:437:ARG:NH2	2.39	0.56
1:B:38:LEU:HD21	1:B:55:PRO:HG2	1.86	0.56
1:C:375:GLU:HA	1:C:400:ILE:HD13	1.87	0.56
1:C:310:GLN:O	1:C:390:ALA:CB	2.52	0.56
1:B:42:LEU:HD23	1:C:574:GLN:HE21	1.71	0.56
1:C:344:VAL:HG12	3:C:602:NDP:H2A	1.86	0.55
1:C:530:ASP:O	1:C:534:GLU:HG2	2.07	0.55
1:C:345:ASP:HB2	3:C:602:NDP:O2X	2.07	0.55
1:C:386:LEU:HG	1:C:396:PHE:CZ	2.41	0.55
1:B:19:ARG:O	1:B:562:ILE:HA	2.06	0.55
1:A:303:SER:O	1:A:340:LYS:HE2	2.07	0.54
1:A:38:LEU:HD21	1:A:55:PRO:HG2	1.89	0.54
1:C:310:GLN:O	1:C:310:GLN:CG	2.54	0.54
1:A:208:GLU:OE2	1:A:224:ARG:HD3	2.08	0.54
1:B:333:PRO:CG	1:B:336:LYS:HG3	2.37	0.54
1:B:386:LEU:HG	1:B:396:PHE:CZ	2.44	0.53
1:D:251:LEU:HD12	1:D:252:ILE:N	2.24	0.53
1:B:517:ARG:HG2	4:B:816:HOH:O	2.09	0.53
1:D:136:THR:HB	1:D:221:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:TRP:H	1:B:574:GLN:NE2	2.06	0.52
1:A:529:LYS:HE3	1:A:546:LYS:HB2	1.91	0.52
1:C:367:GLU:O	1:C:368:HIS:HB2	2.09	0.52
1:C:439:ILE:HG22	1:C:509:LEU:HD11	1.92	0.52
1:D:530:ASP:O	1:D:534:GLU:HG2	2.10	0.52
1:C:23:GLN:NE2	4:C:703:HOH:O	2.42	0.52
1:A:208:GLU:HG2	1:A:225:ARG:HG3	1.91	0.51
1:A:104:ILE:O	1:A:108:MET:HG3	2.11	0.51
1:B:23:GLN:NE2	4:B:707:HOH:O	2.44	0.51
1:A:283:THR:HG23	3:A:602:NDP:H41N	1.93	0.51
1:B:517:ARG:CG	4:B:816:HOH:O	2.59	0.51
1:C:28:LEU:C	1:C:28:LEU:HD23	2.31	0.51
1:B:113:THR:CG2	1:B:167:LEU:HD11	2.41	0.50
1:B:329:LYS:HD2	1:B:489:LEU:HD21	1.92	0.50
1:D:398:GLU:HG3	1:D:433:ILE:HG12	1.93	0.50
1:D:338:ILE:HG22	1:D:366:HIS:HE1	1.75	0.50
1:B:439:ILE:HG22	1:B:509:LEU:HD11	1.92	0.50
1:D:193:MET:HE1	1:D:473:LEU:CA	2.41	0.50
1:D:158:ILE:HG12	1:D:199:LEU:HB3	1.93	0.49
1:D:375:GLU:HG3	1:D:400:ILE:HG13	1.93	0.49
1:C:403:ASP:HB3	1:C:407:PHE:CE2	2.48	0.49
1:C:17:ARG:HH21	1:C:19:ARG:HB3	1.77	0.49
1:C:403:ASP:HB3	1:C:407:PHE:HE2	1.78	0.49
1:D:442:SER:O	1:D:461:GLN:HA	2.13	0.48
1:A:61:GLN:HG3	1:A:559:TYR:CE2	2.47	0.48
1:C:450:THR:HG22	1:C:456:THR:HG23	1.94	0.48
1:B:118:LEU:HA	1:B:121:GLN:HE21	1.77	0.48
1:A:136:THR:HG21	1:B:56:PRO:HB3	1.95	0.48
1:A:391:ALA:HA	1:A:417:SER:HB3	1.96	0.48
1:A:451:LEU:HD11	1:A:457:LEU:HD11	1.95	0.48
1:B:61:GLN:HG3	1:B:559:TYR:CE2	2.48	0.48
1:A:19:ARG:O	1:A:19:ARG:HG3	2.14	0.48
1:B:19:ARG:NH1	1:B:196:GLN:NE2	2.61	0.48
1:A:217:LEU:HD21	1:B:66:LEU:HD23	1.96	0.47
1:B:42:LEU:CD2	1:C:574:GLN:HE21	2.27	0.47
1:C:380:GLU:HG3	1:C:381:ILE:HG13	1.97	0.47
1:D:512:PRO:HG2	1:D:515:THR:HG23	1.97	0.47
1:A:49:ASN:HB3	1:D:22:HIS:CE1	2.49	0.47
1:B:167:LEU:HB3	1:B:168:GLY:H	1.58	0.47
1:C:283:THR:HG23	3:C:602:NDP:H41N	1.96	0.47
1:D:498:GLN:HB2	1:D:511:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HB	1:A:221:LEU:HD11	1.97	0.47
1:A:30:ARG:HB3	1:B:30:ARG:HB3	1.97	0.46
1:A:165:ARG:NH2	3:A:602:NDP:O1A	2.48	0.46
1:B:351:VAL:HG21	1:B:370:GLU:HG2	1.96	0.46
1:D:122:GLN:O	1:D:126:VAL:HG22	2.15	0.46
1:C:253:GLN:HG3	1:C:276:PHE:CZ	2.50	0.46
1:C:498:GLN:HB2	1:C:511:PRO:HG3	1.98	0.46
1:D:187:TYR:HE2	1:D:472:ALA:CB	2.27	0.46
1:A:66:LEU:HD23	1:B:217:LEU:HD21	1.98	0.46
1:D:23:GLN:NE2	4:D:707:HOH:O	2.48	0.46
1:D:189:ALA:O	1:D:517:ARG:HD2	2.16	0.46
1:A:579:LYS:HA	1:A:579:LYS:HE3	1.98	0.46
1:C:19:ARG:O	1:C:562:ILE:HA	2.16	0.45
1:C:129:LYS:HA	1:C:130:PRO:HD2	1.67	0.45
1:C:397:SER:H	1:C:400:ILE:HG13	1.81	0.45
1:D:468:PHE:N	1:D:469:PRO:CD	2.79	0.45
1:A:236:ASP:O	1:A:240:GLU:HG3	2.17	0.45
1:B:128:ARG:HD3	4:B:763:HOH:O	2.16	0.45
1:B:120:CYS:O	1:B:175:ASN:HB3	2.17	0.45
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.98	0.45
1:B:450:THR:HB	1:B:456:THR:OG1	2.16	0.45
1:C:432:LYS:HA	1:C:432:LYS:HE3	1.98	0.45
1:B:240:GLU:O	1:B:244:SER:HB3	2.17	0.45
1:C:67:ARG:HB2	1:D:217:LEU:HD22	1.99	0.45
1:D:295:LEU:HD11	1:D:302:LEU:HD13	1.98	0.45
1:A:313:GLY:HA3	3:A:602:NDP:O5B	2.17	0.45
1:C:400:ILE:H	1:C:400:ILE:HG12	1.64	0.44
1:C:417:SER:HA	3:C:602:NDP:H1D	1.99	0.44
1:D:62:GLU:HG3	1:D:98:ARG:NH2	2.32	0.44
1:D:328:GLU:HA	1:D:332:LEU:O	2.17	0.44
1:B:60:SER:HB3	1:C:578:THR:HG22	1.99	0.44
1:C:360:GLU:C	1:C:362:GLU:H	2.19	0.44
1:A:481:ARG:HG2	1:A:481:ARG:HH11	1.82	0.44
1:C:465:SER:O	1:C:516:ILE:HD11	2.17	0.44
1:A:481:ARG:HG2	1:A:481:ARG:NH1	2.32	0.44
1:D:351:VAL:O	1:D:354:ARG:HB2	2.18	0.44
1:B:456:THR:HG22	1:B:458:TYR:CE1	2.52	0.44
1:A:466:TYR:HA	1:A:516:ILE:HD11	2.00	0.43
1:B:367:GLU:O	1:B:368:HIS:HB2	2.17	0.43
1:A:471:VAL:O	1:A:475:VAL:HG23	2.18	0.43
1:B:416:LEU:O	3:B:602:NDP:H2N	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HA	1:A:563:LEU:HD21	1.99	0.43
1:C:358:THR:OG1	1:C:361:LYS:HG3	2.18	0.43
1:A:574:GLN:HE21	1:D:42:LEU:CD2	2.30	0.43
1:A:91:ARG:HG3	1:B:129:LYS:HD3	2.00	0.43
1:B:310:GLN:HE21	1:B:310:GLN:HA	1.83	0.43
1:D:325:MET:SD	1:D:485:ASP:HB3	2.58	0.43
1:D:177:MET:O	1:D:180:PRO:HD2	2.18	0.43
1:C:19:ARG:HG3	1:C:562:ILE:HG22	2.00	0.43
1:D:193:MET:HE3	1:D:193:MET:HB2	1.86	0.43
1:C:450:THR:HA	1:C:455:GLN:O	2.18	0.43
1:C:310:GLN:NE2	4:C:702:HOH:O	2.26	0.43
1:C:416:LEU:O	3:C:602:NDP:H2N	2.19	0.43
1:C:310:GLN:HA	1:C:310:GLN:HE21	1.84	0.42
1:D:320:ALA:O	1:D:324:VAL:HG23	2.19	0.42
1:C:354:ARG:HG2	1:C:355:ALA:N	2.34	0.42
1:D:525:GLU:OE2	1:D:547:GLU:HG2	2.19	0.42
1:B:172:LEU:O	1:B:175:ASN:HB2	2.19	0.42
1:C:120:CYS:O	1:C:175:ASN:HB3	2.20	0.42
1:A:82:TYR:O	1:A:86:MET:HG2	2.20	0.42
1:C:578:THR:OG1	1:C:579:LYS:N	2.50	0.42
1:A:47:GLN:HG2	1:A:563:LEU:HD22	2.02	0.42
1:A:375:GLU:HA	1:A:400:ILE:HD13	1.97	0.42
1:B:358:THR:O	1:B:362:GLU:HG2	2.20	0.42
1:C:312:ALA:HA	1:C:316:ALA:HB3	2.02	0.42
1:C:354:ARG:O	1:C:357:LEU:HB2	2.19	0.42
1:A:396:PHE:CG	1:A:424:GLU:HB3	2.54	0.42
1:A:463:ASN:OD1	1:A:465:SER:HB2	2.20	0.41
1:B:104:ILE:HG13	1:B:108:MET:HG3	2.01	0.41
1:C:42:LEU:O	1:C:46:GLN:HG3	2.20	0.41
1:A:56:PRO:HB3	1:B:136:THR:HG21	2.03	0.41
1:A:531:ALA:HA	1:A:536:THR:OG1	2.20	0.41
1:A:36:LYS:O	1:A:37:ASP:HB2	2.21	0.41
1:B:563:LEU:HD23	1:B:563:LEU:HA	1.84	0.41
1:C:354:ARG:HG2	1:C:355:ALA:H	1.85	0.41
1:D:303:SER:O	1:D:340:LYS:NZ	2.53	0.41
1:A:426:SER:HA	1:A:446:PHE:CZ	2.55	0.41
1:B:575:LYS:HG2	1:B:576:ILE:N	2.35	0.41
1:D:245:LYS:HE3	4:D:718:HOH:O	2.19	0.41
1:D:386:LEU:HG	1:D:396:PHE:CZ	2.56	0.41
1:A:193:MET:HE1	1:A:473:LEU:HA	2.01	0.41
1:A:503:HIS:O	1:A:506:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HB3	1:C:168:GLY:H	1.61	0.41
1:A:309:PHE:HB2	1:A:343:LEU:HD23	2.03	0.41
1:C:359:GLN:O	1:C:362:GLU:HB2	2.21	0.40
1:C:410:ARG:HA	1:C:437:ARG:O	2.21	0.40
1:A:350:ILE:HD13	1:A:361:LYS:HB3	2.03	0.40
1:C:465:SER:HA	1:C:468:PHE:CE2	2.55	0.40
1:A:109:PRO:HA	1:A:113:THR:O	2.21	0.40
1:C:108:MET:N	1:C:109:PRO:CD	2.85	0.40
1:A:19:ARG:CZ	1:A:196:GLN:HE22	2.34	0.40
1:B:378:VAL:HG21	1:B:400:ILE:HG23	2.03	0.40
1:C:136:THR:HB	1:C:221:LEU:HD11	2.02	0.40
1:D:155:ILE:HB	1:D:246:TYR:CD1	2.56	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	562/572 (98%)	542 (96%)	20 (4%)	0	100	100
1	B	562/572 (98%)	547 (97%)	13 (2%)	2 (0%)	34	25
1	C	562/572 (98%)	529 (94%)	30 (5%)	3 (0%)	29	19
1	D	562/572 (98%)	546 (97%)	16 (3%)	0	100	100
All	All	2248/2288 (98%)	2164 (96%)	79 (4%)	5 (0%)	47	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	C	353	GLY
1	C	398	GLU

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Mol	Chain	Res	Type
1	C	332	LEU
1	B	356	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	483/490 (99%)	458 (95%)	25 (5%)	23	14
1	B	483/490 (99%)	458 (95%)	25 (5%)	23	14
1	C	483/490 (99%)	455 (94%)	28 (6%)	20	11
1	D	483/490 (99%)	458 (95%)	25 (5%)	23	14
All	All	1932/1960 (99%)	1829 (95%)	103 (5%)	22	14

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	47	GLN
1	A	74	HIS
1	A	100	LEU
1	A	122	GLN
1	A	167	LEU
1	A	177	MET
1	A	186	LEU
1	A	242	VAL
1	A	253	GLN
1	A	259	ASN
1	A	310	GLN
1	A	325	MET
1	A	352	LYS
1	A	420	THR
1	A	429	GLN
1	A	455	GLN
1	A	480	LEU
1	A	497	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	535	LYS
1	A	547	GLU
1	A	551	ARG
1	A	571	GLU
1	A	575	LYS
1	A	579	LYS
1	B	19	ARG
1	B	47	GLN
1	B	100	LEU
1	B	122	GLN
1	B	129	LYS
1	B	147	LEU
1	B	167	LEU
1	B	186	LEU
1	B	210	GLU
1	B	224	ARG
1	B	242	VAL
1	B	253	GLN
1	B	272	GLN
1	B	301	LYS
1	B	310	GLN
1	B	334	LYS
1	B	335	GLU
1	B	356	SER
1	B	372	LYS
1	B	409	GLU
1	B	450	THR
1	B	533	GLN
1	B	535	LYS
1	B	561	GLN
1	B	571	GLU
1	C	18	ARG
1	C	47	GLN
1	C	73	GLU
1	C	100	LEU
1	C	128	ARG
1	C	147	LEU
1	C	167	LEU
1	C	242	VAL
1	C	253	GLN
1	C	259	ASN
1	C	307	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	310	GLN
1	C	340	LYS
1	C	345	ASP
1	C	346	SER
1	C	351	VAL
1	C	352	LYS
1	C	356	SER
1	C	357	LEU
1	C	402	LYS
1	C	432	LYS
1	C	437	ARG
1	C	450	THR
1	C	451	LEU
1	C	486	ASN
1	C	533	GLN
1	C	544	GLN
1	C	579	LYS
1	D	18	ARG
1	D	19	ARG
1	D	47	GLN
1	D	73	GLU
1	D	74	HIS
1	D	122	GLN
1	D	136	THR
1	D	147	LEU
1	D	167	LEU
1	D	211	GLU
1	D	230	GLU
1	D	242	VAL
1	D	251	LEU
1	D	310	GLN
1	D	347	LYS
1	D	352	LYS
1	D	360	GLU
1	D	369	GLU
1	D	420	THR
1	D	461	GLN
1	D	481	ARG
1	D	517	ARG
1	D	533	GLN
1	D	544	GLN
1	D	547	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	121	GLN
1	A	196	GLN
1	A	310	GLN
1	A	455	GLN
1	A	574	GLN
1	B	23	GLN
1	B	49	ASN
1	B	76	ASN
1	B	121	GLN
1	B	196	GLN
1	B	310	GLN
1	B	574	GLN
1	C	23	GLN
1	C	49	ASN
1	C	121	GLN
1	C	196	GLN
1	C	310	GLN
1	C	366	HIS
1	C	399	GLN
1	C	455	GLN
1	C	486	ASN
1	C	497	GLN
1	C	533	GLN
1	C	544	GLN
1	C	574	GLN
1	D	23	GLN
1	D	310	GLN
1	D	514	ASN
1	D	561	GLN
1	D	574	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	NDP	D	602	-	45,52,52	1.37	3 (6%)	53,80,80	1.37	8 (15%)
3	NDP	A	602	-	45,52,52	1.54	5 (11%)	53,80,80	1.35	7 (13%)
3	NDP	B	602	-	45,52,52	1.40	4 (8%)	53,80,80	1.42	8 (15%)
3	NDP	C	602	-	45,52,52	1.41	4 (8%)	53,80,80	1.50	12 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	602	-	-	4/30/77/77	0/5/5/5
3	NDP	A	602	-	-	4/30/77/77	0/5/5/5
3	NDP	B	602	-	-	5/30/77/77	0/5/5/5
3	NDP	C	602	-	-	5/30/77/77	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NDP	C4N-C3N	-6.12	1.37	1.49
3	D	602	NDP	C4N-C3N	-5.84	1.38	1.49
3	C	602	NDP	C4N-C3N	-5.70	1.38	1.49
3	B	602	NDP	C4N-C3N	-5.05	1.40	1.49
3	B	602	NDP	C4N-C5N	-3.96	1.38	1.48
3	A	602	NDP	C4N-C5N	-3.83	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NDP	C4N-C5N	-3.64	1.39	1.48
3	C	602	NDP	C4N-C5N	-3.60	1.39	1.48
3	A	602	NDP	P2B-O2B	3.47	1.65	1.59
3	D	602	NDP	C6N-C5N	3.36	1.39	1.33
3	B	602	NDP	C6N-C5N	3.04	1.38	1.33
3	A	602	NDP	C6N-C5N	2.75	1.38	1.33
3	C	602	NDP	C6N-C5N	2.74	1.38	1.33
3	C	602	NDP	P2B-O2B	2.68	1.64	1.59
3	B	602	NDP	P2B-O2B	2.48	1.64	1.59
3	A	602	NDP	C7N-N7N	2.23	1.39	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NDP	O3X-P2B-O2X	4.02	123.01	107.64
3	B	602	NDP	O4D-C1D-N1N	4.01	115.90	108.06
3	A	602	NDP	O4D-C1D-N1N	3.64	115.17	108.06
3	B	602	NDP	C3N-C2N-N1N	-3.52	118.07	123.10
3	D	602	NDP	O4B-C1B-C2B	-3.50	100.52	106.59
3	A	602	NDP	C1D-N1N-C2N	-3.36	115.52	121.11
3	C	602	NDP	C1D-N1N-C2N	-3.16	115.85	121.11
3	A	602	NDP	O3D-C3D-C4D	-3.04	102.26	111.05
3	C	602	NDP	C3N-C2N-N1N	-3.01	118.81	123.10
3	C	602	NDP	O3X-P2B-O2X	2.91	118.75	107.64
3	C	602	NDP	O2A-PA-O1A	2.87	126.41	112.24
3	B	602	NDP	C3B-C2B-C1B	-2.86	97.51	102.89
3	A	602	NDP	C3N-C2N-N1N	-2.85	119.03	123.10
3	C	602	NDP	C3B-C2B-C1B	-2.76	97.70	102.89
3	C	602	NDP	C4A-C5A-N7A	2.70	112.22	109.40
3	D	602	NDP	O4D-C1D-N1N	2.67	113.27	108.06
3	C	602	NDP	C2D-C1D-N1N	-2.62	106.74	113.30
3	B	602	NDP	C2D-C1D-N1N	-2.56	106.90	113.30
3	D	602	NDP	O2X-P2B-O2B	-2.53	94.68	105.99
3	D	602	NDP	C1D-N1N-C2N	-2.48	116.98	121.11
3	C	602	NDP	O3B-C3B-C4B	-2.45	103.96	111.05
3	C	602	NDP	O4B-C1B-C2B	-2.36	102.50	106.59
3	D	602	NDP	O3D-C3D-C4D	-2.33	104.32	111.05
3	C	602	NDP	O2N-PN-O1N	2.28	123.49	112.24
3	B	602	NDP	O3B-C3B-C4B	-2.24	104.56	111.05
3	A	602	NDP	O3B-C3B-C4B	-2.23	104.59	111.05
3	D	602	NDP	O2A-PA-O1A	2.17	122.99	112.24
3	D	602	NDP	C3B-C2B-C1B	-2.16	98.83	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NDP	O2A-PA-O1A	2.14	122.82	112.24
3	B	602	NDP	O2A-PA-O1A	2.12	122.70	112.24
3	B	602	NDP	O3X-P2B-O2X	2.10	115.68	107.64
3	B	602	NDP	PN-O3-PA	-2.04	125.81	132.83
3	C	602	NDP	C5B-C4B-C3B	-2.04	107.53	115.18
3	A	602	NDP	O7N-C7N-C3N	-2.02	117.09	120.90
3	C	602	NDP	N6A-C6A-N1A	2.01	122.75	118.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C3B-C2B-O2B-P2B
3	B	602	NDP	O4B-C4B-C5B-O5B
3	B	602	NDP	C3B-C4B-C5B-O5B
3	B	602	NDP	C3B-C2B-O2B-P2B
3	D	602	NDP	C3B-C2B-O2B-P2B
3	C	602	NDP	C1B-C2B-O2B-P2B
3	D	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	O4D-C1D-N1N-C2N
3	B	602	NDP	O4D-C1D-N1N-C2N
3	D	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	C5B-O5B-PA-O1A
3	B	602	NDP	C1B-C2B-O2B-P2B
3	C	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C1B-C2B-O2B-P2B
3	C	602	NDP	C3B-C4B-C5B-O5B
3	A	602	NDP	O4B-C4B-C5B-O5B
3	D	602	NDP	O4B-C4B-C5B-O5B

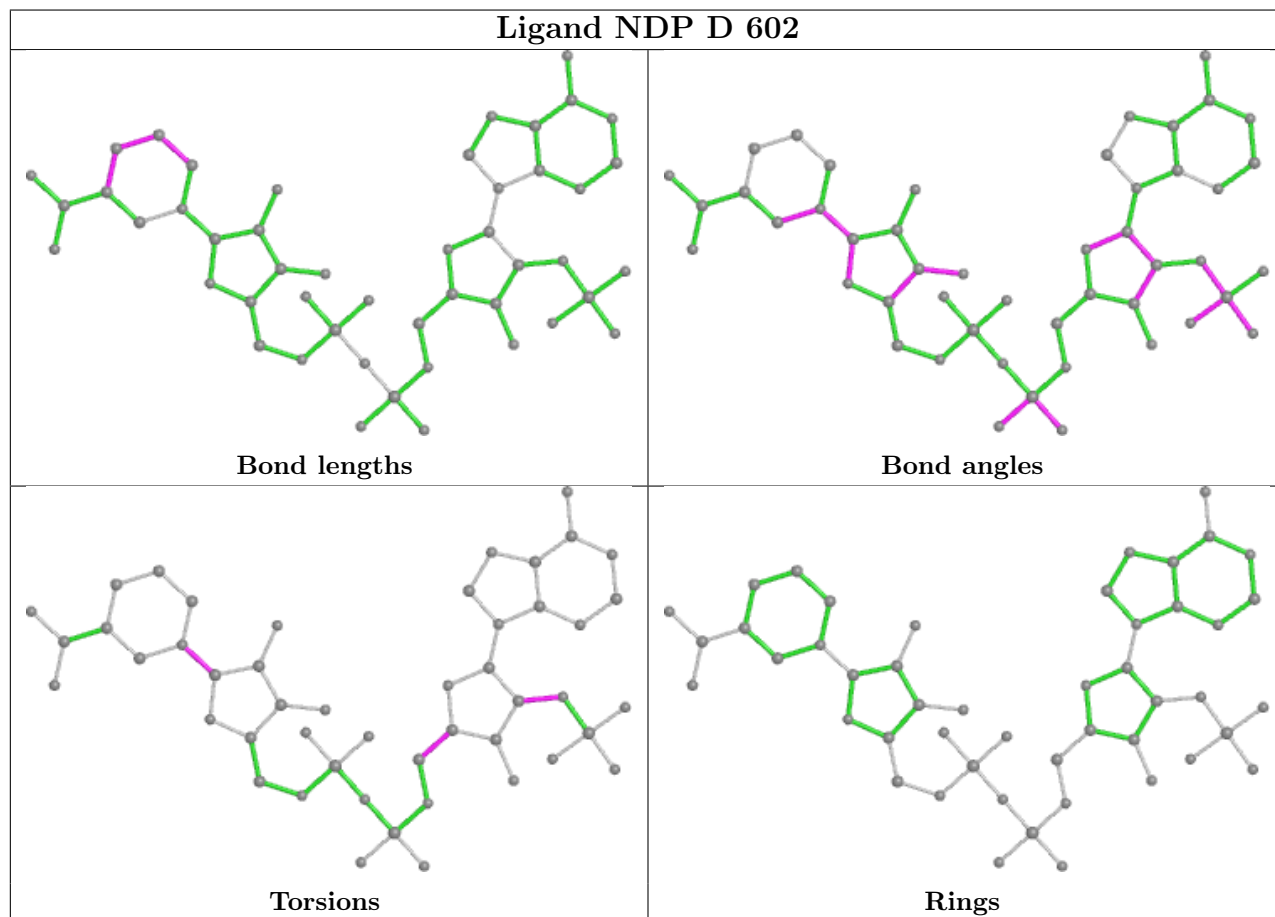
There are no ring outliers.

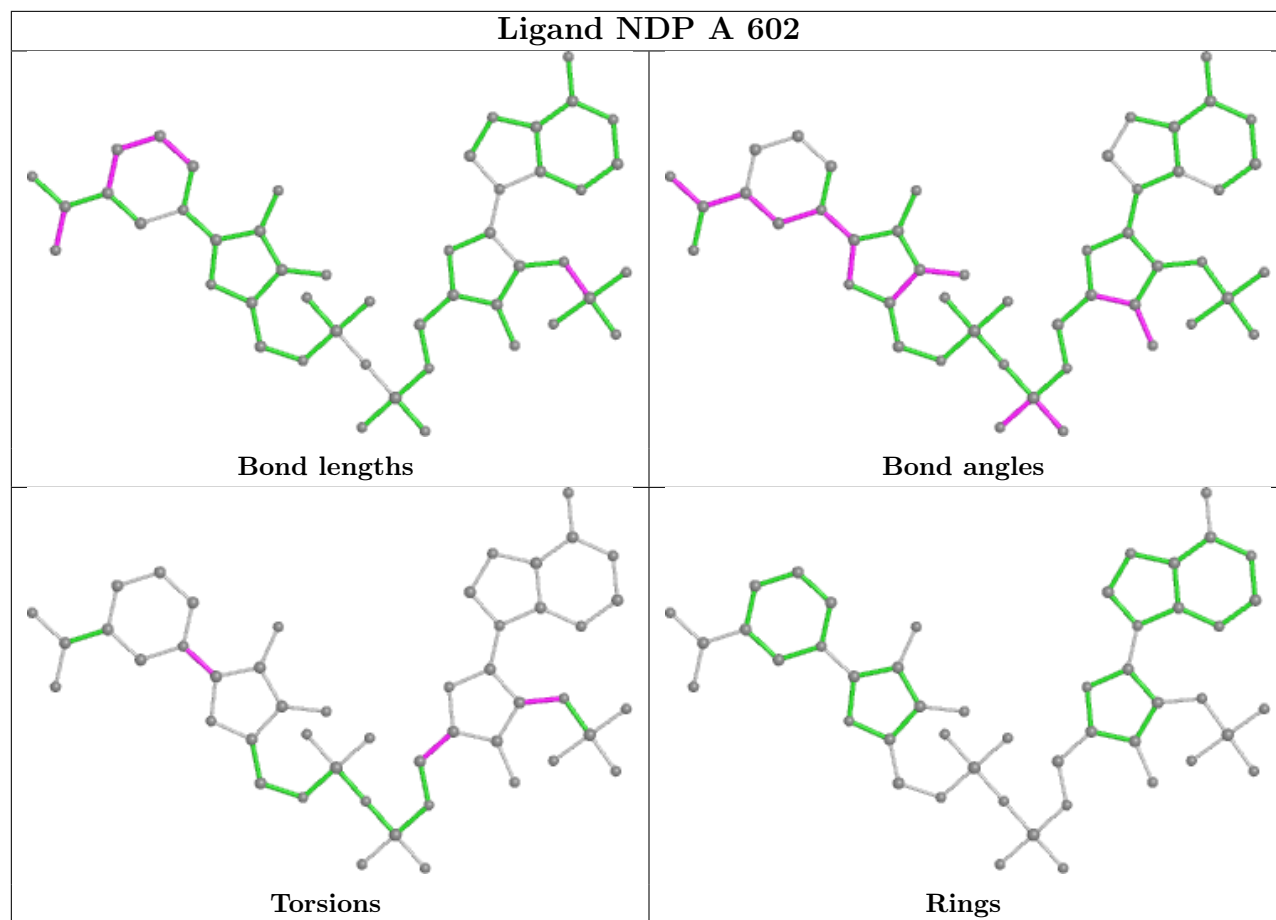
3 monomers are involved in 10 short contacts:

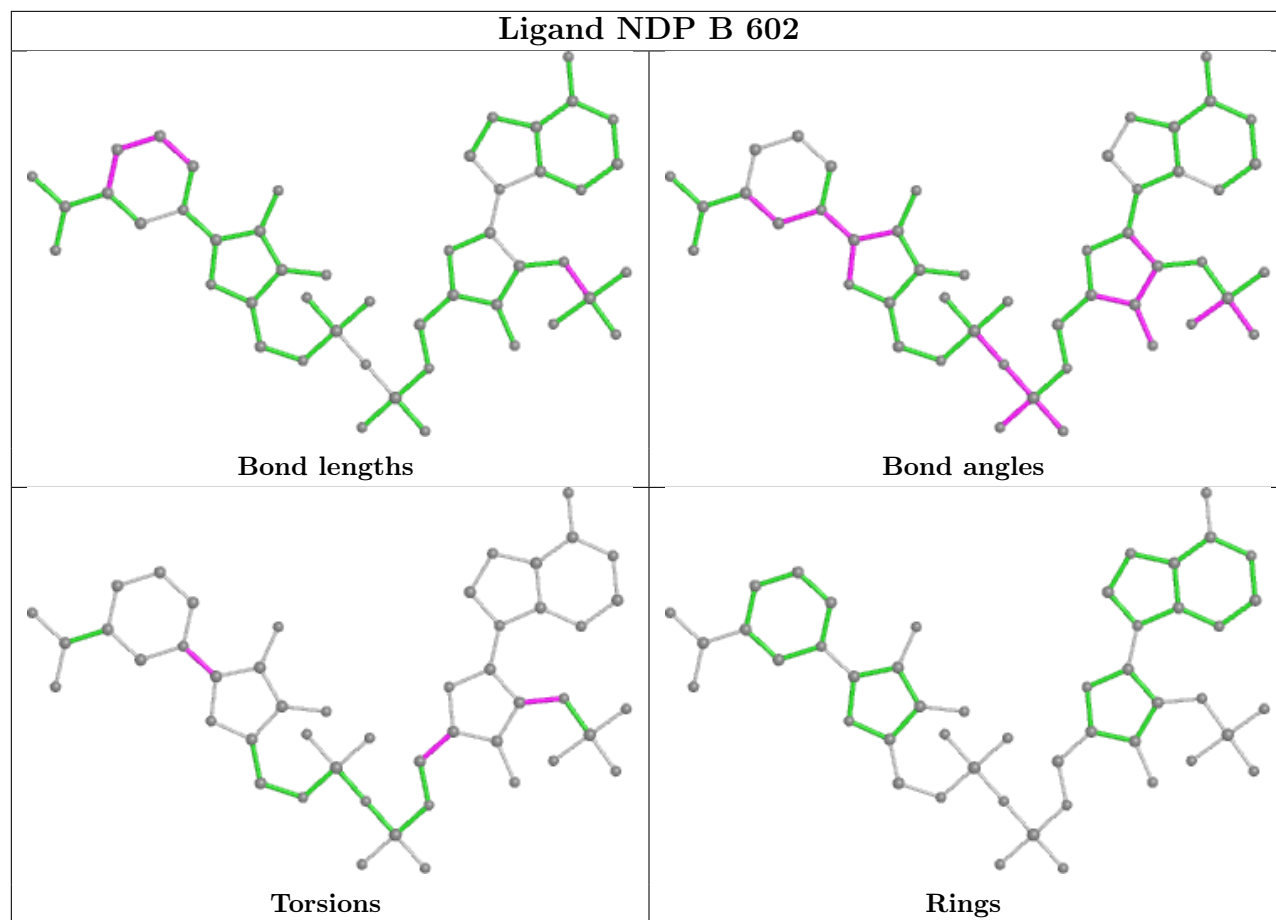
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NDP	3	0
3	B	602	NDP	1	0
3	C	602	NDP	6	0

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

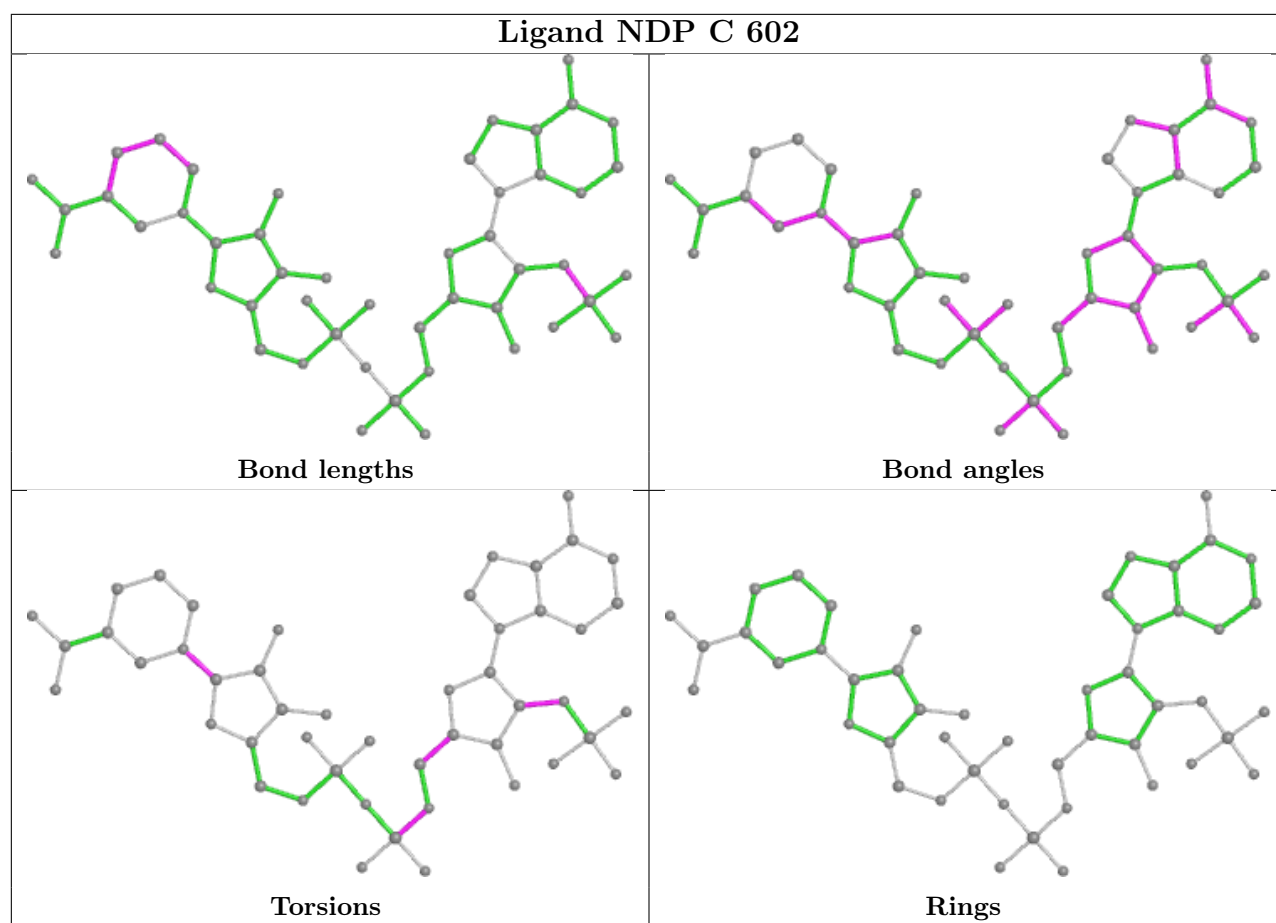
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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	564/572 (98%)	-0.33	5 (0%) 84 85	23, 36, 58, 74	0
1	B	564/572 (98%)	-0.28	6 (1%) 80 81	22, 34, 56, 79	0
1	C	564/572 (98%)	0.08	31 (5%) 25 26	22, 38, 84, 118	0
1	D	564/572 (98%)	-0.20	6 (1%) 80 81	22, 35, 61, 99	0
All	All	2256/2288 (98%)	-0.18	48 (2%) 63 65	22, 35, 65, 118	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	VAL	7.3
1	C	356	SER	5.3
1	C	355	ALA	4.9
1	D	16	PRO	4.8
1	C	366	HIS	4.6
1	B	16	PRO	4.4
1	C	357	LEU	4.2
1	C	454	GLY	3.9
1	C	359	GLN	3.9
1	C	367	GLU	3.8
1	C	339	LYS	3.8
1	C	374	LEU	3.6
1	C	365	ALA	3.4
1	C	370	GLU	3.1
1	C	544	GLN	3.0
1	B	544	GLN	3.0
1	D	355	ALA	2.9
1	C	362	GLU	2.8
1	A	355	ALA	2.7
1	C	352	LYS	2.7
1	C	364	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	16	PRO	2.6
1	A	540	TYR	2.6
1	B	533	GLN	2.6
1	D	579	LYS	2.6
1	A	16	PRO	2.6
1	C	407	PHE	2.5
1	C	372	LYS	2.5
1	B	352	LYS	2.5
1	C	540	TYR	2.4
1	C	354	ARG	2.4
1	C	373	ASN	2.4
1	C	369	GLU	2.3
1	D	572	GLU	2.3
1	C	380	GLU	2.3
1	C	579	LYS	2.3
1	C	368	HIS	2.3
1	C	353	GLY	2.3
1	A	353	GLY	2.2
1	D	353	GLY	2.2
1	C	342	TRP	2.2
1	D	544	GLN	2.2
1	C	371	MET	2.2
1	B	367	GLU	2.1
1	B	579	LYS	2.1
1	A	544	GLN	2.1
1	C	377	ILE	2.1
1	C	378	VAL	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.

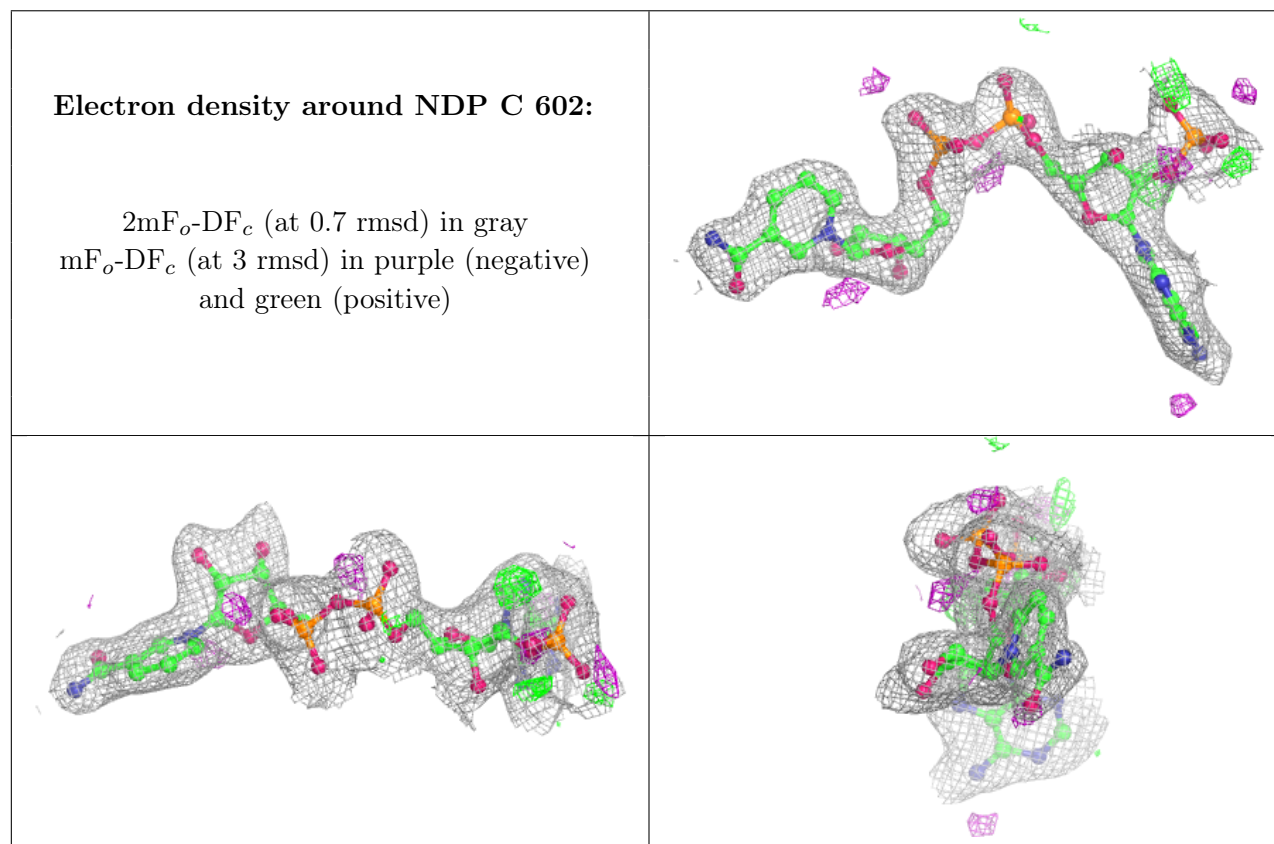
## 6.4 Ligands [i](#)

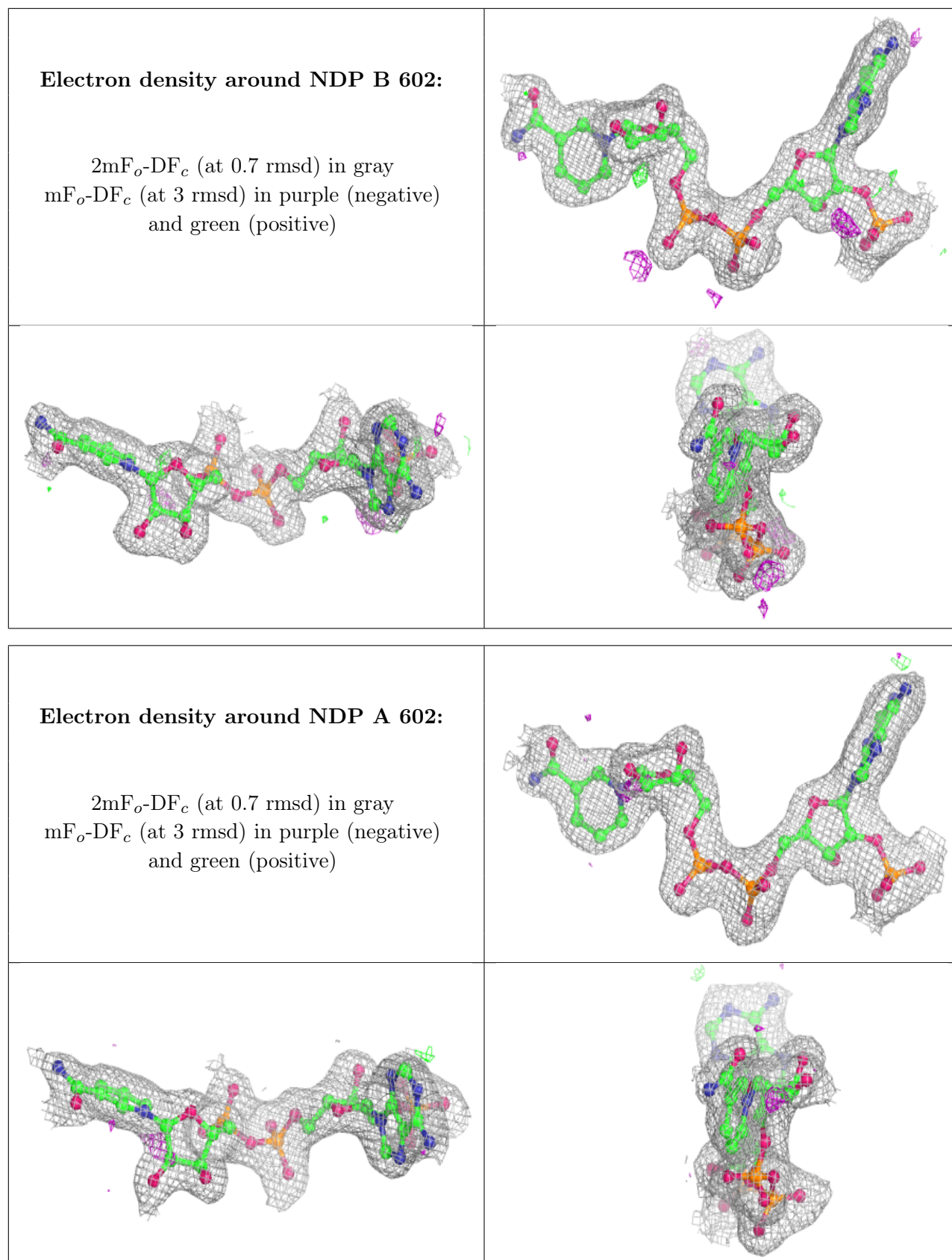
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

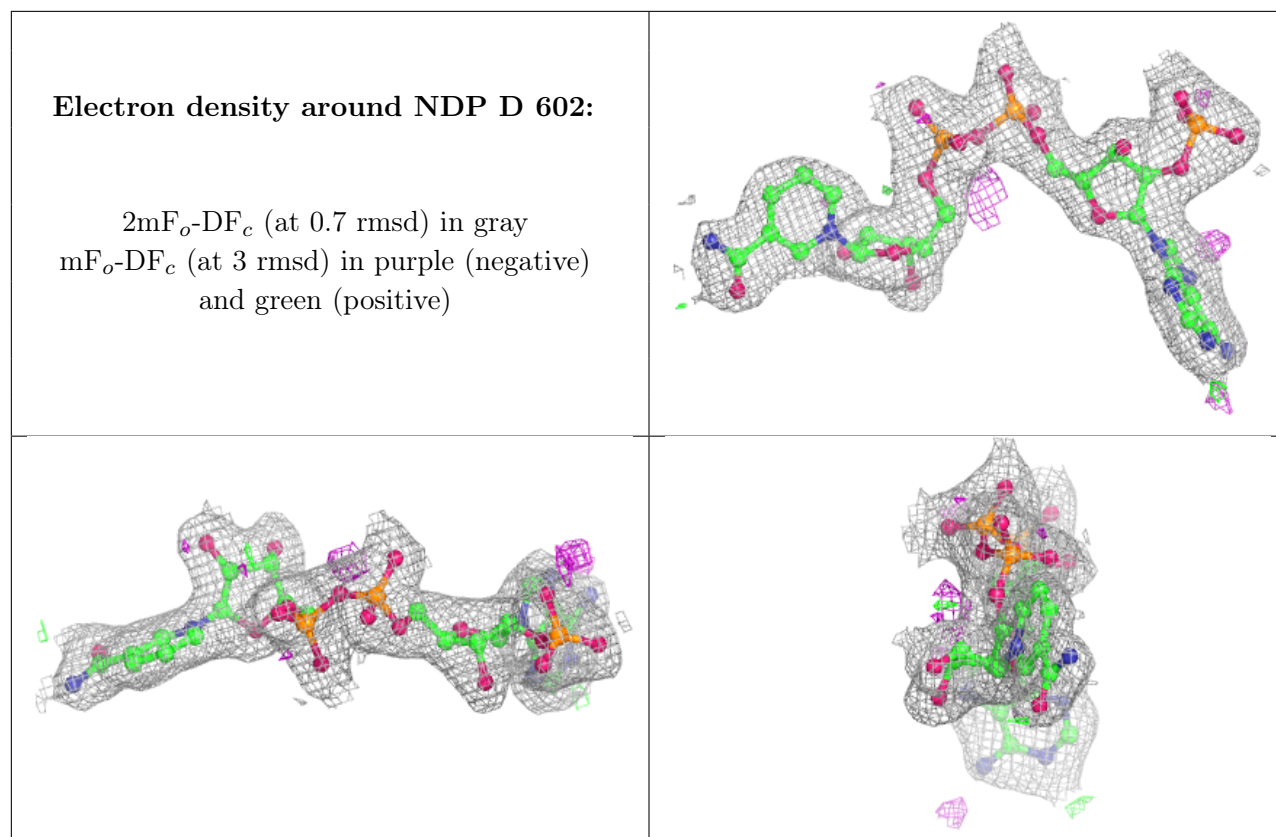
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NDP	C	602	48/48	0.93	0.11	37,51,66,77	0
3	NDP	B	602	48/48	0.97	0.09	26,31,37,39	0
3	NDP	A	602	48/48	0.97	0.10	33,38,42,43	0
3	NDP	D	602	48/48	0.97	0.08	32,39,45,47	0
2	MN	D	601	1/1	0.99	0.12	34,34,34,34	0
2	MN	C	601	1/1	1.00	0.12	34,34,34,34	0
2	MN	A	601	1/1	1.00	0.11	36,36,36,36	0
2	MN	B	601	1/1	1.00	0.13	30,30,30,30	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 [i](#)

There are no such residues in this entry.