



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 PM UTC

PDB ID : 8J1G / pdb_00008j1g
Title : Structure of amino acid dehydrogenase in complex with NADPH
Authors : Sakuraba, H.; Ohshima, T.
Deposited on : 2023-04-12
Resolution : 2.50 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

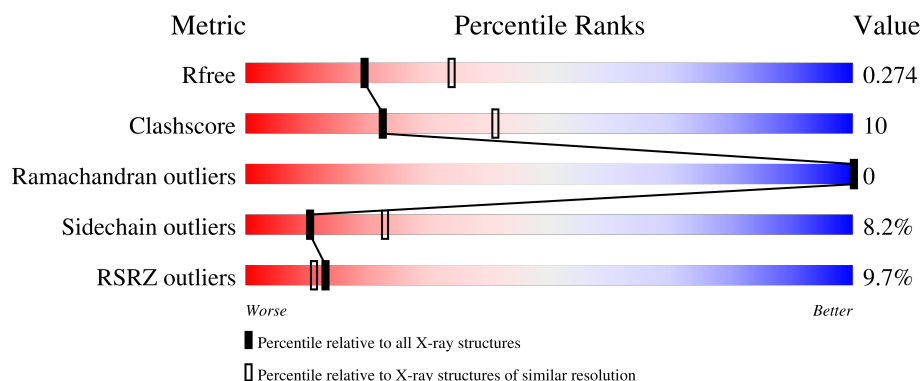
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	336	7% 67% 24% 8%
1	B	336	5% 65% 25% 7%
1	C	336	10% 67% 17% 13%
1	D	336	14% 67% 24% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	1003	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9489 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 Ornithine cyclodeaminase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2320	1471	408	430	11			
1	B	312	Total	C	N	O	S	0	0	0
			2346	1485	413	437	11			
1	C	293	Total	C	N	O	S	0	0	0
			2220	1409	392	408	11			
1	D	306	Total	C	N	O	S	0	0	0
			2310	1464	407	428	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	ASP	-	expression tag	UNP A0A7Y0ZV07
A	317	PRO	-	expression tag	UNP A0A7Y0ZV07
A	318	ASN	-	expression tag	UNP A0A7Y0ZV07
A	319	SER	-	expression tag	UNP A0A7Y0ZV07
A	320	SER	-	expression tag	UNP A0A7Y0ZV07
A	321	SER	-	expression tag	UNP A0A7Y0ZV07
A	322	VAL	-	expression tag	UNP A0A7Y0ZV07
A	323	ASP	-	expression tag	UNP A0A7Y0ZV07
A	324	LYS	-	expression tag	UNP A0A7Y0ZV07
A	325	LEU	-	expression tag	UNP A0A7Y0ZV07
A	326	ALA	-	expression tag	UNP A0A7Y0ZV07
A	327	ALA	-	expression tag	UNP A0A7Y0ZV07
A	328	ALA	-	expression tag	UNP A0A7Y0ZV07
A	329	LEU	-	expression tag	UNP A0A7Y0ZV07
A	330	GLU	-	expression tag	UNP A0A7Y0ZV07
A	331	HIS	-	expression tag	UNP A0A7Y0ZV07
A	332	HIS	-	expression tag	UNP A0A7Y0ZV07
A	333	HIS	-	expression tag	UNP A0A7Y0ZV07
A	334	HIS	-	expression tag	UNP A0A7Y0ZV07
A	335	HIS	-	expression tag	UNP A0A7Y0ZV07
A	336	HIS	-	expression tag	UNP A0A7Y0ZV07

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Chain	Residue	Modelled	Actual	Comment	Reference
B	316	ASP	-	expression tag	UNP A0A7Y0ZV07
B	317	PRO	-	expression tag	UNP A0A7Y0ZV07
B	318	ASN	-	expression tag	UNP A0A7Y0ZV07
B	319	SER	-	expression tag	UNP A0A7Y0ZV07
B	320	SER	-	expression tag	UNP A0A7Y0ZV07
B	321	SER	-	expression tag	UNP A0A7Y0ZV07
B	322	VAL	-	expression tag	UNP A0A7Y0ZV07
B	323	ASP	-	expression tag	UNP A0A7Y0ZV07
B	324	LYS	-	expression tag	UNP A0A7Y0ZV07
B	325	LEU	-	expression tag	UNP A0A7Y0ZV07
B	326	ALA	-	expression tag	UNP A0A7Y0ZV07
B	327	ALA	-	expression tag	UNP A0A7Y0ZV07
B	328	ALA	-	expression tag	UNP A0A7Y0ZV07
B	329	LEU	-	expression tag	UNP A0A7Y0ZV07
B	330	GLU	-	expression tag	UNP A0A7Y0ZV07
B	331	HIS	-	expression tag	UNP A0A7Y0ZV07
B	332	HIS	-	expression tag	UNP A0A7Y0ZV07
B	333	HIS	-	expression tag	UNP A0A7Y0ZV07
B	334	HIS	-	expression tag	UNP A0A7Y0ZV07
B	335	HIS	-	expression tag	UNP A0A7Y0ZV07
B	336	HIS	-	expression tag	UNP A0A7Y0ZV07
C	316	ASP	-	expression tag	UNP A0A7Y0ZV07
C	317	PRO	-	expression tag	UNP A0A7Y0ZV07
C	318	ASN	-	expression tag	UNP A0A7Y0ZV07
C	319	SER	-	expression tag	UNP A0A7Y0ZV07
C	320	SER	-	expression tag	UNP A0A7Y0ZV07
C	321	SER	-	expression tag	UNP A0A7Y0ZV07
C	322	VAL	-	expression tag	UNP A0A7Y0ZV07
C	323	ASP	-	expression tag	UNP A0A7Y0ZV07
C	324	LYS	-	expression tag	UNP A0A7Y0ZV07
C	325	LEU	-	expression tag	UNP A0A7Y0ZV07
C	326	ALA	-	expression tag	UNP A0A7Y0ZV07
C	327	ALA	-	expression tag	UNP A0A7Y0ZV07
C	328	ALA	-	expression tag	UNP A0A7Y0ZV07
C	329	LEU	-	expression tag	UNP A0A7Y0ZV07
C	330	GLU	-	expression tag	UNP A0A7Y0ZV07
C	331	HIS	-	expression tag	UNP A0A7Y0ZV07
C	332	HIS	-	expression tag	UNP A0A7Y0ZV07
C	333	HIS	-	expression tag	UNP A0A7Y0ZV07
C	334	HIS	-	expression tag	UNP A0A7Y0ZV07
C	335	HIS	-	expression tag	UNP A0A7Y0ZV07
C	336	HIS	-	expression tag	UNP A0A7Y0ZV07

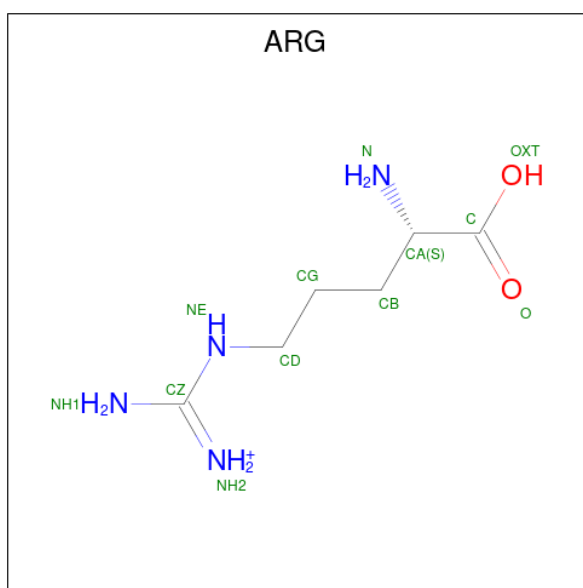
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Chain	Residue	Modelled	Actual	Comment	Reference
D	316	ASP	-	expression tag	UNP A0A7Y0ZV07
D	317	PRO	-	expression tag	UNP A0A7Y0ZV07
D	318	ASN	-	expression tag	UNP A0A7Y0ZV07
D	319	SER	-	expression tag	UNP A0A7Y0ZV07
D	320	SER	-	expression tag	UNP A0A7Y0ZV07
D	321	SER	-	expression tag	UNP A0A7Y0ZV07
D	322	VAL	-	expression tag	UNP A0A7Y0ZV07
D	323	ASP	-	expression tag	UNP A0A7Y0ZV07
D	324	LYS	-	expression tag	UNP A0A7Y0ZV07
D	325	LEU	-	expression tag	UNP A0A7Y0ZV07
D	326	ALA	-	expression tag	UNP A0A7Y0ZV07
D	327	ALA	-	expression tag	UNP A0A7Y0ZV07
D	328	ALA	-	expression tag	UNP A0A7Y0ZV07
D	329	LEU	-	expression tag	UNP A0A7Y0ZV07
D	330	GLU	-	expression tag	UNP A0A7Y0ZV07
D	331	HIS	-	expression tag	UNP A0A7Y0ZV07
D	332	HIS	-	expression tag	UNP A0A7Y0ZV07
D	333	HIS	-	expression tag	UNP A0A7Y0ZV07
D	334	HIS	-	expression tag	UNP A0A7Y0ZV07
D	335	HIS	-	expression tag	UNP A0A7Y0ZV07
D	336	HIS	-	expression tag	UNP A0A7Y0ZV07

- # NDP

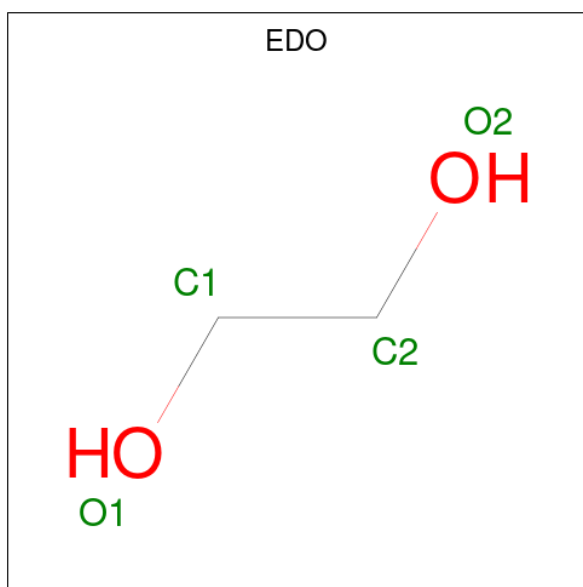
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		
3	C	1	Total	C	N	O	0	0
			12	6	4	2		
3	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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		

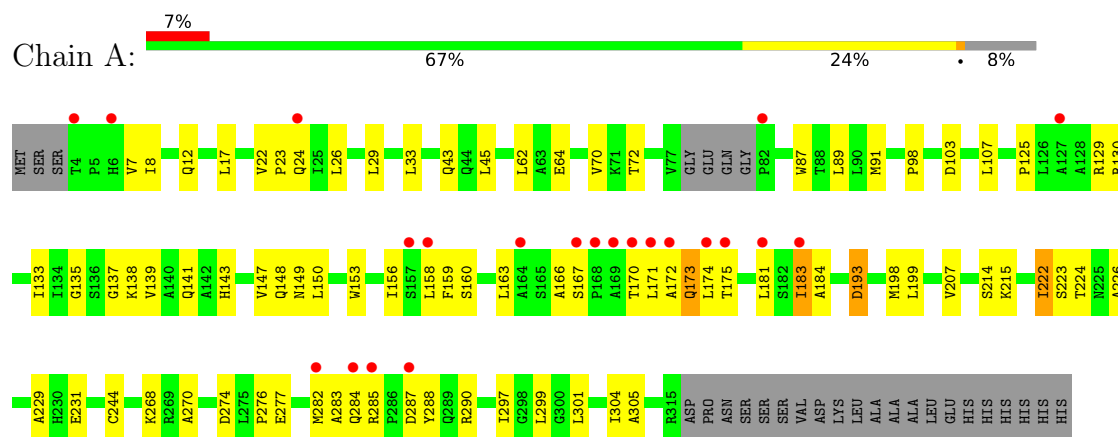
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	17	Total	O	0	0
			17	17		
5	C	7	Total	O	0	0
			7	7		
5	D	10	Total	O	0	0
			10	10		

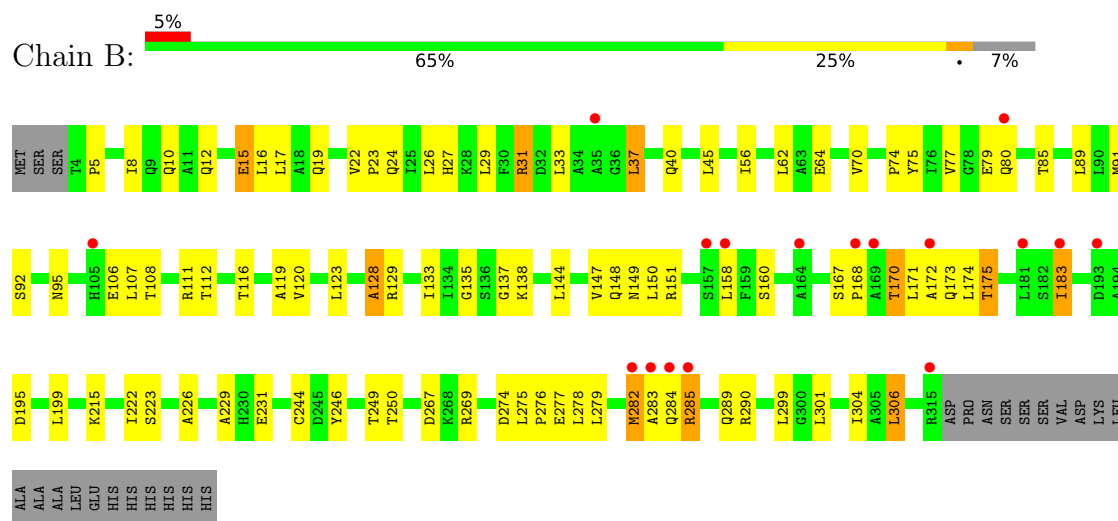
3 Residue-property plots [i](#)

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.

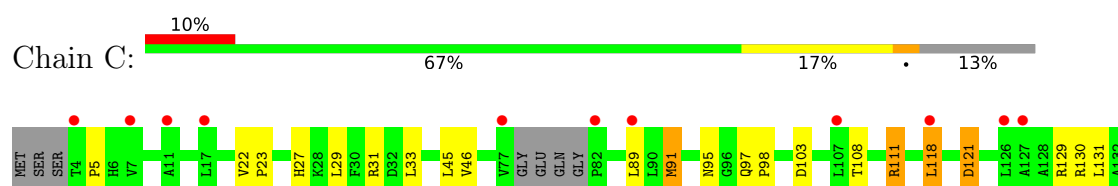
• Molecule 1: Ornithine cyclodeaminase family protein

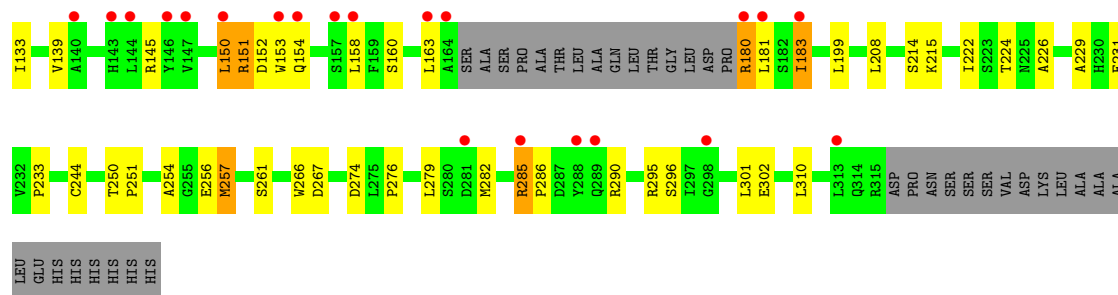


• Molecule 1: Ornithine cyclodeaminase family protein

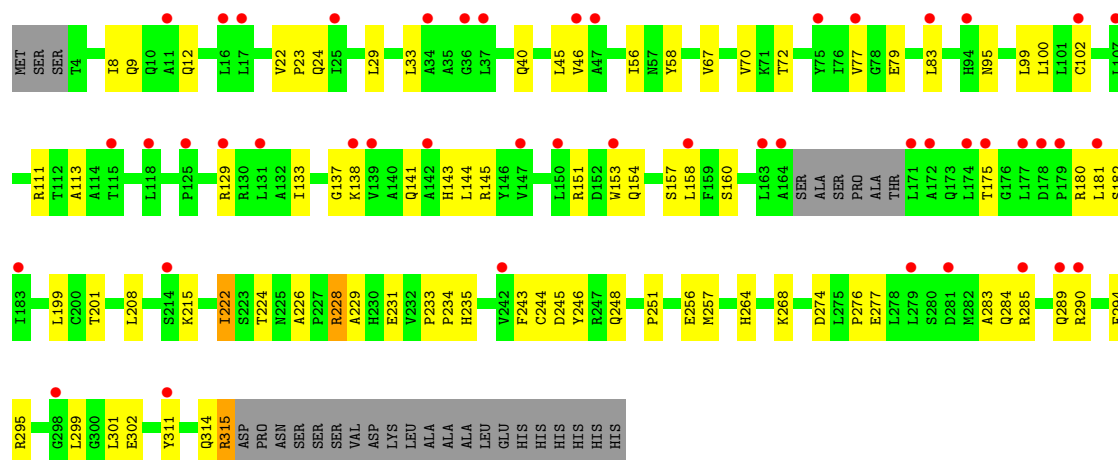


• Molecule 1: Ornithine cyclodeaminase family protein





• Molecule 1: Ornithine cyclodeaminase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 70.31Å 100.14Å 88.65° 72.53° 86.53°	Depositor
Resolution (Å)	47.80 – 2.50 47.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.80-2.50) 98.7 (47.80-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.225 , 0.274 0.235 , 0.274	Depositor DCC
R_{free} test set	2774 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.230 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9489	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, EDO

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	0.68	0/2369	1.10	1/3236 (0.0%)
1	B	0.67	0/2396	1.14	4/3274 (0.1%)
1	C	0.54	0/2266	0.93	0/3091
1	D	0.52	0/2358	0.90	1/3219 (0.0%)
All	All	0.61	0/9389	1.02	6/12820 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	N-CA-C	-5.95	102.08	109.64
1	B	10	GLN	N-CA-C	5.33	117.53	111.02
1	A	287	ASP	N-CA-C	-5.33	103.00	110.35
1	B	128	ALA	N-CA-C	-5.33	101.85	110.32
1	B	31	ARG	N-CA-C	-5.30	105.15	111.03
1	D	289	GLN	N-CA-C	-5.04	107.27	113.41

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	2320	0	2341	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2346	0	2361	67	0
1	C	2220	0	2239	42	0
1	D	2310	0	2326	41	0
2	A	48	0	26	4	0
2	B	48	0	26	4	0
2	C	48	0	26	2	0
2	D	48	0	26	2	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
4	A	4	0	6	2	0
4	B	4	0	6	5	0
5	A	11	0	0	0	0
5	B	17	0	0	1	0
5	C	7	0	0	0	0
5	D	10	0	0	3	0
All	All	9489	0	9431	198	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 10.

All (198) 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:89:LEU:HD21	1:A:91:MET:HE3	1.52	0.89
1:A:222:ILE:O	2:A:1001:NDP:H2N	1.81	0.81
1:C:226:ALA:HB3	1:C:229:ALA:HB2	1.63	0.80
1:B:89:LEU:HD21	1:B:91:MET:HE2	1.63	0.80
1:D:226:ALA:HB3	1:D:229:ALA:HB2	1.66	0.78
1:B:37:LEU:HG	1:B:64:GLU:HB3	1.66	0.77
1:B:299:LEU:HA	4:B:1003:EDO:H12	1.67	0.75
1:B:226:ALA:HB3	1:B:229:ALA:HB2	1.68	0.74
1:C:129:ARG:HB3	1:C:154:GLN:HG2	1.70	0.73
1:B:40:GLN:NE2	4:B:1003:EDO:C2	2.52	0.72
1:A:172:ALA:HA	1:A:175:THR:HG22	1.70	0.72
1:C:163:LEU:HB3	1:C:183:ILE:HD11	1.73	0.70
1:A:72:THR:CG2	1:B:91:MET:HE3	2.22	0.69
1:B:8:ILE:HG23	1:B:12:GLN:HB3	1.73	0.68
1:A:17:LEU:HD13	1:A:107:LEU:HD22	1.75	0.68
1:B:40:GLN:HB2	1:B:301:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:O	2:D:1001:NDP:H2N	1.94	0.67
1:C:257:MET:HE3	1:C:266:TRP:CH2	2.31	0.65
1:D:151:ARG:HB2	1:D:153:TRP:CE2	2.31	0.65
1:A:148:GLN:HG3	1:A:149:ASN:OD1	1.96	0.65
1:D:9:GLN:HB3	5:D:1105:HOH:O	1.96	0.64
1:B:148:GLN:HG3	1:B:149:ASN:OD1	1.99	0.63
1:B:40:GLN:NE2	4:B:1003:EDO:H21	2.12	0.63
1:D:144:LEU:HD21	1:D:181:LEU:HD11	1.82	0.62
1:C:222:ILE:O	2:C:1001:NDP:H2N	2.00	0.61
1:C:29:LEU:HD11	1:C:301:LEU:HB3	1.80	0.61
1:D:245:ASP:HB2	1:D:299:LEU:HD11	1.80	0.61
1:A:226:ALA:HB3	1:A:229:ALA:HB2	1.82	0.61
1:B:222:ILE:O	2:B:1001:NDP:H2N	2.01	0.61
1:B:282:MET:HE1	5:B:1113:HOH:O	2.01	0.60
1:A:173:GLN:HG2	1:A:174:LEU:N	2.16	0.60
1:A:199:LEU:HD13	1:A:231:GLU:HB3	1.84	0.59
1:B:167:SER:O	1:B:171:LEU:HD12	2.03	0.59
1:C:208:LEU:O	1:C:233:PRO:HD3	2.03	0.59
1:A:29:LEU:HD11	1:A:301:LEU:HB3	1.85	0.59
1:A:43:GLN:HB3	4:A:1003:EDO:H11	1.86	0.58
1:A:139:VAL:HG21	2:A:1001:NDP:H52N	1.85	0.58
1:B:17:LEU:HD13	1:B:107:LEU:HD22	1.85	0.58
1:B:244:CYS:O	1:B:274:ASP:HA	2.04	0.58
1:C:257:MET:HE3	1:C:266:TRP:HH2	1.67	0.58
1:C:133:ILE:HB	1:C:158:LEU:HB3	1.87	0.57
1:C:27:HIS:CE1	1:C:31:ARG:HD2	2.40	0.57
1:C:108:THR:HA	1:C:111:ARG:HD3	1.86	0.57
1:A:72:THR:HG23	1:B:91:MET:HE3	1.87	0.57
1:B:171:LEU:HA	1:B:174:LEU:HD12	1.87	0.57
1:B:8:ILE:CG2	1:B:12:GLN:HB3	2.35	0.56
1:D:144:LEU:CD2	1:D:181:LEU:HD11	2.35	0.56
1:C:118:LEU:CD2	1:C:279:LEU:HD11	2.36	0.55
1:A:244:CYS:O	1:A:274:ASP:HA	2.07	0.55
1:B:171:LEU:HD23	1:B:183:ILE:HD13	1.88	0.55
1:A:87:TRP:CZ2	1:A:103:ASP:HB2	2.41	0.55
1:B:267:ASP:OD2	1:B:269:ARG:NH1	2.40	0.55
1:B:246:TYR:CD2	1:B:249:THR:HG23	2.42	0.54
1:B:119:ALA:O	1:B:123:LEU:HB2	2.08	0.54
1:C:139:VAL:HG21	2:C:1001:NDP:H52N	1.89	0.53
1:A:299:LEU:HA	4:A:1003:EDO:H12	1.88	0.53
1:A:163:LEU:HA	1:A:166:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:GLU:CD	1:D:295:ARG:HE	2.17	0.53
1:C:151:ARG:HB2	1:C:153:TRP:CE2	2.43	0.53
1:B:75:TYR:HE1	1:B:77:VAL:HG22	1.73	0.53
1:D:45:LEU:HD23	1:D:46:VAL:N	2.24	0.53
1:C:131:LEU:HD13	1:C:153:TRP:CZ2	2.44	0.53
1:A:130:ARG:HD3	1:A:193:ASP:O	2.09	0.52
1:A:29:LEU:CD1	1:A:305:ALA:HB2	2.39	0.52
1:B:199:LEU:HD13	1:B:231:GLU:HB3	1.92	0.52
1:C:111:ARG:HG3	1:C:302:GLU:HB3	1.92	0.52
1:D:133:ILE:HB	1:D:158:LEU:HB3	1.92	0.52
1:C:95:ASN:OD1	1:C:97:GLN:N	2.37	0.51
1:D:33:LEU:HD23	1:D:276:PRO:HG3	1.91	0.51
1:A:166:ALA:HB3	1:A:171:LEU:HD21	1.93	0.51
1:A:147:VAL:HG21	1:A:198:MET:SD	2.51	0.50
1:B:147:VAL:O	1:B:147:VAL:HG12	2.09	0.50
1:C:121:ASP:HB2	1:C:150:LEU:HD11	1.93	0.50
1:B:40:GLN:HB2	1:B:301:LEU:CD1	2.42	0.50
1:B:133:ILE:HB	1:B:158:LEU:HB3	1.92	0.50
1:D:40:GLN:HB2	1:D:301:LEU:CD1	2.41	0.50
1:B:62:LEU:HD12	1:B:304:ILE:HG22	1.93	0.50
1:B:27:HIS:ND1	1:B:279:LEU:HD13	2.27	0.49
1:A:33:LEU:HD23	1:A:276:PRO:HG3	1.94	0.49
1:B:89:LEU:HD21	1:B:91:MET:CE	2.40	0.49
1:C:5:PRO:HB3	1:C:98:PRO:O	2.12	0.49
1:A:133:ILE:HB	1:A:158:LEU:HB3	1.94	0.49
1:B:33:LEU:HD23	1:B:276:PRO:HG3	1.94	0.49
1:D:157:SER:HA	1:D:182:SER:O	2.12	0.49
1:A:156:ILE:O	1:A:181:LEU:HA	2.13	0.49
1:C:91:MET:HE3	1:D:72:THR:HG21	1.94	0.49
1:C:89:LEU:HG	1:C:91:MET:HE1	1.95	0.48
1:C:256:GLU:CD	1:C:295:ARG:HE	2.21	0.48
1:D:113:ALA:HA	1:D:143:HIS:CE1	2.47	0.48
1:D:40:GLN:HB2	1:D:301:LEU:HD12	1.95	0.48
1:B:22:VAL:HB	1:B:23:PRO:HD3	1.95	0.48
1:B:275:LEU:N	1:B:276:PRO:HD2	2.29	0.48
1:B:249:THR:OG1	1:B:250:THR:N	2.47	0.47
1:B:37:LEU:CG	1:B:64:GLU:HB3	2.42	0.47
1:C:254:ALA:HB3	1:C:257:MET:HG3	1.96	0.47
1:B:150:LEU:O	1:B:151:ARG:HD3	2.14	0.47
1:B:29:LEU:HD11	1:B:301:LEU:HB3	1.96	0.47
1:A:147:VAL:HA	1:A:150:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PRO:O	1:B:171:LEU:HB2	2.15	0.47
1:A:207:VAL:HG12	2:A:1001:NDP:N6A	2.30	0.47
1:B:40:GLN:NE2	4:B:1003:EDO:H22	2.30	0.47
1:C:163:LEU:CB	1:C:183:ILE:HD11	2.44	0.47
1:D:22:VAL:HB	1:D:23:PRO:HD3	1.96	0.47
1:D:244:CYS:O	1:D:274:ASP:HA	2.15	0.46
1:B:74:PRO:HD2	1:B:85:THR:OG1	2.16	0.46
1:C:22:VAL:HB	1:C:23:PRO:HD3	1.98	0.46
1:D:228:ARG:HD3	5:D:1107:HOH:O	2.14	0.46
1:A:7:VAL:HG11	1:B:5:PRO:HD2	1.98	0.46
1:C:244:CYS:O	1:C:274:ASP:HA	2.16	0.46
1:B:111:ARG:HB3	1:B:306:LEU:HD22	1.97	0.46
1:C:45:LEU:HD23	1:C:46:VAL:N	2.30	0.46
1:C:163:LEU:HB3	1:C:183:ILE:CD1	2.44	0.46
1:A:223:SER:HB2	1:A:231:GLU:CD	2.41	0.46
1:C:103:ASP:C	1:C:103:ASP:OD1	2.59	0.45
1:D:311:TYR:CE1	1:D:315:ARG:HG3	2.51	0.45
1:B:167:SER:HB2	1:B:170:THR:HB	1.98	0.45
1:D:243:PHE:O	1:D:294:PHE:HA	2.17	0.45
1:C:108:THR:HA	1:C:111:ARG:CD	2.46	0.45
1:A:171:LEU:HA	1:A:174:LEU:HD12	1.98	0.45
1:C:33:LEU:HD23	1:C:276:PRO:HG3	1.97	0.45
1:A:166:ALA:CB	1:A:171:LEU:HD21	2.47	0.45
1:B:144:LEU:O	1:B:148:GLN:HB3	2.17	0.45
1:D:201:THR:HA	2:D:1001:NDP:O4B	2.17	0.45
1:A:91:MET:CE	1:A:98:PRO:HB3	2.47	0.45
1:C:222:ILE:O	1:C:224:THR:HG23	2.16	0.45
1:D:277:GLU:HB3	1:D:283:ALA:HB2	1.98	0.45
1:A:91:MET:HE2	1:A:98:PRO:HB3	1.99	0.44
1:B:147:VAL:HA	1:B:150:LEU:HD12	1.98	0.44
1:B:277:GLU:HB3	1:B:283:ALA:HB2	1.99	0.44
1:D:151:ARG:O	1:D:153:TRP:CD1	2.70	0.44
1:D:246:TYR:CE2	1:D:248:GLN:HB2	2.52	0.44
1:A:277:GLU:HB3	1:A:283:ALA:HB2	1.99	0.44
1:C:199:LEU:HD13	1:C:231:GLU:HB3	1.99	0.44
1:B:299:LEU:HA	4:B:1003:EDO:C1	2.43	0.44
1:A:148:GLN:O	1:A:153:TRP:CD1	2.71	0.44
1:A:163:LEU:HD13	1:A:183:ILE:HD13	2.00	0.44
1:A:135:GLY:HA2	2:A:1001:NDP:H1B	2.00	0.44
1:A:143:HIS:O	1:A:147:VAL:HG23	2.17	0.44
1:D:137:GLY:O	1:D:141:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:C	1:A:181:LEU:HD23	2.42	0.44
1:A:62:LEU:HD12	1:A:304:ILE:HG22	2.00	0.44
1:A:64:GLU:OE1	1:A:64:GLU:N	2.49	0.43
1:B:40:GLN:OE1	1:B:301:LEU:HB2	2.18	0.43
1:B:274:ASP:OD1	1:B:274:ASP:C	2.61	0.43
1:D:235:HIS:HB3	1:D:264:HIS:CE1	2.53	0.43
1:B:135:GLY:HA2	2:B:1001:NDP:H1B	1.99	0.43
1:D:208:LEU:O	1:D:233:PRO:HD3	2.18	0.43
1:D:199:LEU:HD13	1:D:231:GLU:HB3	2.00	0.43
1:C:250:THR:N	1:C:251:PRO:CD	2.81	0.43
1:A:22:VAL:HB	1:A:23:PRO:HD3	1.99	0.43
1:B:108:THR:O	1:B:112:THR:OG1	2.31	0.43
1:D:129:ARG:HB3	1:D:154:GLN:HG2	1.99	0.43
1:B:45:LEU:HD12	1:B:56:ILE:HD11	2.00	0.43
1:B:223:SER:HA	2:B:1001:NDP:H1D	2.01	0.43
1:A:103:ASP:OD1	1:A:103:ASP:C	2.61	0.43
1:B:92:SER:HB3	1:B:95:ASN:OD1	2.18	0.43
1:B:116:THR:O	1:B:120:VAL:HG23	2.18	0.42
1:C:151:ARG:HA	1:C:151:ARG:HD3	1.62	0.42
1:D:251:PRO:HA	1:D:257:MET:SD	2.58	0.42
1:B:167:SER:O	1:B:168:PRO:C	2.62	0.42
1:A:159:PHE:HB2	1:A:184:ALA:HB3	2.01	0.42
1:B:31:ARG:HG2	1:B:31:ARG:NH1	2.34	0.42
1:C:261:SER:HA	1:C:266:TRP:O	2.19	0.42
1:B:64:GLU:OE1	1:B:64:GLU:N	2.51	0.42
1:D:29:LEU:HD11	1:D:301:LEU:HB3	2.00	0.42
1:C:151:ARG:HB2	1:C:153:TRP:CZ2	2.54	0.42
1:D:234:PRO:HD2	5:D:1110:HOH:O	2.19	0.42
1:D:222:ILE:O	1:D:224:THR:HG23	2.20	0.42
1:A:137:GLY:O	1:A:141:GLN:HG3	2.20	0.41
1:A:8:ILE:HG23	1:A:12:GLN:HB3	2.02	0.41
1:A:125:PRO:HD3	1:A:288:TYR:CZ	2.55	0.41
1:B:172:ALA:HA	1:B:175:THR:HB	2.01	0.41
1:C:91:MET:CE	1:D:72:THR:HG21	2.50	0.41
1:D:67:VAL:HG12	1:D:99:LEU:HD12	2.02	0.41
1:B:133:ILE:O	1:B:158:LEU:HA	2.20	0.41
1:D:95:ASN:OD1	1:D:95:ASN:C	2.63	0.41
1:D:56:ILE:HG22	1:D:58:TYR:CE1	2.56	0.41
1:A:148:GLN:O	1:A:153:TRP:HD1	2.02	0.41
1:B:89:LEU:CD2	1:B:91:MET:HE2	2.42	0.41
1:B:128:ALA:HB1	1:B:195:ASP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:CD2	1:C:91:MET:HE1	2.51	0.41
1:A:139:VAL:HG11	1:A:222:ILE:HD13	2.02	0.41
1:D:100:LEU:HD21	1:D:102:CYS:HB2	2.01	0.41
1:A:284:GLN:H	1:A:284:GLN:HG2	1.53	0.41
1:B:15:GLU:O	1:B:19:GLN:HG3	2.21	0.41
1:C:180:ARG:HG2	1:C:180:ARG:HH11	1.86	0.41
1:A:268:LYS:C	1:A:270:ALA:N	2.77	0.41
1:A:167:SER:O	1:A:171:LEU:HG	2.20	0.40
1:C:285:ARG:CD	1:C:286:PRO:HD2	2.52	0.40
1:D:111:ARG:HD3	1:D:302:GLU:OE1	2.22	0.40
1:A:149:ASN:OD1	1:A:149:ASN:N	2.52	0.40
1:B:137:GLY:HA3	2:B:1001:NDP:O1N	2.22	0.40
1:D:8:ILE:HG23	1:D:12:GLN:HB3	2.02	0.40
1:A:224:THR:HG22	1:A:297:ILE:HG22	2.02	0.40
1:B:12:GLN:O	1:B:16:LEU:HG	2.22	0.40
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.85	0.40
1:C:129:ARG:NH2	1:C:152:ASP:HB2	2.36	0.40
1:B:278:LEU:HD23	1:B:283:ALA:HB3	2.04	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	304/336 (90%)	292 (96%)	12 (4%)	0	100	100
1	B	310/336 (92%)	301 (97%)	9 (3%)	0	100	100
1	C	287/336 (85%)	279 (97%)	8 (3%)	0	100	100
1	D	302/336 (90%)	286 (95%)	16 (5%)	0	100	100
All	All	1203/1344 (90%)	1158 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	244/267 (91%)	227 (93%)	17 (7%)	14	29
1	B	246/267 (92%)	224 (91%)	22 (9%)	9	20
1	C	233/267 (87%)	212 (91%)	21 (9%)	9	19
1	D	242/267 (91%)	223 (92%)	19 (8%)	11	24
All	All	965/1068 (90%)	886 (92%)	79 (8%)	10	23

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	26	LEU
1	A	45	LEU
1	A	70	VAL
1	A	129	ARG
1	A	138	LYS
1	A	160	SER
1	A	170	THR
1	A	173	GLN
1	A	183	ILE
1	A	193	ASP
1	A	214	SER
1	A	215	LYS
1	A	222	ILE
1	A	282	MET
1	A	285	ARG
1	A	290	ARG
1	B	15	GLU
1	B	24	GLN
1	B	26	LEU
1	B	37	LEU
1	B	70	VAL
1	B	79	GLU
1	B	80	GLN

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Mol	Chain	Res	Type
1	B	106	GLU
1	B	129	ARG
1	B	138	LYS
1	B	160	SER
1	B	170	THR
1	B	173	GLN
1	B	175	THR
1	B	183	ILE
1	B	215	LYS
1	B	282	MET
1	B	284	GLN
1	B	285	ARG
1	B	289	GLN
1	B	290	ARG
1	B	306	LEU
1	C	91	MET
1	C	111	ARG
1	C	118	LEU
1	C	121	ASP
1	C	130	ARG
1	C	145	ARG
1	C	150	LEU
1	C	151	ARG
1	C	160	SER
1	C	180	ARG
1	C	181	LEU
1	C	183	ILE
1	C	214	SER
1	C	215	LYS
1	C	257	MET
1	C	267	ASP
1	C	282	MET
1	C	285	ARG
1	C	290	ARG
1	C	296	SER
1	C	310	LEU
1	D	24	GLN
1	D	70	VAL
1	D	77	VAL
1	D	79	GLU
1	D	83	LEU
1	D	138	LYS

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Mol	Chain	Res	Type
1	D	145	ARG
1	D	160	SER
1	D	175	THR
1	D	180	ARG
1	D	215	LYS
1	D	222	ILE
1	D	228	ARG
1	D	268	LYS
1	D	284	GLN
1	D	285	ARG
1	D	290	ARG
1	D	314	GLN
1	D	315	ARG

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	97	GLN
1	A	314	GLN
1	B	97	GLN
1	B	141	GLN
1	C	27	HIS
1	C	105	HIS
1	D	43	GLN
1	D	97	GLN
1	D	149	ASN

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

10 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	1003	-	3,3,3	1.12	0	2,2,2	0.64	0
3	ARG	A	1002	-	10,11,11	0.64	0	9,13,13	0.63	0
2	NDP	C	1001	-	51,52,52	1.18	6 (11%)	71,80,80	1.58	12 (16%)
4	EDO	A	1003	-	3,3,3	0.41	0	2,2,2	0.24	0
3	ARG	D	1002	-	10,11,11	0.60	0	9,13,13	0.69	0
2	NDP	A	1001	-	51,52,52	1.17	5 (9%)	71,80,80	1.61	12 (16%)
2	NDP	B	1001	-	51,52,52	1.18	6 (11%)	71,80,80	1.56	12 (16%)
2	NDP	D	1001	-	51,52,52	1.18	6 (11%)	71,80,80	1.59	12 (16%)
3	ARG	C	1002	-	10,11,11	0.77	0	9,13,13	0.44	0
3	ARG	B	1002	-	10,11,11	0.81	1 (10%)	9,13,13	0.30	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	1003	-	-	1/1/1/1	-
3	ARG	A	1002	-	-	3/11/11/11	-
2	NDP	C	1001	-	-	8/34/77/77	0/5/5/5
4	EDO	A	1003	-	-	1/1/1/1	-
3	ARG	D	1002	-	-	2/11/11/11	-
2	NDP	A	1001	-	-	9/34/77/77	0/5/5/5
2	NDP	B	1001	-	-	6/34/77/77	0/5/5/5
2	NDP	D	1001	-	-	6/34/77/77	0/5/5/5
3	ARG	C	1002	-	-	1/11/11/11	-
3	ARG	B	1002	-	-	3/11/11/11	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NDP	C5A-C4A	4.58	1.47	1.39
2	D	1001	NDP	C5A-C4A	4.52	1.47	1.39
2	A	1001	NDP	C5A-C4A	4.45	1.47	1.39
2	B	1001	NDP	C5A-C4A	4.45	1.47	1.39
2	B	1001	NDP	C5A-C6A	2.68	1.48	1.41
2	A	1001	NDP	C5A-C6A	2.64	1.48	1.41
2	D	1001	NDP	C5A-C6A	2.61	1.48	1.41
2	C	1001	NDP	C5A-C6A	2.60	1.48	1.41
2	D	1001	NDP	C5A-N7A	-2.37	1.34	1.39
2	A	1001	NDP	C5A-N7A	-2.36	1.34	1.39
2	C	1001	NDP	C5A-N7A	-2.33	1.34	1.39
2	D	1001	NDP	C8A-N7A	2.32	1.36	1.31
2	B	1001	NDP	C5A-N7A	-2.29	1.34	1.39
2	B	1001	NDP	C8A-N7A	2.29	1.36	1.31
2	C	1001	NDP	C8A-N7A	2.28	1.36	1.31
2	A	1001	NDP	C8A-N7A	2.23	1.36	1.31
2	A	1001	NDP	C4A-N9A	-2.10	1.33	1.37
2	B	1001	NDP	C4A-N9A	-2.09	1.33	1.37
2	D	1001	NDP	C4A-N9A	-2.07	1.33	1.37
3	B	1002	ARG	O-C	2.07	1.28	1.22
2	C	1001	NDP	C4A-N9A	-2.07	1.33	1.37
2	D	1001	NDP	C6N-C5N	2.04	1.39	1.33
2	B	1001	NDP	C6N-C5N	2.02	1.39	1.33
2	C	1001	NDP	C6N-C5N	2.01	1.39	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	NDP	C5A-C4A-N3A	-5.57	119.05	126.72
2	B	1001	NDP	C5A-C4A-N3A	-5.54	119.09	126.72
2	C	1001	NDP	C5A-C4A-N3A	-5.52	119.11	126.72
2	A	1001	NDP	C5A-C4A-N3A	-5.46	119.19	126.72
2	B	1001	NDP	N3A-C4A-N9A	4.43	134.69	127.17
2	D	1001	NDP	N3A-C4A-N9A	4.41	134.66	127.17
2	C	1001	NDP	N3A-C4A-N9A	4.40	134.65	127.17
2	A	1001	NDP	N3A-C4A-N9A	4.38	134.62	127.17
2	C	1001	NDP	C2A-N3A-C4A	3.60	120.63	111.83
2	B	1001	NDP	C2A-N3A-C4A	3.60	120.62	111.83
2	D	1001	NDP	C2A-N3A-C4A	3.57	120.54	111.83
2	A	1001	NDP	C2A-N3A-C4A	3.55	120.50	111.83
2	C	1001	NDP	C4A-C5A-N7A	-3.49	106.59	110.58
2	B	1001	NDP	C4A-C5A-N7A	-3.49	106.59	110.58
2	D	1001	NDP	C4A-C5A-N7A	-3.48	106.60	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NDP	C2B-C1B-N9A	-3.44	108.09	113.75
2	A	1001	NDP	C4A-C5A-N7A	-3.43	106.66	110.58
2	D	1001	NDP	C2B-C1B-N9A	-3.25	108.40	113.75
2	C	1001	NDP	N3A-C2A-N1A	-3.25	123.66	128.58
2	B	1001	NDP	N3A-C2A-N1A	-3.23	123.69	128.58
2	A	1001	NDP	N3A-C2A-N1A	-3.19	123.75	128.58
2	D	1001	NDP	N3A-C2A-N1A	-3.17	123.79	128.58
2	B	1001	NDP	C4A-N9A-C8A	3.02	108.91	105.74
2	A	1001	NDP	C4A-N9A-C8A	2.97	108.85	105.74
2	A	1001	NDP	O4B-C1B-N9A	2.95	113.75	108.09
2	C	1001	NDP	C4A-N9A-C8A	2.90	108.78	105.74
2	D	1001	NDP	C4A-N9A-C8A	2.87	108.75	105.74
2	C	1001	NDP	C3D-C2D-C1D	2.78	106.72	101.46
2	C	1001	NDP	C2B-C1B-N9A	-2.74	109.23	113.75
2	B	1001	NDP	C3D-C2D-C1D	2.56	106.31	101.46
2	A	1001	NDP	C5A-N7A-C8A	2.56	107.47	103.45
2	C	1001	NDP	C5A-N7A-C8A	2.55	107.45	103.45
2	B	1001	NDP	C5A-N7A-C8A	2.54	107.45	103.45
2	D	1001	NDP	C5A-N7A-C8A	2.54	107.44	103.45
2	D	1001	NDP	O4B-C1B-N9A	2.53	112.96	108.09
2	D	1001	NDP	C3D-C2D-C1D	2.47	106.14	101.46
2	A	1001	NDP	C3D-C2D-C1D	2.30	105.81	101.46
2	C	1001	NDP	C6A-C5A-N7A	2.23	136.38	132.09
2	B	1001	NDP	C6A-C5A-N7A	2.20	136.33	132.09
2	A	1001	NDP	N9A-C8A-N7A	-2.19	110.83	113.94
2	B	1001	NDP	N9A-C8A-N7A	-2.19	110.83	113.94
2	A	1001	NDP	C6A-C5A-N7A	2.18	136.28	132.09
2	D	1001	NDP	C6A-C5A-N7A	2.17	136.28	132.09
2	C	1001	NDP	O4B-C1B-N9A	2.16	112.24	108.09
2	D	1001	NDP	N9A-C8A-N7A	-2.13	110.92	113.94
2	C	1001	NDP	N9A-C8A-N7A	-2.11	110.94	113.94
2	B	1001	NDP	C2B-C1B-N9A	-2.04	110.39	113.75
2	B	1001	NDP	O4B-C1B-N9A	2.04	112.00	108.09

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NDP	C3D-C4D-C5D-O5D
3	A	1002	ARG	C-CA-CB-CG
3	B	1002	ARG	N-CA-CB-CG
2	B	1001	NDP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	C	1001	NDP	C3D-C4D-C5D-O5D
3	D	1002	ARG	NE-CD-CG-CB
2	A	1001	NDP	O4D-C4D-C5D-O5D
2	C	1001	NDP	C3B-C2B-O2B-P2B
2	C	1001	NDP	O4D-C4D-C5D-O5D
3	C	1002	ARG	NE-CD-CG-CB
2	D	1001	NDP	C3D-C4D-C5D-O5D
2	C	1001	NDP	C1B-C2B-O2B-P2B
2	B	1001	NDP	O4D-C4D-C5D-O5D
2	A	1001	NDP	PN-O3-PA-O5B
3	B	1002	ARG	C-CA-CB-CG
2	A	1001	NDP	C2B-O2B-P2B-O1X
2	D	1001	NDP	O4D-C4D-C5D-O5D
4	B	1003	EDO	O1-C1-C2-O2
2	D	1001	NDP	O4D-C1D-N1N-C2N
2	C	1001	NDP	O4D-C1D-N1N-C2N
2	B	1001	NDP	O4D-C1D-N1N-C2N
2	A	1001	NDP	O4D-C1D-N1N-C2N
2	C	1001	NDP	C2N-C3N-C7N-N7N
2	B	1001	NDP	C2B-O2B-P2B-O1X
2	C	1001	NDP	C2B-O2B-P2B-O1X
2	A	1001	NDP	C2D-C1D-N1N-C2N
2	B	1001	NDP	C2D-C1D-N1N-C2N
3	D	1002	ARG	C-CA-CB-CG
3	A	1002	ARG	NE-CD-CG-CB
2	D	1001	NDP	O4B-C4B-C5B-O5B
3	B	1002	ARG	OXT-C-CA-N
2	C	1001	NDP	PA-O3-PN-O2N
3	A	1002	ARG	OXT-C-CA-N
2	A	1001	NDP	C3B-C2B-O2B-P2B
2	D	1001	NDP	C2D-C1D-N1N-C2N
4	A	1003	EDO	O1-C1-C2-O2
2	A	1001	NDP	O4B-C4B-C5B-O5B
2	A	1001	NDP	PA-O3-PN-O2N
2	D	1001	NDP	PA-O3-PN-O2N
2	B	1001	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 19 short contacts:

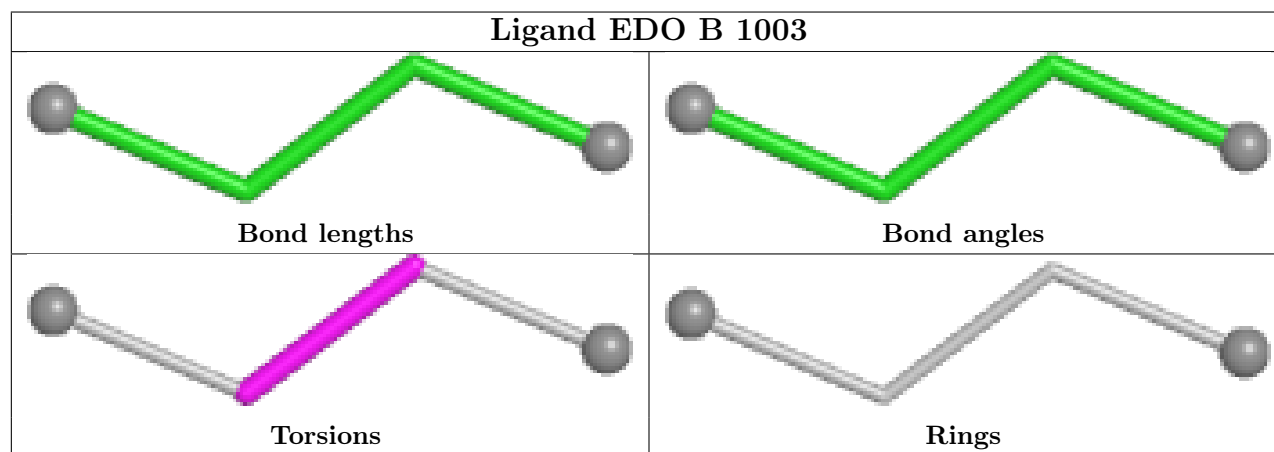
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	EDO	5	0

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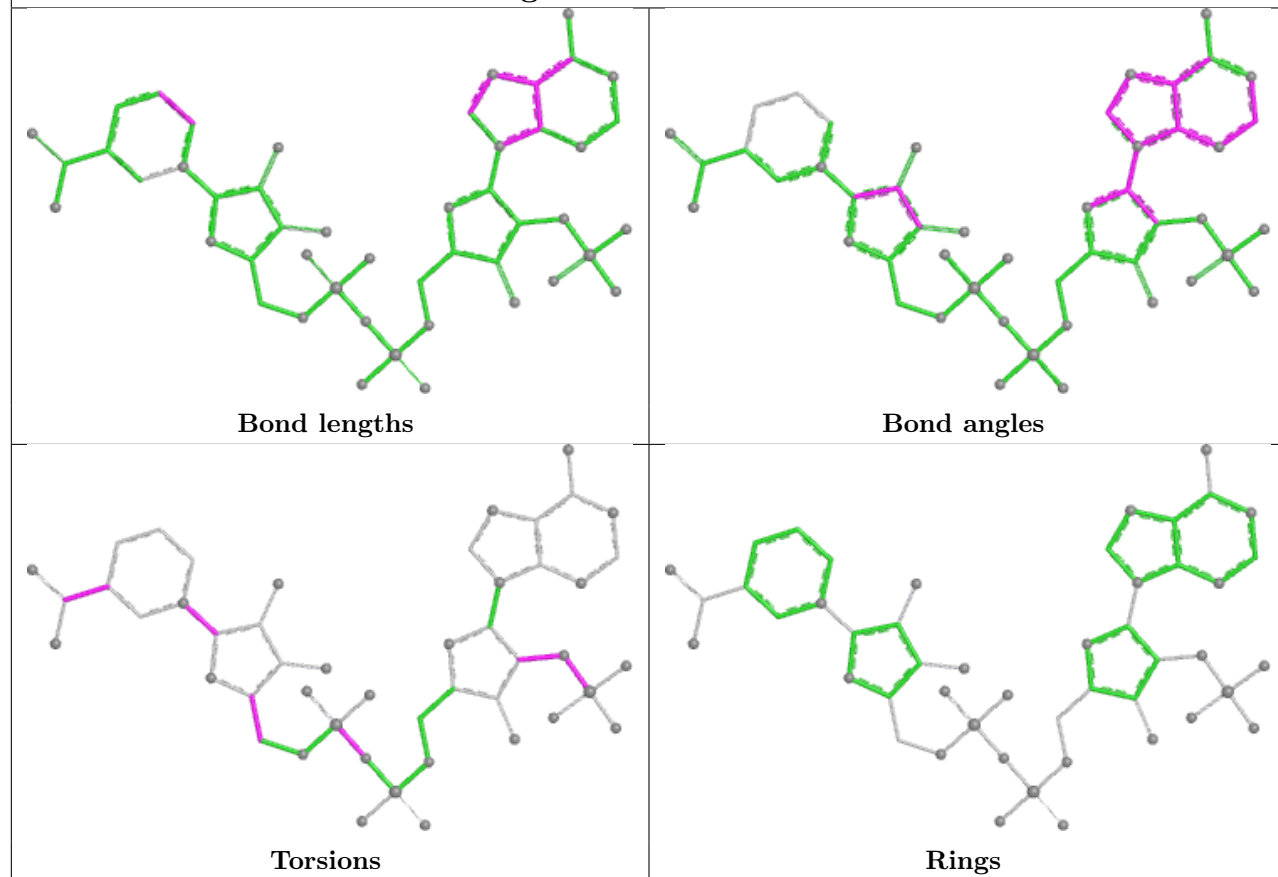
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	NDP	2	0
4	A	1003	EDO	2	0
2	A	1001	NDP	4	0
2	B	1001	NDP	4	0
2	D	1001	NDP	2	0

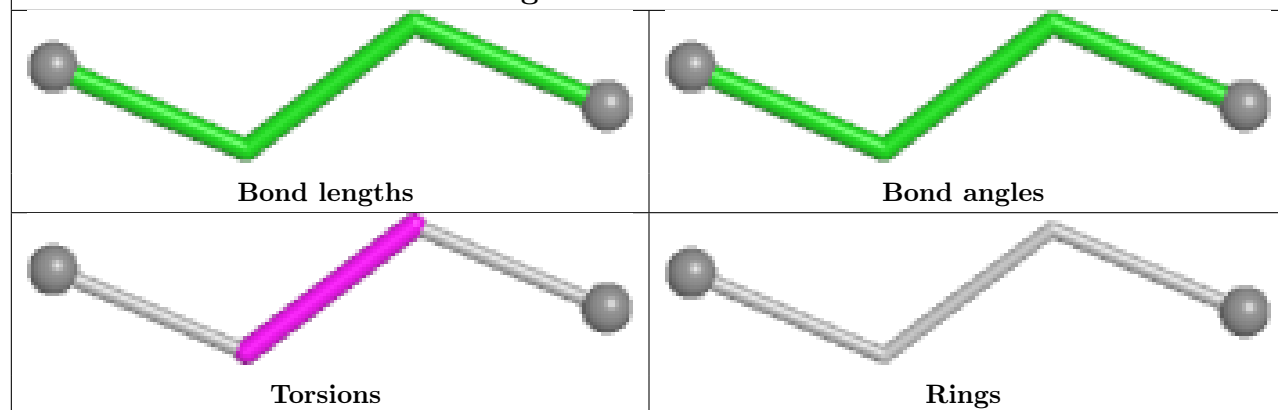
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

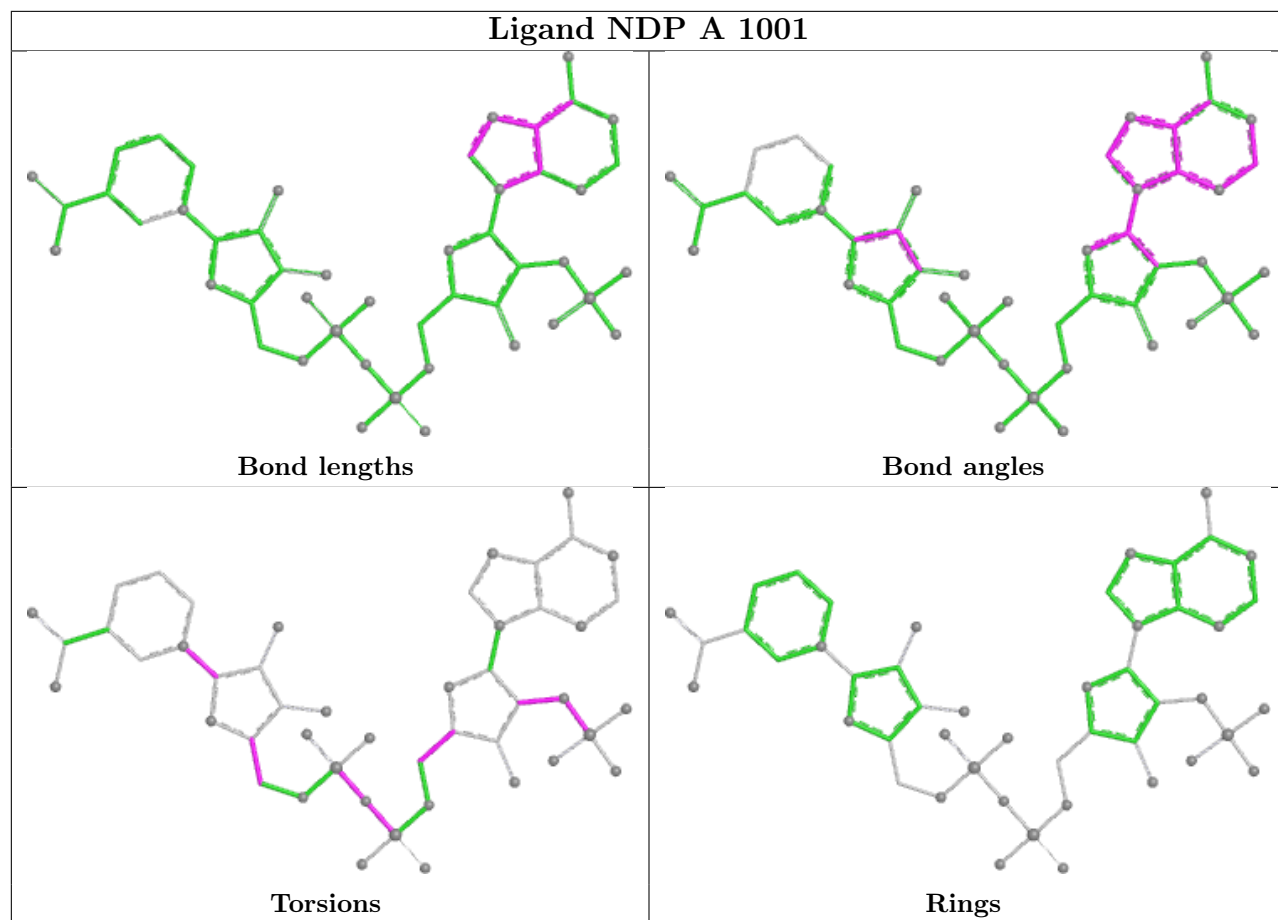


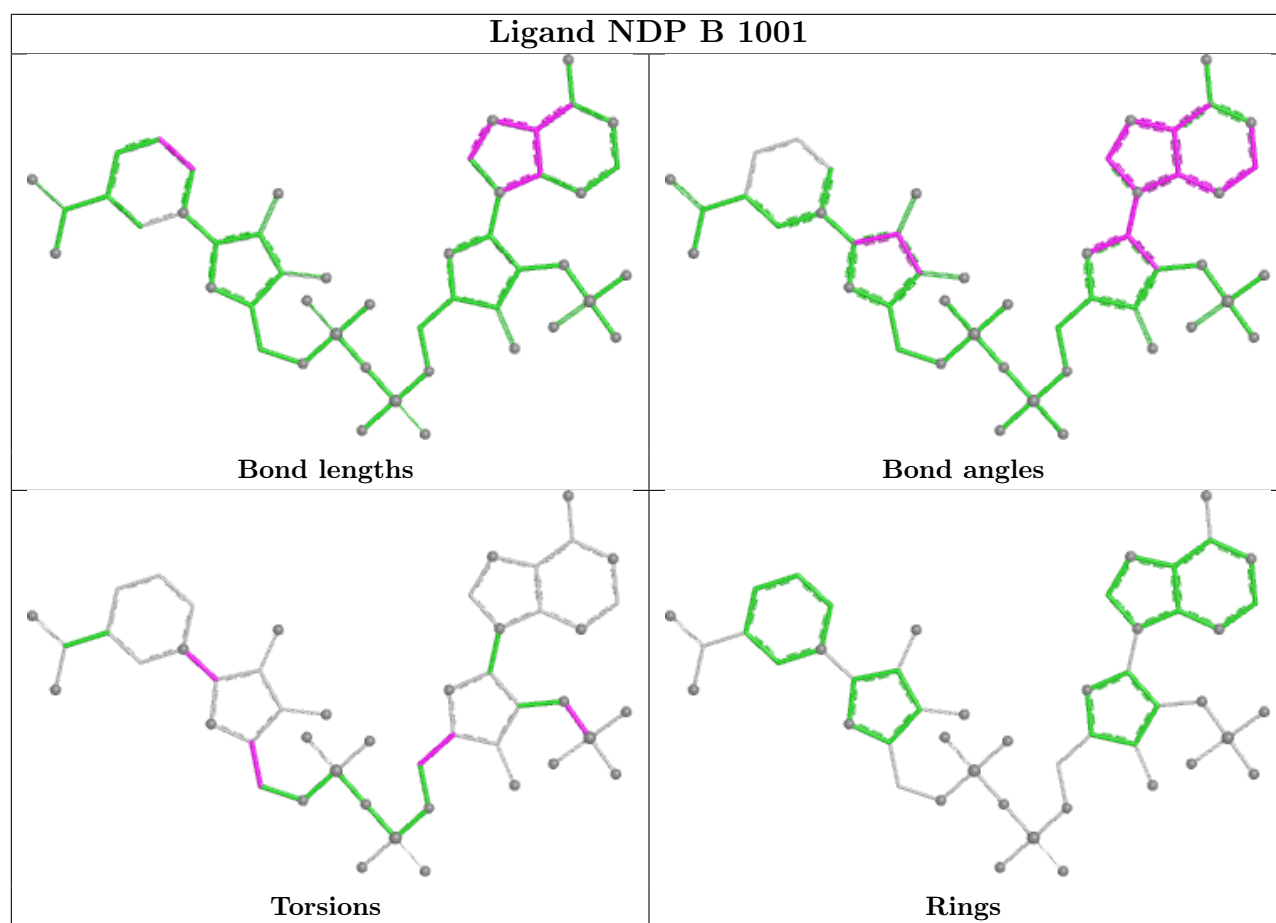
Ligand NDP C 1001

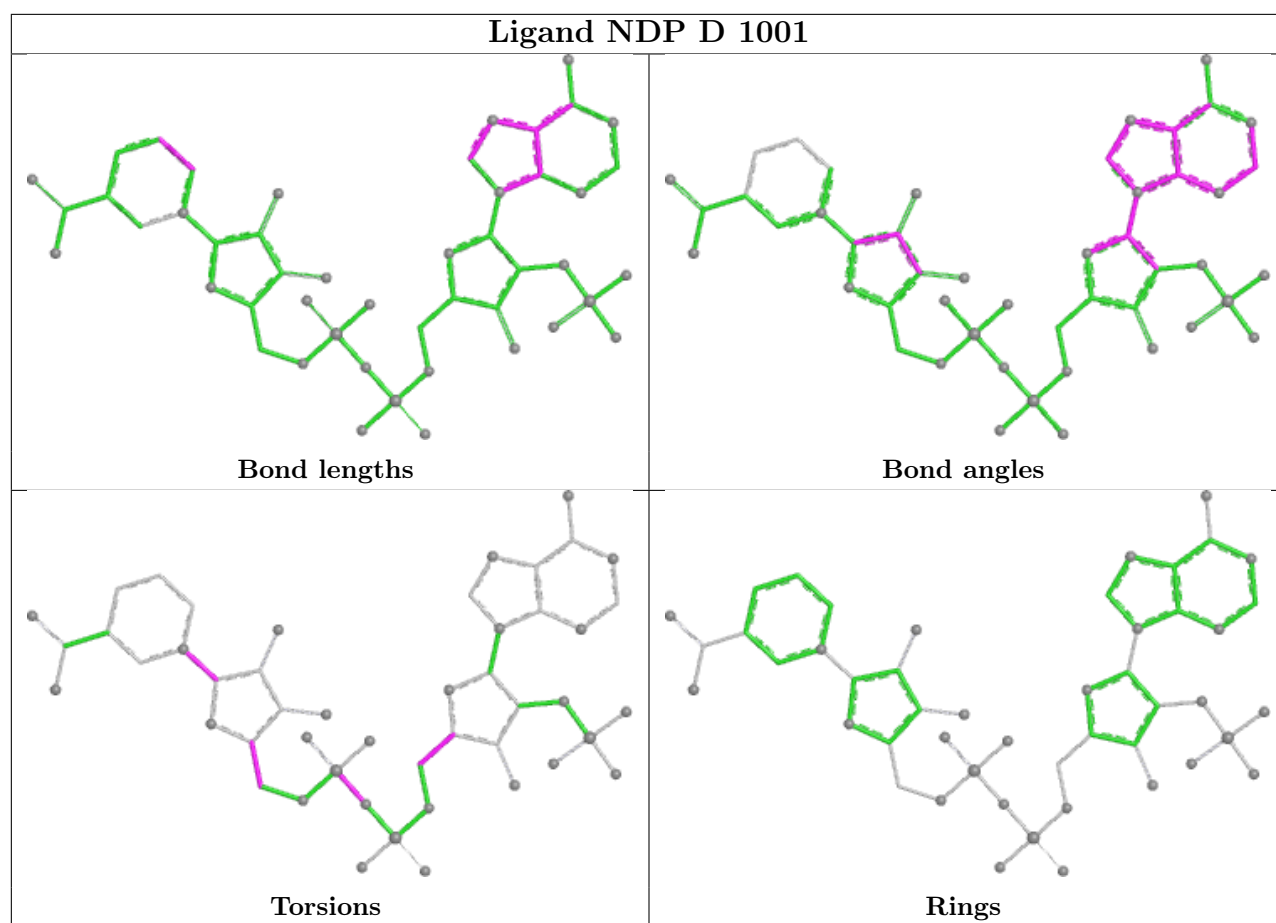


Ligand EDO A 1003









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	308/336 (91%)	0.66	22 (7%) 22 19	47, 66, 105, 146	0
1	B	312/336 (92%)	0.54	17 (5%) 31 27	44, 66, 108, 133	0
1	C	293/336 (87%)	0.99	32 (10%) 10 9	54, 87, 122, 145	0
1	D	306/336 (91%)	1.26	47 (15%) 5 4	56, 96, 135, 167	0
All	All	1219/1344 (90%)	0.86	118 (9%) 13 11	44, 78, 124, 167	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	LEU	4.9
1	D	279	LEU	4.2
1	D	102	CYS	3.9
1	D	172	ALA	3.8
1	A	174	LEU	3.8
1	B	158	LEU	3.8
1	D	171	LEU	3.8
1	C	157	SER	3.8
1	C	147	VAL	3.7
1	D	164	ALA	3.7
1	A	158	LEU	3.7
1	C	181	LEU	3.7
1	C	164	ALA	3.6
1	C	289	GLN	3.6
1	B	169	ALA	3.5
1	D	118	LEU	3.5
1	D	289	GLN	3.5
1	C	82	PRO	3.4
1	D	158	LEU	3.4
1	D	163	LEU	3.3
1	C	127	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	3.3
1	C	158	LEU	3.3
1	A	172	ALA	3.2
1	A	181	LEU	3.1
1	C	150	LEU	3.1
1	D	178	ASP	3.1
1	C	288	TYR	3.0
1	B	284	GLN	2.9
1	A	169	ALA	2.9
1	D	83	LEU	2.9
1	A	285	ARG	2.8
1	A	6	HIS	2.8
1	B	172	ALA	2.8
1	C	285	ARG	2.8
1	A	167	SER	2.7
1	D	175	THR	2.7
1	D	174	LEU	2.7
1	D	34	ALA	2.7
1	A	82	PRO	2.7
1	D	311	TYR	2.7
1	A	127	ALA	2.6
1	C	107	LEU	2.6
1	D	77	VAL	2.6
1	D	147	VAL	2.6
1	C	77	VAL	2.5
1	B	283	ALA	2.5
1	D	47	ALA	2.5
1	C	4	THR	2.5
1	A	157	SER	2.5
1	C	180	ARG	2.5
1	B	282	MET	2.5
1	D	183	ILE	2.4
1	C	313	LEU	2.4
1	D	179	PRO	2.4
1	D	129	ARG	2.4
1	A	170	THR	2.4
1	C	144	LEU	2.4
1	A	282	MET	2.4
1	B	35	ALA	2.4
1	C	11	ALA	2.4
1	C	183	ILE	2.4
1	A	171	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	HIS	2.3
1	D	11	ALA	2.3
1	A	168	PRO	2.3
1	C	298	GLY	2.3
1	D	150	LEU	2.3
1	A	175	THR	2.3
1	D	17	LEU	2.3
1	D	37	LEU	2.3
1	D	107	LEU	2.3
1	B	285	ARG	2.3
1	B	164	ALA	2.2
1	D	25	ILE	2.2
1	C	154	GLN	2.2
1	C	17	LEU	2.2
1	A	287	ASP	2.2
1	C	153	TRP	2.2
1	D	290	ARG	2.2
1	B	168	PRO	2.2
1	D	75	TYR	2.2
1	D	125	PRO	2.2
1	D	131	LEU	2.2
1	A	183	ILE	2.2
1	B	80	GLN	2.1
1	C	163	LEU	2.1
1	B	183	ILE	2.1
1	C	146	TYR	2.1
1	C	281	ASP	2.1
1	D	281	ASP	2.1
1	D	94	HIS	2.1
1	B	181	LEU	2.1
1	C	118	LEU	2.1
1	D	36	GLY	2.1
1	C	143	HIS	2.1
1	A	284	GLN	2.1
1	A	4	THR	2.1
1	D	298	GLY	2.1
1	D	285	ARG	2.1
1	D	214	SER	2.1
1	D	46	VAL	2.1
1	D	139	VAL	2.1
1	D	142	ALA	2.1
1	D	16	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	153	TRP	2.1
1	C	140	ALA	2.0
1	C	89	LEU	2.0
1	D	138	LYS	2.0
1	A	24	GLN	2.0
1	B	315	ARG	2.0
1	C	7	VAL	2.0
1	D	242	VAL	2.0
1	A	164	ALA	2.0
1	C	126	LEU	2.0
1	D	115	THR	2.0
1	B	193	ASP	2.0
1	B	157	SER	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](#)

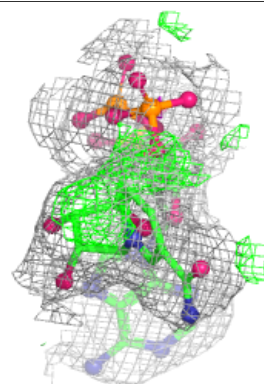
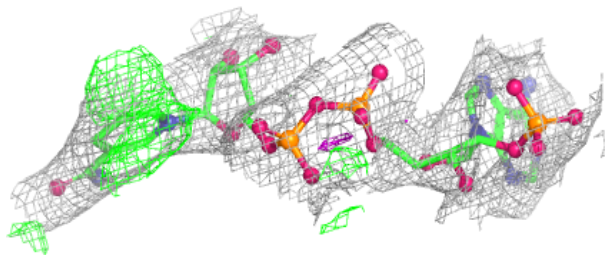
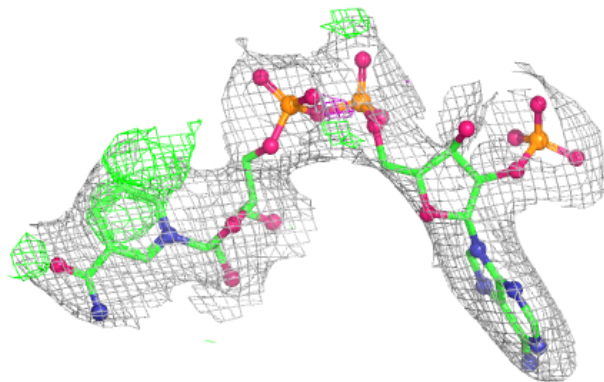
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ARG	C	1002	12/12	0.83	0.17	76,83,92,99	0
2	NDP	D	1001	48/48	0.84	0.13	77,95,111,119	0
2	NDP	C	1001	48/48	0.85	0.13	72,86,99,103	0
3	ARG	B	1002	12/12	0.89	0.13	53,57,65,66	0
3	ARG	D	1002	12/12	0.89	0.13	65,80,84,85	0
3	ARG	A	1002	12/12	0.90	0.12	48,58,60,62	0
2	NDP	B	1001	48/48	0.91	0.11	57,68,78,83	0
2	NDP	A	1001	48/48	0.92	0.10	51,65,79,86	0
4	EDO	A	1003	4/4	0.93	0.16	45,45,45,45	0
4	EDO	B	1003	4/4	0.95	0.15	43,43,43,43	0

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

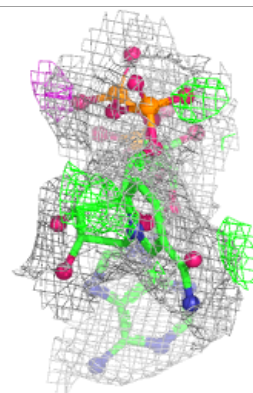
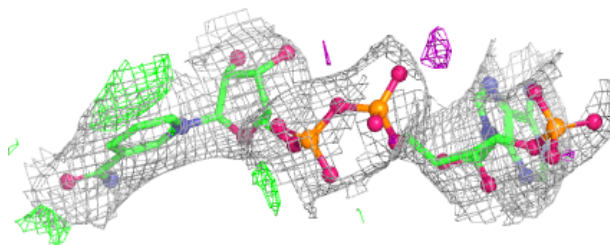
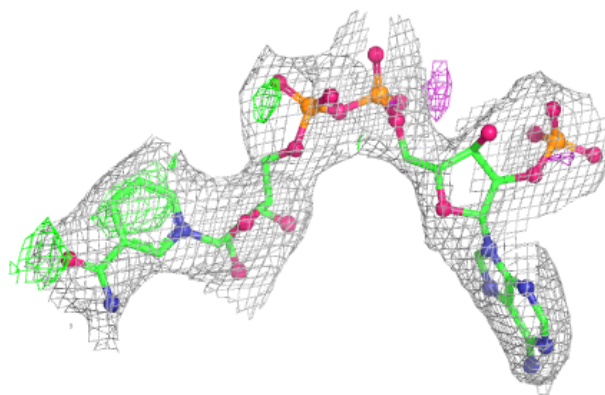
Electron density around NDP D 1001:

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

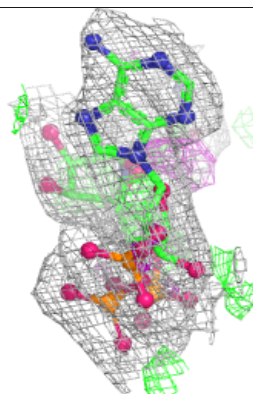
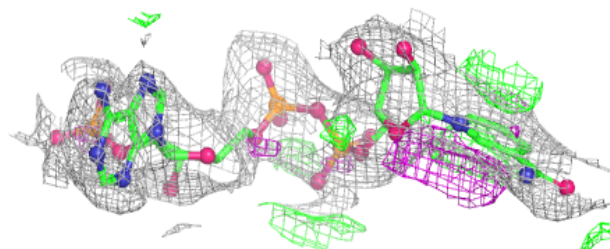
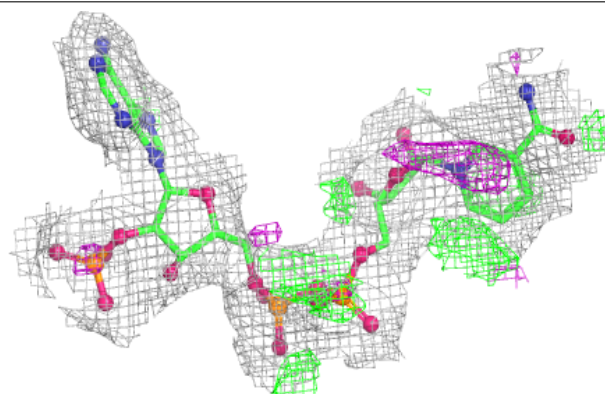


Electron density around NDP C 1001:

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

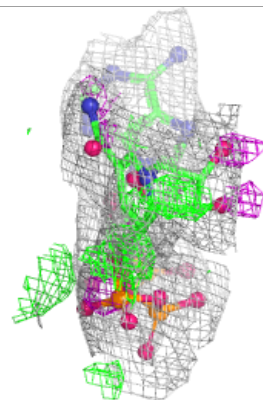
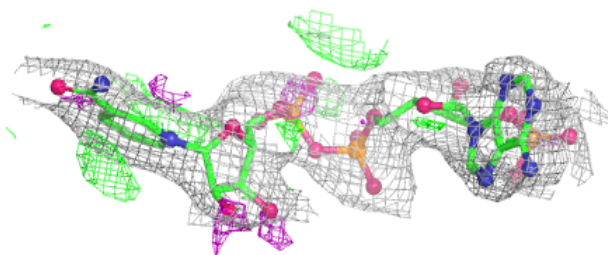
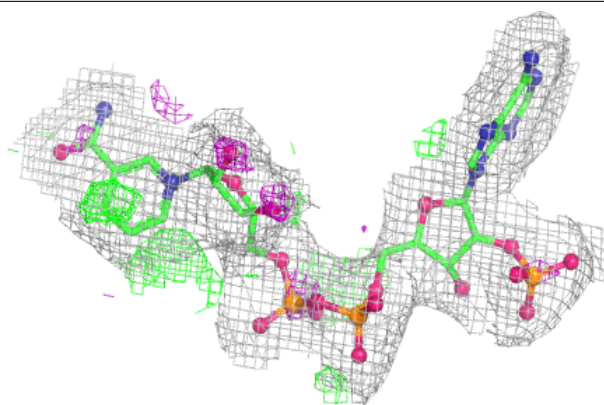
**Electron density around NDP B 1001:**

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



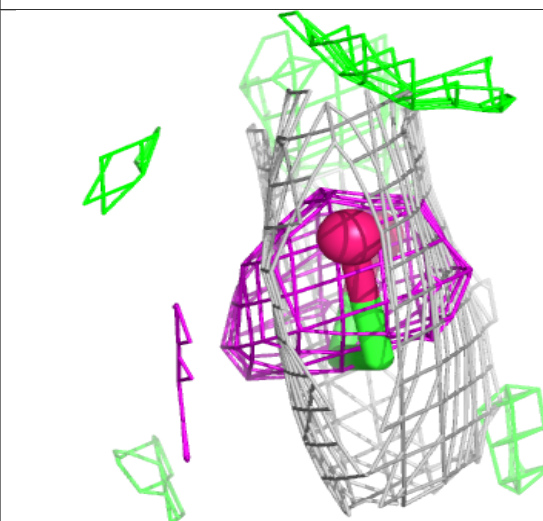
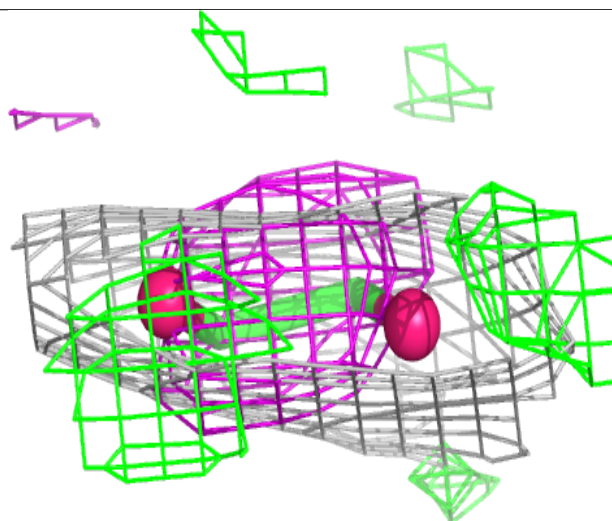
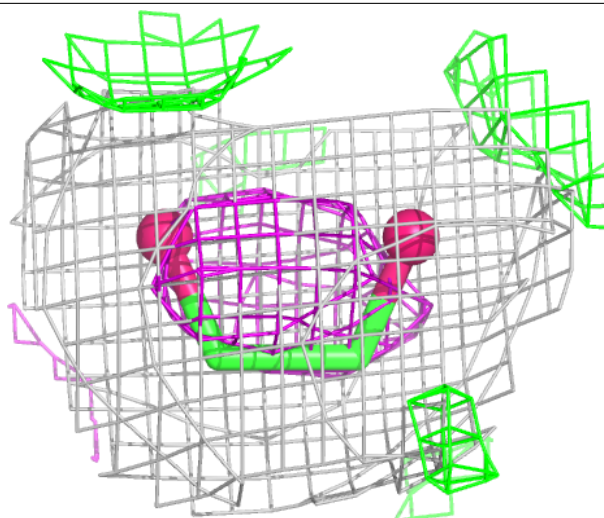
Electron density around NDP A 1001:

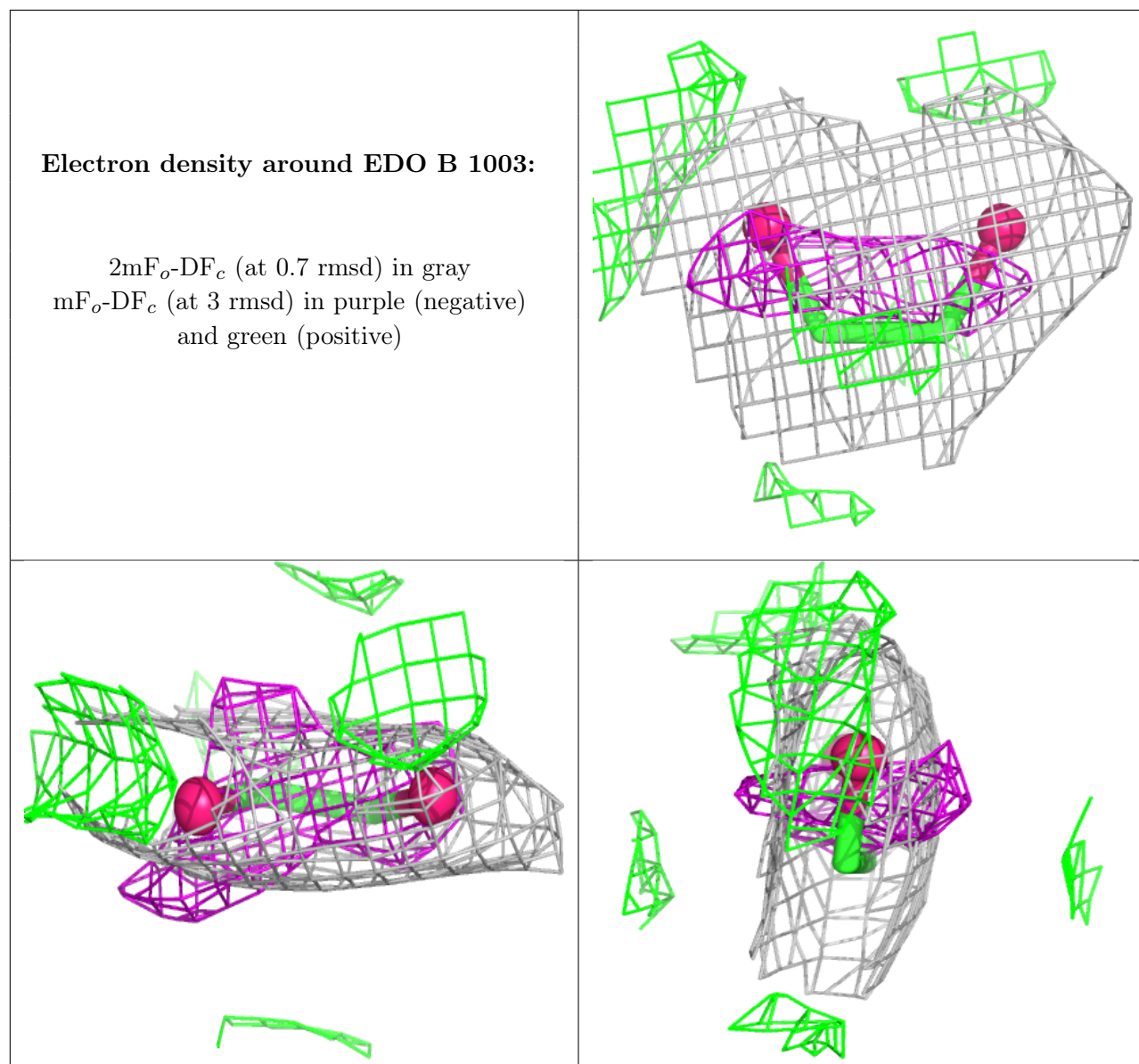
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EDO A 1003:

$2mF_o-DF_c$ (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.