



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:40 PM UTC

PDB ID : 4GAE / pdb_00004gae
Title : Crystal structure of plasmodium dxr in complex with a pyridine-containing inhibitor
Authors : Diao, J.; Xue, J.; Cai, G.; Deng, L.; Song, Y.
Deposited on : 2012-07-25
Resolution : 2.30 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

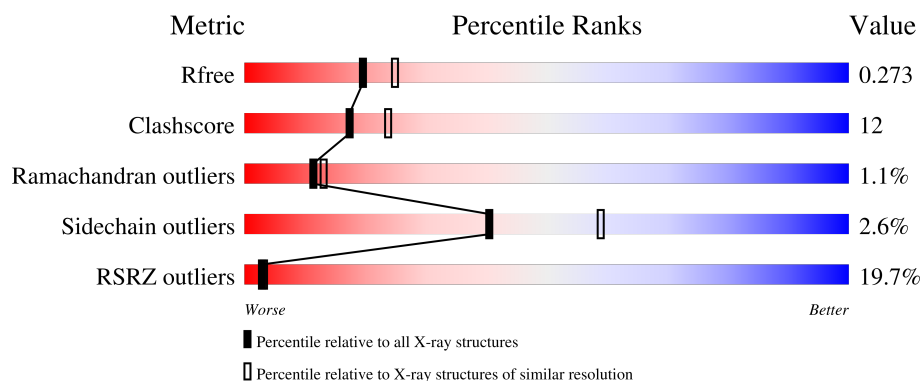
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	426	
1	B	426	

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
8	EDO	A	507	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6931 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3324	2132	549	623	20			
1	B	410	Total	C	N	O	S	0	0	0
			3276	2103	537	616	20			

There are 26 discrepancies between the modelled and reference sequences:

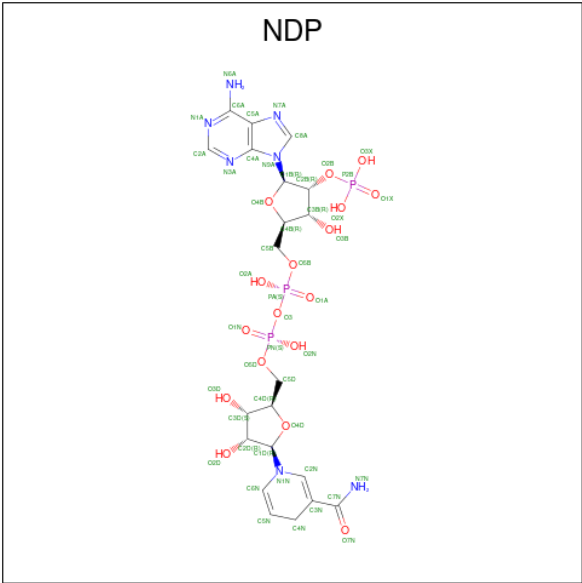
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	expression tag	UNP O96693
A	64	ARG	-	expression tag	UNP O96693
A	65	GLY	-	expression tag	UNP O96693
A	66	SER	-	expression tag	UNP O96693
A	67	HIS	-	expression tag	UNP O96693
A	68	HIS	-	expression tag	UNP O96693
A	69	HIS	-	expression tag	UNP O96693
A	70	HIS	-	expression tag	UNP O96693
A	71	HIS	-	expression tag	UNP O96693
A	72	HIS	-	expression tag	UNP O96693
A	73	GLY	-	expression tag	UNP O96693
A	74	SER	-	expression tag	UNP O96693
A	247	ILE	LEU	engineered mutation	UNP O96693
B	63	MET	-	expression tag	UNP O96693
B	64	ARG	-	expression tag	UNP O96693
B	65	GLY	-	expression tag	UNP O96693
B	66	SER	-	expression tag	UNP O96693
B	67	HIS	-	expression tag	UNP O96693
B	68	HIS	-	expression tag	UNP O96693
B	69	HIS	-	expression tag	UNP O96693
B	70	HIS	-	expression tag	UNP O96693
B	71	HIS	-	expression tag	UNP O96693
B	72	HIS	-	expression tag	UNP O96693
B	73	GLY	-	expression tag	UNP O96693
B	74	SER	-	expression tag	UNP O96693

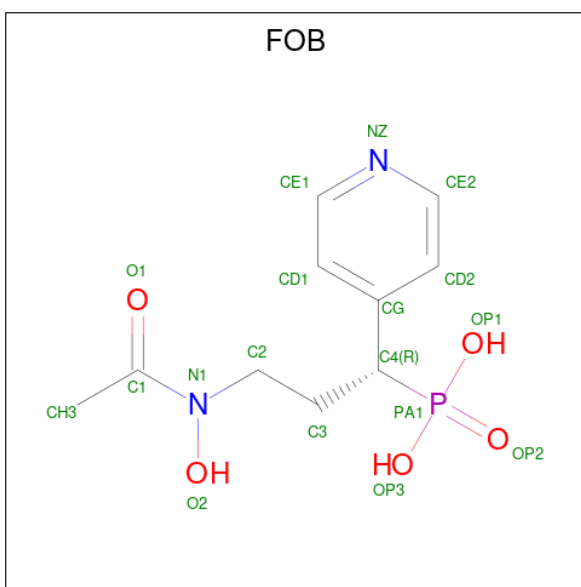
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Chain	Residue	Modelled	Actual	Comment	Reference
B	247	ILE	LEU	engineered mutation	UNP O96693

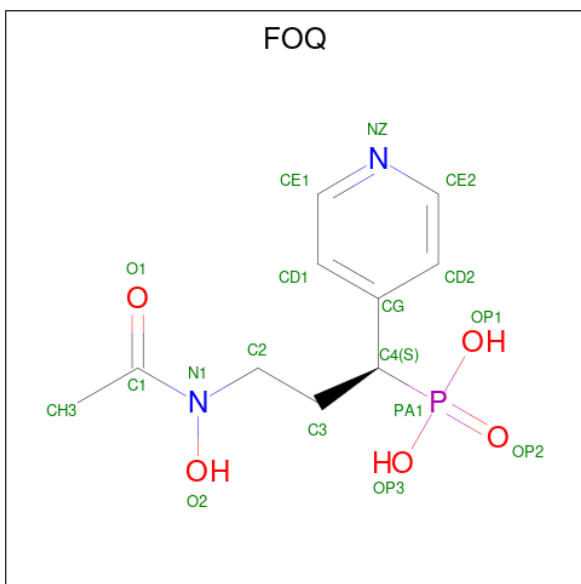
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			18	10	2	5	1		
3	B	1	Total	C	N	O	P	0	1
			18	10	2	5	1		

- Molecule 4 is [(1S)-3-[acetyl(hydroxy)amino]-1-(pyridin-4-yl)propyl]phosphonic acid (CCD ID: FOQ) (formula: C₁₀H₁₅N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			18	10	2	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	1
			18	10	2	5	1		

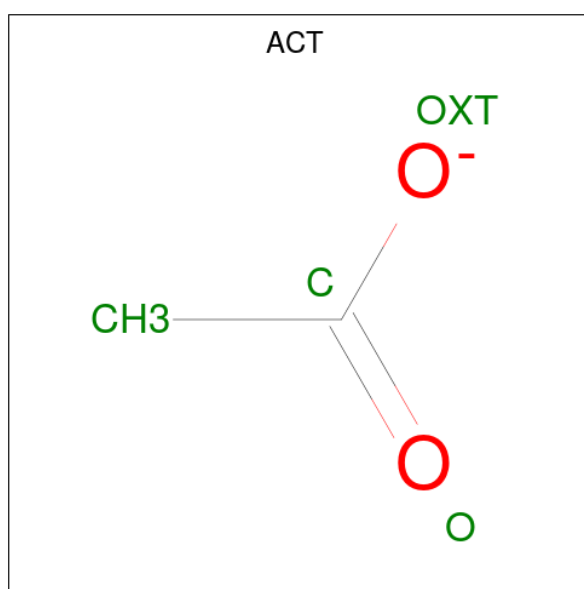
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	3	Total	Mn	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	67	Total	O	0	0
			67	67		
9	B	71	Total	O	0	0
			71	71		

I460	I461	Y462	M463	F464	H465	M466	SER	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.36Å 77.28Å 109.41Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	44.64 – 2.30 44.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.0 (44.64-2.30) 89.1 (44.64-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.29Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.230 , 0.273 0.230 , 0.273	Depositor DCC
R_{free} test set	1698 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6931	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FOB, MN, CL, FOQ, EDO, ACT

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	0.42	0/3389	0.91	6/4575 (0.1%)
1	B	0.46	0/3339	0.93	8/4509 (0.2%)
All	All	0.44	0/6728	0.92	14/9084 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	LEU	N-CA-C	9.65	121.88	111.36
1	A	336	LYS	N-CA-C	7.21	120.01	111.71
1	A	235	SER	N-CA-C	-6.91	103.83	111.36
1	A	310	MET	N-CA-C	-6.67	104.08	111.82
1	B	310	MET	N-CA-C	-6.38	104.75	112.54
1	B	202	LEU	N-CA-C	6.30	118.98	108.96
1	B	223	LYS	N-CA-C	6.29	120.42	112.87
1	B	235	SER	N-CA-C	-6.16	104.64	111.36
1	A	460	SER	N-CA-C	5.99	117.81	111.28
1	B	336	LYS	N-CA-C	5.70	118.26	111.71
1	B	339	ILE	N-CA-C	-5.65	106.31	111.67
1	A	80	VAL	N-CA-C	5.56	117.93	108.86
1	A	228	ILE	N-CA-C	-5.29	101.81	108.05
1	B	118	VAL	N-CA-C	5.27	115.99	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3324	0	3369	98	0
1	B	3276	0	3322	76	0
2	A	48	0	26	3	0
2	B	48	0	26	1	0
3	A	18	0	12	1	0
3	B	18	0	12	0	0
4	A	18	0	12	0	0
4	B	18	0	12	0	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	1	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
8	A	4	0	6	0	0
8	B	8	0	12	0	0
9	A	67	0	0	0	0
9	B	71	0	0	3	0
All	All	6931	0	6815	170	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 12.

All (170) 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:295:LYS:HD2	1:B:358:PRO:HG2	1.36	1.04
1:B:269:SER:HB2	1:B:312:LYS:HE3	1.50	0.92
1:A:165:MET:HE1	1:A:192:TYR:CB	2.12	0.79
1:A:156:PRO:HG2	1:A:158:ILE:HD11	1.65	0.79
1:B:295:LYS:CD	1:B:358:PRO:HG2	2.11	0.78
1:A:165:MET:HE3	1:A:169:CYS:SG	2.25	0.77
1:B:283:LYS:NZ	1:B:283:LYS:HB2	1.98	0.77
1:B:485:HIS:O	1:B:486:ASN:C	2.28	0.77
1:B:269:SER:CB	1:B:312:LYS:HE3	2.16	0.76
1:A:205:LYS:HB3	1:A:205:LYS:HZ3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG11	1:A:140:VAL:HB	1.71	0.72
1:A:340:ILE:HD12	1:A:391:PHE:HZ	1.55	0.71
1:A:243:ASN:O	1:A:247:ILE:HG12	1.92	0.69
1:A:165:MET:HE1	1:A:192:TYR:HB3	1.75	0.69
1:B:274:PHE:CZ	1:B:290:ALA:HB2	2.27	0.69
1:A:135:ILE:HG12	1:A:140:VAL:HG23	1.74	0.68
1:B:264:LYS:HE2	1:B:266:PHE:CE1	2.29	0.67
1:B:283:LYS:HB2	1:B:283:LYS:HZ2	1.57	0.67
1:A:205:LYS:HB3	1:A:205:LYS:NZ	2.10	0.67
1:A:269:SER:HB2	1:A:312:LYS:HE3	1.76	0.67
1:B:165:MET:HE3	1:B:169:CYS:SG	2.35	0.66
1:B:135:ILE:HG12	1:B:140:VAL:HG23	1.78	0.66
1:A:158:ILE:HD12	1:A:158:ILE:N	2.11	0.65
1:A:282:LEU:O	1:A:285:VAL:HG22	1.96	0.65
1:B:397:GLU:HB2	9:B:665:HOH:O	1.97	0.64
1:B:291:LEU:O	1:B:303:THR:HG21	1.98	0.64
1:A:206:GLU:HG3	1:A:420:ASN:HD21	1.63	0.63
1:B:165:MET:HE1	1:B:192:TYR:CB	2.29	0.63
1:A:202:LEU:HD23	1:A:208:ILE:HD11	1.80	0.62
1:A:165:MET:HE1	1:A:192:TYR:HB2	1.80	0.62
1:B:292:LYS:O	1:B:292:LYS:HG2	1.99	0.61
1:B:116:LYS:HA	1:B:135:ILE:HD11	1.81	0.61
1:B:245:LYS:HD3	1:B:259:ILE:O	2.00	0.60
1:B:483:ASN:C	1:B:485:HIS:H	2.09	0.59
1:A:111:ALA:HB2	1:A:132:TYR:HB2	1.83	0.59
1:B:191:MET:O	1:B:195:MET:HG3	2.02	0.59
1:A:72:HIS:NE2	1:A:74:SER:HB3	2.18	0.58
1:A:197:ASN:HA	1:A:225:ALA:HB2	1.85	0.57
1:A:355:MET:HE3	1:B:353:SER:HB3	1.85	0.57
1:A:71:HIS:HB3	1:B:258:LYS:NZ	2.19	0.57
1:A:425:ILE:O	1:A:429:LEU:HD13	2.04	0.57
1:A:86:THR:HG23	1:A:114:VAL:HG11	1.86	0.57
1:A:340:ILE:HD12	1:A:391:PHE:CZ	2.38	0.57
1:A:165:MET:CE	1:A:169:CYS:SG	2.93	0.56
1:A:310:MET:O	1:A:310:MET:HE3	2.04	0.56
1:B:165:MET:HE1	1:B:192:TYR:HB2	1.86	0.56
1:A:114:VAL:HG22	1:A:121:LEU:HD22	1.88	0.56
1:A:403:LYS:HE3	1:A:407:GLN:NE2	2.21	0.56
1:B:118:VAL:HG21	1:B:140:VAL:HB	1.87	0.55
1:B:247:ILE:HD13	1:B:370:TRP:CZ2	2.41	0.55
1:B:251:CYS:O	1:B:252:LEU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ALA:HB1	1:B:475:LYS:HG3	1.88	0.55
1:A:425:ILE:HD11	1:A:475:LYS:HD2	1.86	0.55
1:A:72:HIS:CE1	1:A:74:SER:HB3	2.41	0.55
1:B:197:ASN:HA	1:B:225:ALA:HB2	1.87	0.55
1:B:430:PHE:CG	1:B:440:ILE:HD11	2.42	0.54
1:A:269:SER:CB	1:A:312:LYS:HE3	2.37	0.54
1:A:252:LEU:HA	1:A:321:PHE:O	2.08	0.54
1:B:145:LYS:HG2	1:B:158:ILE:HD12	1.89	0.53
1:B:295:LYS:CE	1:B:358:PRO:HG2	2.38	0.53
1:B:243:ASN:O	1:B:247:ILE:HG12	2.07	0.53
1:B:287:SER:O	1:B:291:LEU:HG	2.07	0.53
1:A:109:VAL:HG21	1:A:128:PHE:HB3	1.92	0.52
1:A:311:ASN:ND2	3:A:502[A]:FOB:H8	2.25	0.52
1:B:165:MET:HE2	1:B:166:LYS:HA	1.92	0.52
1:A:73:GLY:O	1:A:75:LYS:HG3	2.09	0.52
1:A:242:ASP:HB3	1:A:244:ASN:OD1	2.09	0.52
1:A:205:LYS:NZ	1:A:231:ASP:OD2	2.39	0.52
1:B:295:LYS:HE3	1:B:358:PRO:CG	2.40	0.52
1:B:257:SER:HB2	1:B:262:ILE:HB	1.92	0.52
1:A:296:TRP:HZ3	2:A:501:NDP:O7N	1.93	0.51
1:A:135:ILE:HG21	1:A:141:TYR:HA	1.91	0.51
1:A:348:ASP:O	1:A:349:LYS:HB2	2.10	0.51
1:B:264:LYS:HG2	1:B:265:ILE:N	2.25	0.51
1:A:113:TYR:OH	1:A:136:HIS:HD2	1.93	0.51
1:A:264:LYS:HE2	1:A:266:PHE:CZ	2.46	0.51
1:B:266:PHE:HB2	1:B:343:CYS:HB2	1.93	0.51
1:B:442:SER:O	1:B:446:GLN:HG3	2.11	0.51
1:A:420:ASN:O	1:A:424:GLU:HG3	2.11	0.50
1:A:296:TRP:CH2	1:A:360:MET:HG2	2.45	0.50
1:B:80:VAL:HG12	1:B:81:ALA:N	2.27	0.50
1:B:310:MET:HE1	1:B:405:ALA:HB2	1.93	0.50
1:A:141:TYR:HE1	1:A:158:ILE:HG22	1.75	0.50
1:A:109:VAL:HG23	1:A:109:VAL:O	2.11	0.50
1:B:296:TRP:NE1	1:B:298:MET:HG2	2.27	0.50
1:A:156:PRO:HG2	1:A:158:ILE:CD1	2.40	0.49
1:A:75:LYS:HE2	1:A:104:GLU:HG3	1.95	0.49
1:B:296:TRP:HE1	1:B:298:MET:HG2	1.77	0.49
1:A:119:ASN:O	1:A:122:TYR:HB3	2.12	0.49
1:B:264:LYS:HE2	1:B:266:PHE:CZ	2.46	0.49
1:A:114:VAL:HG23	1:A:135:ILE:HD12	1.95	0.48
1:A:359:ASP:OD1	1:A:361:GLN:HG3	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:O	1:B:467:ILE:HG13	2.12	0.48
1:A:176:LYS:HG3	1:A:199:ILE:HB	1.94	0.48
1:A:228:ILE:HG21	1:A:367:SER:HA	1.95	0.48
1:B:458:GLU:HG2	9:B:646:HOH:O	2.13	0.48
1:B:348:ASP:O	1:B:349:LYS:HB2	2.12	0.47
1:A:245:LYS:NZ	6:A:505:CL:CL	2.82	0.47
1:A:93:ALA:O	1:A:96:ILE:HG22	2.14	0.47
1:A:296:TRP:CZ3	2:A:501:NDP:O7N	2.67	0.47
1:B:403:LYS:O	1:B:407:GLN:HG3	2.15	0.47
1:A:266:PHE:HB2	1:A:343:CYS:HB2	1.96	0.47
1:A:165:MET:O	1:A:165:MET:HE2	2.15	0.47
1:A:120:GLU:O	1:A:124:GLN:HG3	2.15	0.46
1:A:464:MET:HE3	1:A:468:LEU:HG	1.97	0.46
1:B:482:TYR:O	1:B:485:HIS:N	2.48	0.46
1:A:144:LEU:O	1:A:148:VAL:HG23	2.16	0.46
1:A:75:LYS:C	1:A:76:LYS:HD2	2.40	0.46
1:B:250:LYS:HG2	9:B:660:HOH:O	2.14	0.46
1:A:310:MET:HE1	1:A:405:ALA:HB2	1.98	0.46
1:A:360:MET:HE2	2:A:501:NDP:H42N	1.98	0.46
1:A:71:HIS:HB3	1:B:258:LYS:HZ2	1.80	0.46
1:A:425:ILE:HD11	1:A:475:LYS:HB3	1.99	0.45
1:B:213:PHE:CE1	1:B:456:VAL:HG11	2.52	0.45
1:B:295:LYS:CE	1:B:358:PRO:CG	2.94	0.45
1:A:304:ILE:HB	1:A:427:ASN:HD21	1.83	0.44
1:B:282:LEU:O	1:B:285:VAL:HG22	2.17	0.44
1:A:115:ASN:ND2	1:A:116:LYS:HG3	2.32	0.44
1:B:295:LYS:HE3	1:B:358:PRO:HG3	2.00	0.44
1:A:206:GLU:HG3	1:A:420:ASN:ND2	2.30	0.44
1:B:143:GLU:O	1:B:147:LEU:HG	2.18	0.44
1:A:230:VAL:O	1:A:231:ASP:C	2.60	0.44
1:A:75:LYS:O	1:A:76:LYS:HD2	2.18	0.44
1:A:356:TYR:CG	1:A:357:TYR:N	2.86	0.43
1:B:141:TYR:CG	1:B:160:CYS:SG	3.11	0.43
1:B:247:ILE:CD1	1:B:370:TRP:CZ2	3.01	0.43
1:B:446:GLN:HB2	1:B:481:ILE:HD13	2.00	0.43
1:B:165:MET:HE2	1:B:165:MET:C	2.43	0.43
1:B:146:GLU:OE2	1:B:146:GLU:HA	2.17	0.43
1:B:282:LEU:HD11	1:B:398:HIS:HB3	2.01	0.43
1:B:340:ILE:HD12	1:B:391:PHE:HZ	1.83	0.43
1:A:106:VAL:HG13	1:A:107:PHE:CD2	2.54	0.43
1:B:113:TYR:OH	1:B:136:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE3	1:B:353:SER:CB	2.48	0.43
1:B:141:TYR:CD1	1:B:160:CYS:SG	3.10	0.43
1:B:254:ASP:O	1:B:255:ASN:HB2	2.19	0.43
1:A:135:ILE:O	1:A:135:ILE:HG23	2.19	0.42
1:A:158:ILE:N	1:A:158:ILE:CD1	2.80	0.42
1:A:233:GLU:H	1:A:233:GLU:CD	2.25	0.42
1:A:446:GLN:HB2	1:A:481:ILE:HD13	2.01	0.42
1:A:214:PHE:HE1	1:A:460:SER:HB2	1.85	0.42
1:B:214:PHE:HE1	1:B:460:SER:HB2	1.85	0.42
1:A:341:HIS:O	1:A:342:SER:CB	2.68	0.42
1:A:97:ILE:HG23	1:A:107:PHE:HB2	2.02	0.42
1:A:430:PHE:CG	1:A:440:ILE:HD11	2.55	0.42
1:A:348:ASP:O	1:A:349:LYS:CB	2.68	0.42
1:A:418:VAL:CG1	1:A:447:VAL:HG12	2.50	0.42
1:B:206:GLU:HG3	1:B:420:ASN:HD21	1.84	0.42
1:A:289:ASN:N	1:A:289:ASN:HD22	2.18	0.41
1:A:296:TRP:CD1	1:A:296:TRP:N	2.88	0.41
1:A:362:ILE:HB	1:A:363:PRO:CD	2.50	0.41
1:A:109:VAL:CG2	1:A:128:PHE:HB3	2.50	0.41
1:B:176:LYS:HG2	1:B:199:ILE:HB	2.02	0.41
1:B:464:MET:O	1:B:464:MET:HE3	2.19	0.41
1:A:287:SER:O	1:A:291:LEU:HG	2.21	0.41
1:A:388:THR:O	1:A:389:LEU:HD23	2.20	0.41
1:B:237:ILE:O	1:B:241:LEU:HG	2.21	0.41
1:B:264:LYS:HG2	1:B:265:ILE:H	1.85	0.41
1:A:164:GLY:O	1:A:168:ILE:HG13	2.20	0.41
1:A:206:GLU:CG	1:A:420:ASN:HD21	2.31	0.41
1:B:194:ILE:HD11	1:B:227:ILE:HD11	2.02	0.41
1:B:360:MET:HE2	2:B:501:NDP:H42N	2.03	0.41
1:A:96:ILE:HG12	1:A:365:LEU:HB2	2.03	0.41
1:B:247:ILE:O	1:B:247:ILE:HG22	2.19	0.41
1:A:158:ILE:HD12	1:A:158:ILE:H	1.84	0.40
1:A:357:TYR:CE2	1:A:381:LEU:HA	2.56	0.40
1:A:86:THR:CG2	1:A:114:VAL:HG11	2.50	0.40
1:A:75:LYS:HD3	1:A:105:ASN:O	2.21	0.40
1:A:426:ALA:HB1	1:A:440:ILE:HG23	2.03	0.40
1:B:227:ILE:HD12	1:B:252:LEU:HD13	2.03	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	414/426 (97%)	385 (93%)	24 (6%)	5 (1%)	10	12
1	B	408/426 (96%)	386 (95%)	18 (4%)	4 (1%)	12	15
All	All	822/852 (96%)	771 (94%)	42 (5%)	9 (1%)	11	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	PRO
1	A	342	SER
1	A	453	SER
1	A	105	ASN
1	B	342	SER
1	B	485	HIS
1	A	161	GLY
1	A	294	PRO
1	B	161	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/391 (98%)	372 (97%)	10 (3%)	40	59
1	B	377/391 (96%)	367 (97%)	10 (3%)	39	58
All	All	759/782 (97%)	739 (97%)	20 (3%)	40	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	139	SER
1	A	158	ILE
1	A	165	MET
1	A	205	LYS
1	A	213	PHE
1	A	216	LYS
1	A	252	LEU
1	A	296	TRP
1	A	372	ASP
1	B	92	ASN
1	B	114	VAL
1	B	163	GLU
1	B	165	MET
1	B	216	LYS
1	B	217	LYS
1	B	252	LEU
1	B	283	LYS
1	B	284	ASN
1	B	292	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	124	GLN
1	A	136	HIS
1	A	172	ASN
1	A	255	ASN
1	A	260	ASN
1	A	289	ASN
1	A	293	HIS
1	A	341	HIS
1	A	407	GLN
1	A	420	ASN
1	A	432	ASN
1	A	433	ASN
1	B	92	ASN
1	B	108	ASN
1	B	136	HIS
1	B	150	ASN

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Mol	Chain	Res	Type
1	B	185	GLN
1	B	197	ASN
1	B	244	ASN
1	B	253	GLN
1	B	255	ASN
1	B	261	ASN
1	B	289	ASN
1	B	407	GLN
1	B	420	ASN
1	B	433	ASN
1	B	452	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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
2	NDP	B	501	-	51,52,52	1.59	9 (17%)	71,80,80	1.68	12 (16%)
7	ACT	A	506	-	3,3,3	1.09	0	3,3,3	0.83	0
7	ACT	B	507	-	3,3,3	1.09	0	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FOB	A	502[A]	5	16,18,18	2.30	5 (31%)	16,25,25	2.62	4 (25%)
2	NDP	A	501	-	51,52,52	1.47	7 (13%)	71,80,80	1.65	12 (16%)
4	FOQ	B	503[B]	5	16,18,18	2.29	6 (37%)	16,25,25	1.65	3 (18%)
8	EDO	B	509	-	3,3,3	0.52	0	2,2,2	0.32	0
4	FOQ	A	503[B]	5	16,18,18	2.21	6 (37%)	16,25,25	1.70	4 (25%)
8	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.35	0
8	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.36	0
3	FOB	B	502[A]	5	16,18,18	2.29	6 (37%)	16,25,25	2.68	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	501	-	-	4/34/77/77	0/5/5/5
3	FOB	A	502[A]	5	-	5/19/19/19	0/1/1/1
2	NDP	A	501	-	-	4/34/77/77	0/5/5/5
4	FOQ	B	503[B]	5	-	3/19/19/19	0/1/1/1
8	EDO	B	509	-	-	0/1/1/1	-
4	FOQ	A	503[B]	5	-	4/19/19/19	0/1/1/1
8	EDO	B	508	-	-	1/1/1/1	-
8	EDO	A	507	-	-	0/1/1/1	-
3	FOB	B	502[A]	5	-	8/19/19/19	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	FOB	PA1-C4	-6.37	1.73	1.81
2	B	501	NDP	O7N-C7N	6.09	1.38	1.24
4	B	503[B]	FOQ	PA1-C4	-5.86	1.73	1.81
3	B	502[A]	FOB	PA1-C4	-5.70	1.74	1.81
2	A	501	NDP	O7N-C7N	5.69	1.37	1.24
4	A	503[B]	FOQ	PA1-C4	-5.64	1.74	1.81
2	B	501	NDP	PA-O3	3.67	1.63	1.59
2	B	501	NDP	C2A-N1A	3.66	1.40	1.33
3	B	502[A]	FOB	O2-N1	3.55	1.42	1.40
4	A	503[B]	FOQ	PA1-OP1	-3.48	1.49	1.54
4	B	503[B]	FOQ	O2-N1	3.46	1.42	1.40
3	A	502[A]	FOB	PA1-OP1	-3.37	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	FOB	PA1-OP3	-3.31	1.49	1.54
2	A	501	NDP	C2A-N1A	3.28	1.39	1.33
4	A	503[B]	FOQ	CG-C4	3.20	1.57	1.52
3	A	502[A]	FOB	CG-C4	3.16	1.56	1.52
3	B	502[A]	FOB	CG-C4	3.16	1.56	1.52
4	B	503[B]	FOQ	CG-C4	3.00	1.56	1.52
2	A	501	NDP	PA-O3	2.97	1.62	1.59
2	B	501	NDP	C2A-N3A	2.96	1.39	1.33
4	B	503[B]	FOQ	PA1-OP3	-2.88	1.50	1.54
2	A	501	NDP	C2A-N3A	2.81	1.38	1.33
3	A	502[A]	FOB	CD2-CG	2.68	1.43	1.39
2	A	501	NDP	C6N-C5N	2.63	1.41	1.33
4	A	503[B]	FOQ	PA1-OP3	-2.60	1.50	1.54
3	A	502[A]	FOB	PA1-OP3	-2.59	1.50	1.54
2	B	501	NDP	C6N-C5N	2.56	1.40	1.33
2	A	501	NDP	C4N-C3N	2.54	1.54	1.50
3	B	502[A]	FOB	CD2-CG	2.51	1.43	1.39
4	B	503[B]	FOQ	CD1-CG	2.48	1.43	1.39
2	B	501	NDP	PN-O3	2.45	1.62	1.59
2	B	501	NDP	C4N-C3N	2.38	1.54	1.50
4	A	503[B]	FOQ	CD1-CG	2.35	1.42	1.39
2	B	501	NDP	C8A-N7A	2.32	1.36	1.31
2	A	501	NDP	C8A-N7A	2.25	1.36	1.31
4	B	503[B]	FOQ	PA1-OP1	-2.16	1.51	1.54
4	A	503[B]	FOQ	CD2-CG	2.13	1.42	1.39
3	B	502[A]	FOB	PA1-OP1	-2.11	1.51	1.54
2	B	501	NDP	C6A-N1A	2.04	1.41	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	FOB	C3-C2-N1	-9.37	98.19	111.36
3	A	502[A]	FOB	C3-C2-N1	-9.03	98.67	111.36
2	B	501	NDP	N3A-C2A-N1A	-6.75	118.37	128.58
2	A	501	NDP	N3A-C2A-N1A	-6.74	118.38	128.58
2	B	501	NDP	N9A-C8A-N7A	-4.36	107.75	113.94
2	A	501	NDP	N9A-C8A-N7A	-4.32	107.80	113.94
4	A	503[B]	FOQ	C3-C2-N1	-4.28	105.35	111.36
4	B	503[B]	FOQ	C3-C2-N1	-4.09	105.62	111.36
2	A	501	NDP	C2A-N3A-C4A	3.73	120.94	111.83
2	B	501	NDP	C2A-N3A-C4A	3.66	120.76	111.83
2	A	501	NDP	C5A-C4A-N3A	-3.41	122.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	C6N-N1N-C2N	3.25	122.80	119.32
2	B	501	NDP	C4A-N9A-C8A	3.17	109.07	105.74
2	B	501	NDP	C3N-C7N-N7N	3.13	123.23	117.67
2	A	501	NDP	C5A-N7A-C8A	3.12	108.36	103.45
2	B	501	NDP	C5A-C4A-N3A	-3.08	122.47	126.72
2	A	501	NDP	C6N-N1N-C2N	2.97	122.50	119.32
2	A	501	NDP	C3N-C7N-N7N	2.97	122.95	117.67
2	B	501	NDP	C5A-N7A-C8A	2.96	108.11	103.45
2	A	501	NDP	O7N-C7N-C3N	-2.94	115.36	120.90
2	B	501	NDP	O7N-C7N-C3N	-2.93	115.39	120.90
2	A	501	NDP	C4A-N9A-C8A	2.88	108.76	105.74
4	B	503[B]	FOQ	CE2-NZ-CE1	2.61	122.83	116.86
3	B	502[A]	FOB	CE2-NZ-CE1	2.59	122.79	116.86
4	A	503[B]	FOQ	CE2-NZ-CE1	2.54	122.67	116.86
2	B	501	NDP	C4A-N9A-C1B	-2.54	120.69	126.63
3	A	502[A]	FOB	CE2-NZ-CE1	2.54	122.66	116.86
2	A	501	NDP	N3A-C4A-N9A	2.47	131.37	127.17
2	B	501	NDP	N3A-C4A-N9A	2.26	131.01	127.17
4	A	503[B]	FOQ	O2-N1-C2	2.22	118.96	113.76
3	A	502[A]	FOB	OP3-PA1-OP1	2.19	113.54	107.58
4	A	503[B]	FOQ	OP3-PA1-OP1	2.16	113.44	107.58
2	A	501	NDP	C4A-N9A-C1B	-2.12	121.68	126.63
4	B	503[B]	FOQ	O2-N1-C2	2.11	118.69	113.76
3	A	502[A]	FOB	CD2-CE2-NZ	-2.06	120.08	123.60
2	B	501	NDP	O3D-C3D-C4D	-2.04	105.22	111.08
3	B	502[A]	FOB	OP3-PA1-OP1	2.02	113.06	107.58
2	A	501	NDP	O3D-C3D-C4D	-2.01	105.32	111.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[A]	FOB	CG-C4-PA1-OP1
8	B	508	EDO	O1-C1-C2-O2
3	B	502[A]	FOB	N1-C2-C3-C4
2	A	501	NDP	O4D-C1D-N1N-C6N
4	A	503[B]	FOQ	C3-C2-N1-C1
2	B	501	NDP	O4D-C1D-N1N-C6N
3	A	502[A]	FOB	C3-C4-PA1-OP2
3	B	502[A]	FOB	C3-C4-PA1-OP2
3	B	502[A]	FOB	CG-C4-PA1-OP2
3	B	502[A]	FOB	CG-C4-PA1-OP3

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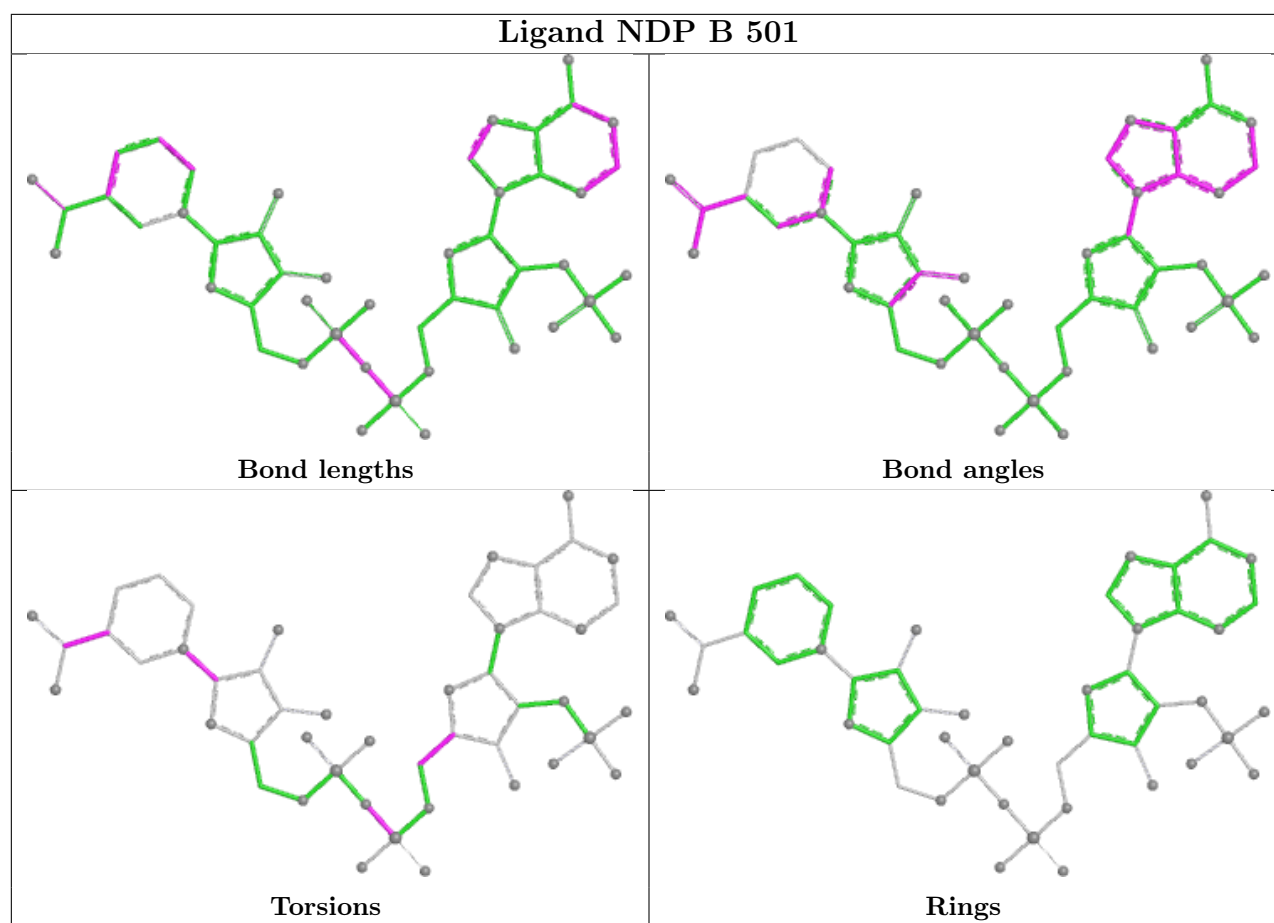
Mol	Chain	Res	Type	Atoms
2	A	501	NDP	PN-O3-PA-O1A
2	A	501	NDP	C2N-C3N-C7N-N7N
2	B	501	NDP	C2N-C3N-C7N-N7N
3	A	502[A]	FOB	N1-C2-C3-C4
2	B	501	NDP	PN-O3-PA-O1A
3	A	502[A]	FOB	CH3-C1-N1-O2
3	B	502[A]	FOB	CH3-C1-N1-O2
4	A	503[B]	FOQ	CH3-C1-N1-O2
4	B	503[B]	FOQ	CH3-C1-N1-O2
4	B	503[B]	FOQ	C3-C2-N1-C1
4	A	503[B]	FOQ	C3-C2-N1-O2
2	B	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	O4B-C4B-C5B-O5B
3	A	502[A]	FOB	O1-C1-N1-O2
3	B	502[A]	FOB	O1-C1-N1-O2
4	A	503[B]	FOQ	O1-C1-N1-O2
4	B	503[B]	FOQ	O1-C1-N1-O2
3	A	502[A]	FOB	CG-C4-PA1-OP2
3	B	502[A]	FOB	C3-C4-PA1-OP1

There are no ring outliers.

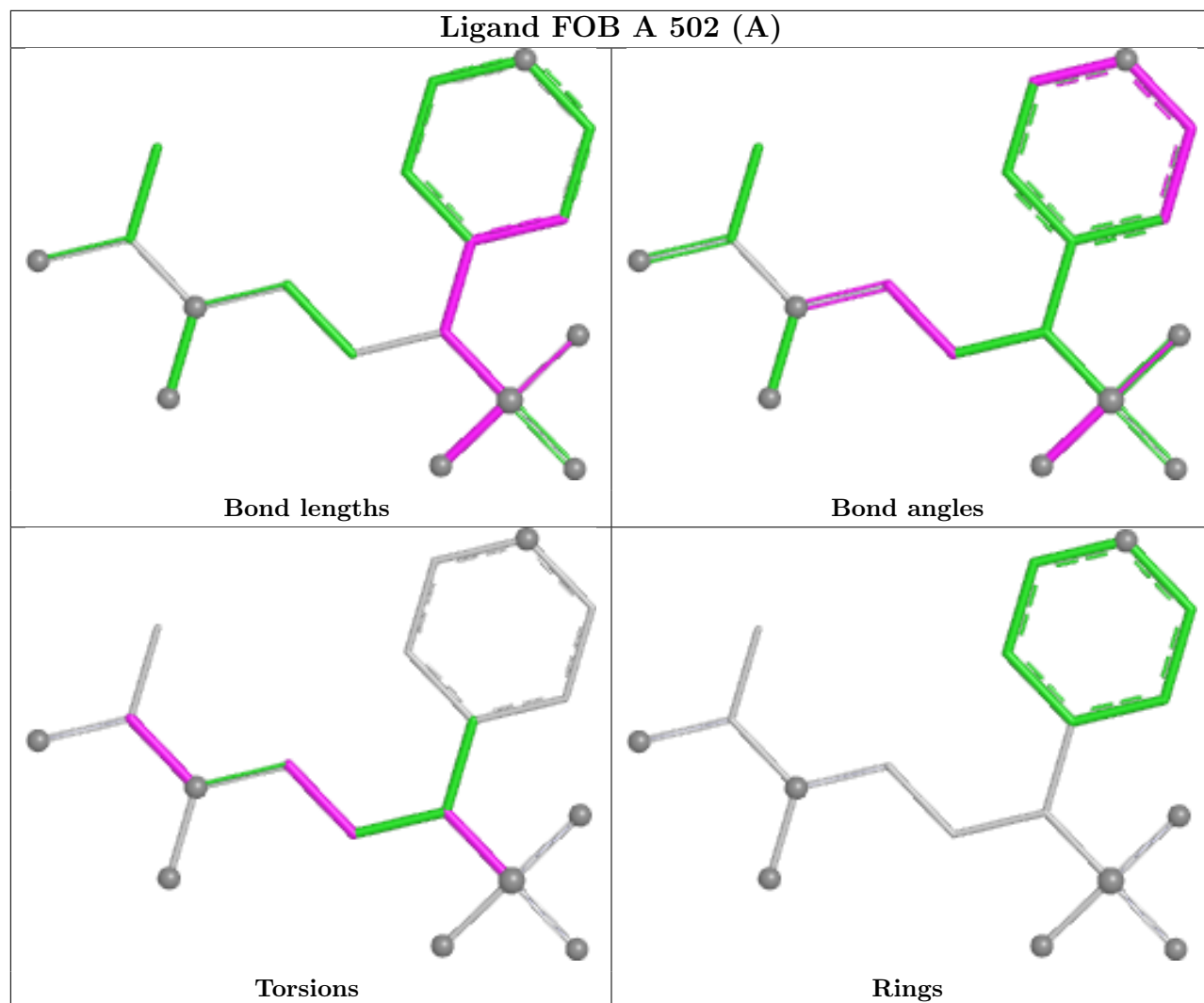
3 monomers are involved in 5 short contacts:

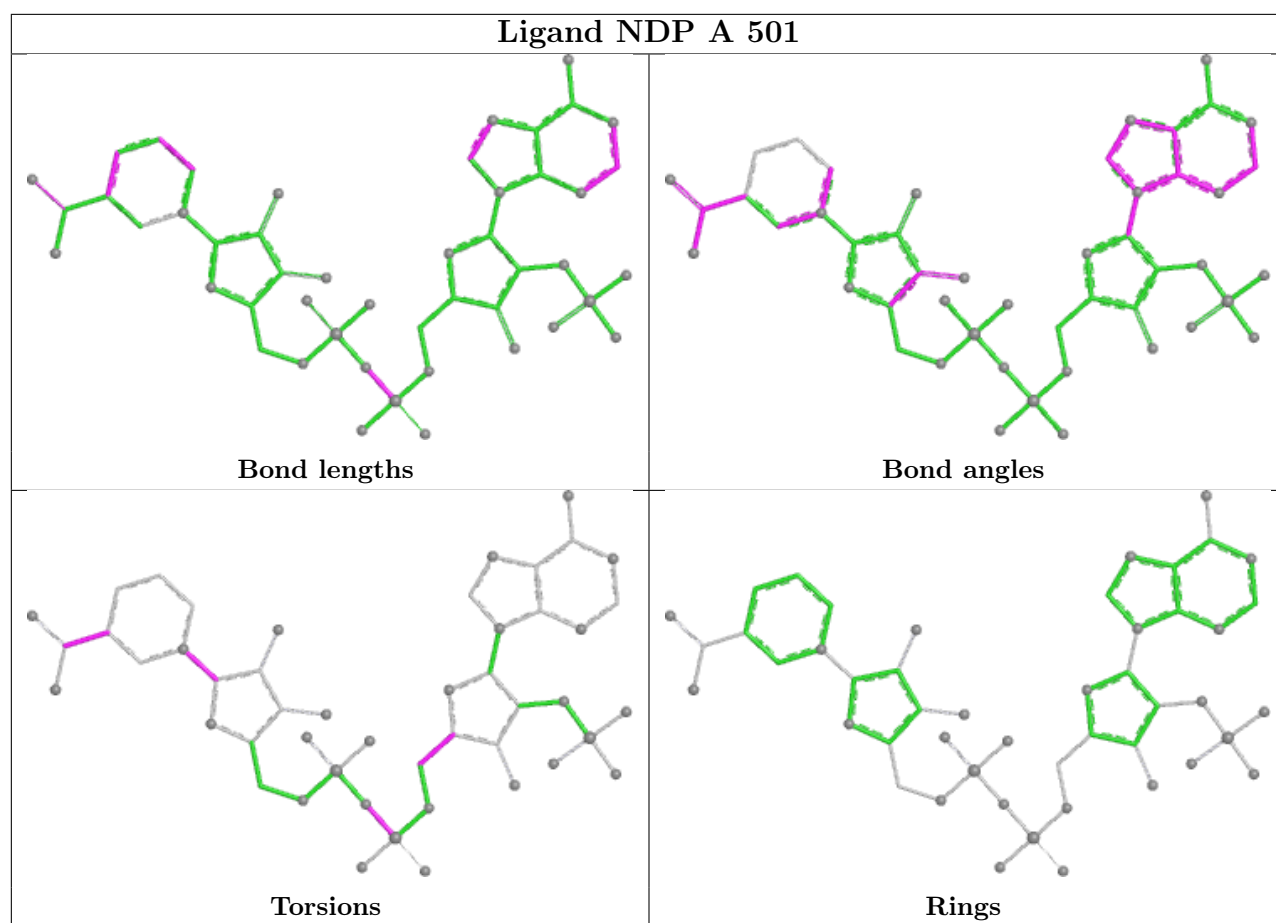
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NDP	1	0
3	A	502[A]	FOB	1	0
2	A	501	NDP	3	0

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.

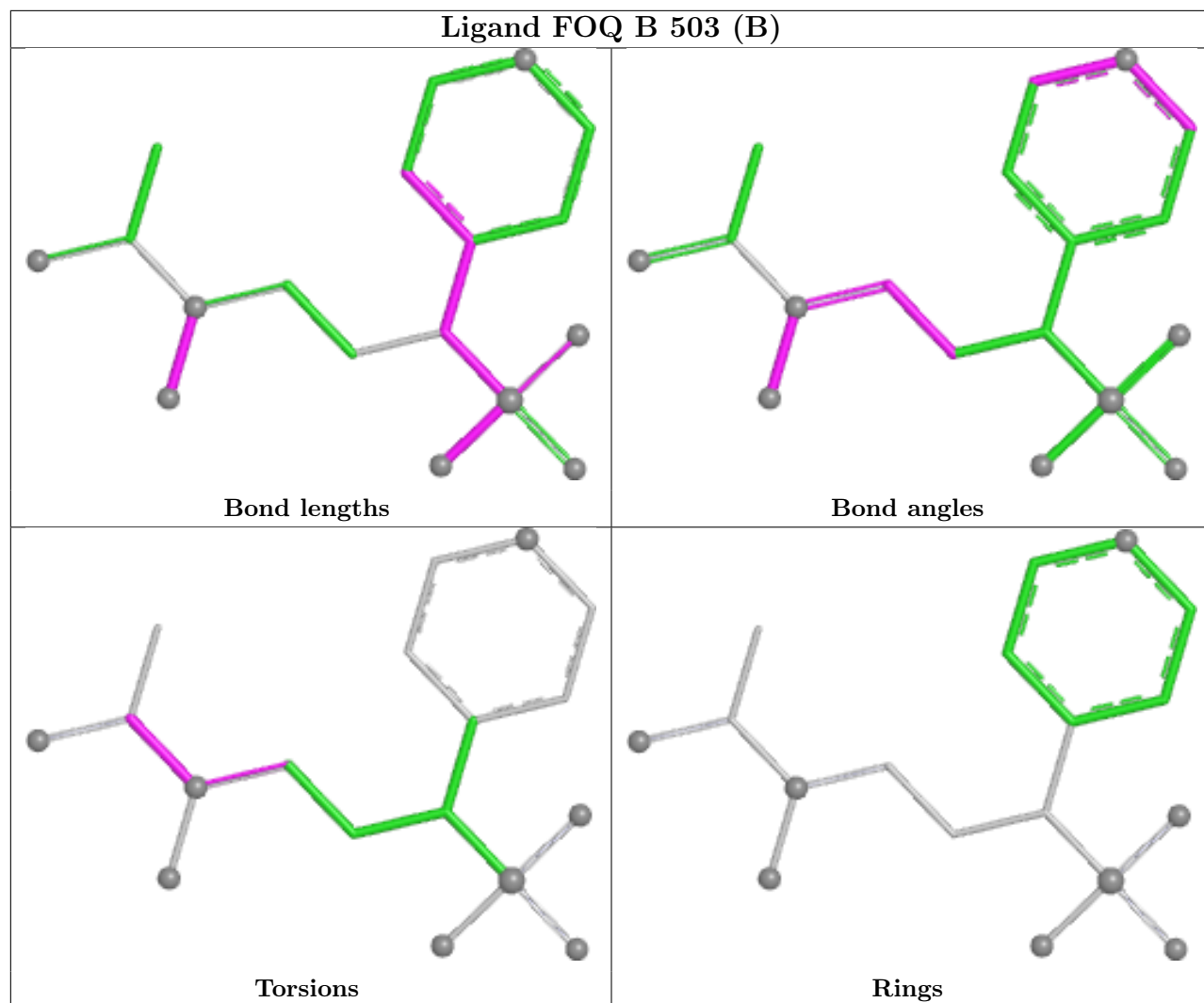


Ligand FOB A 502 (A)

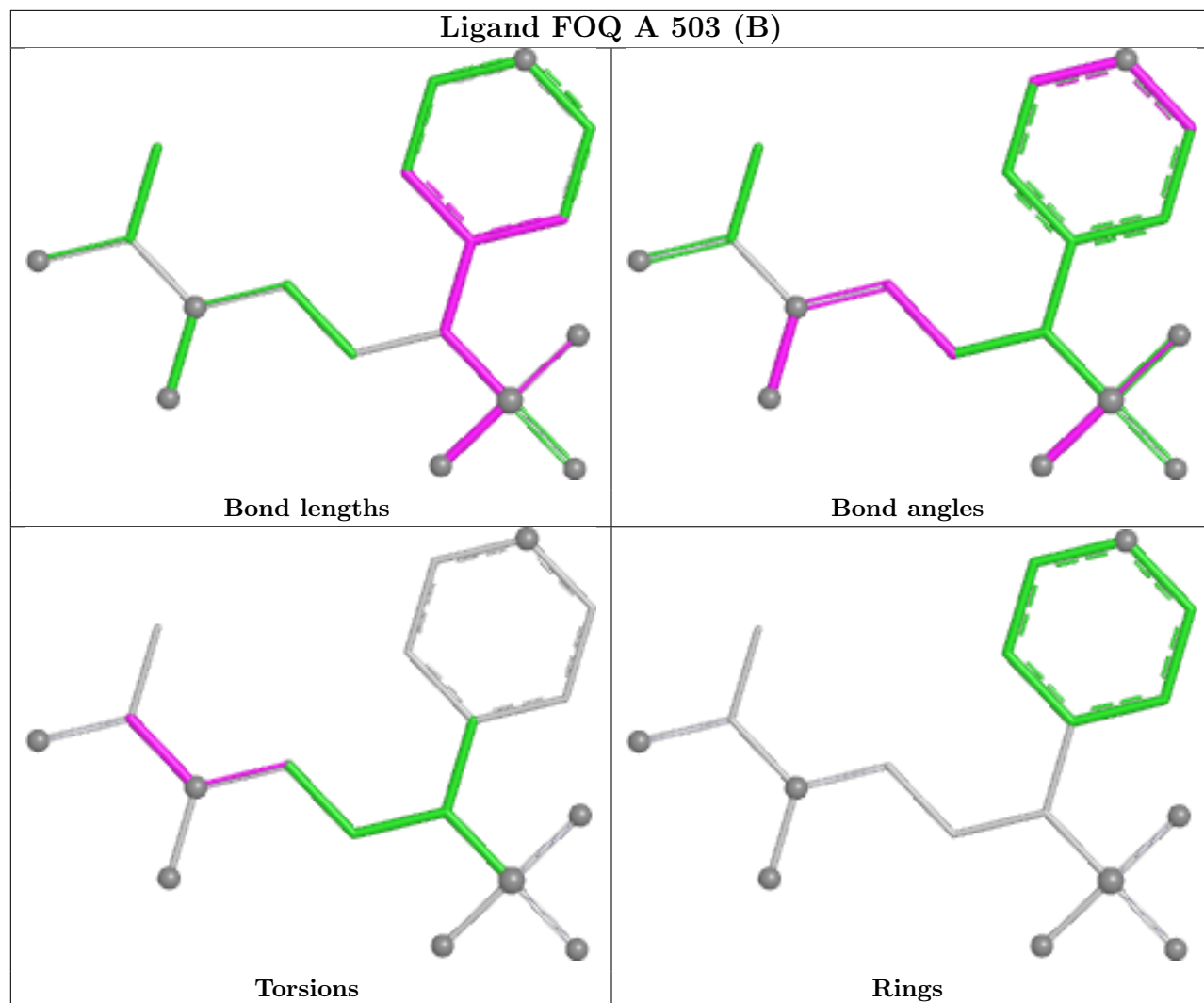


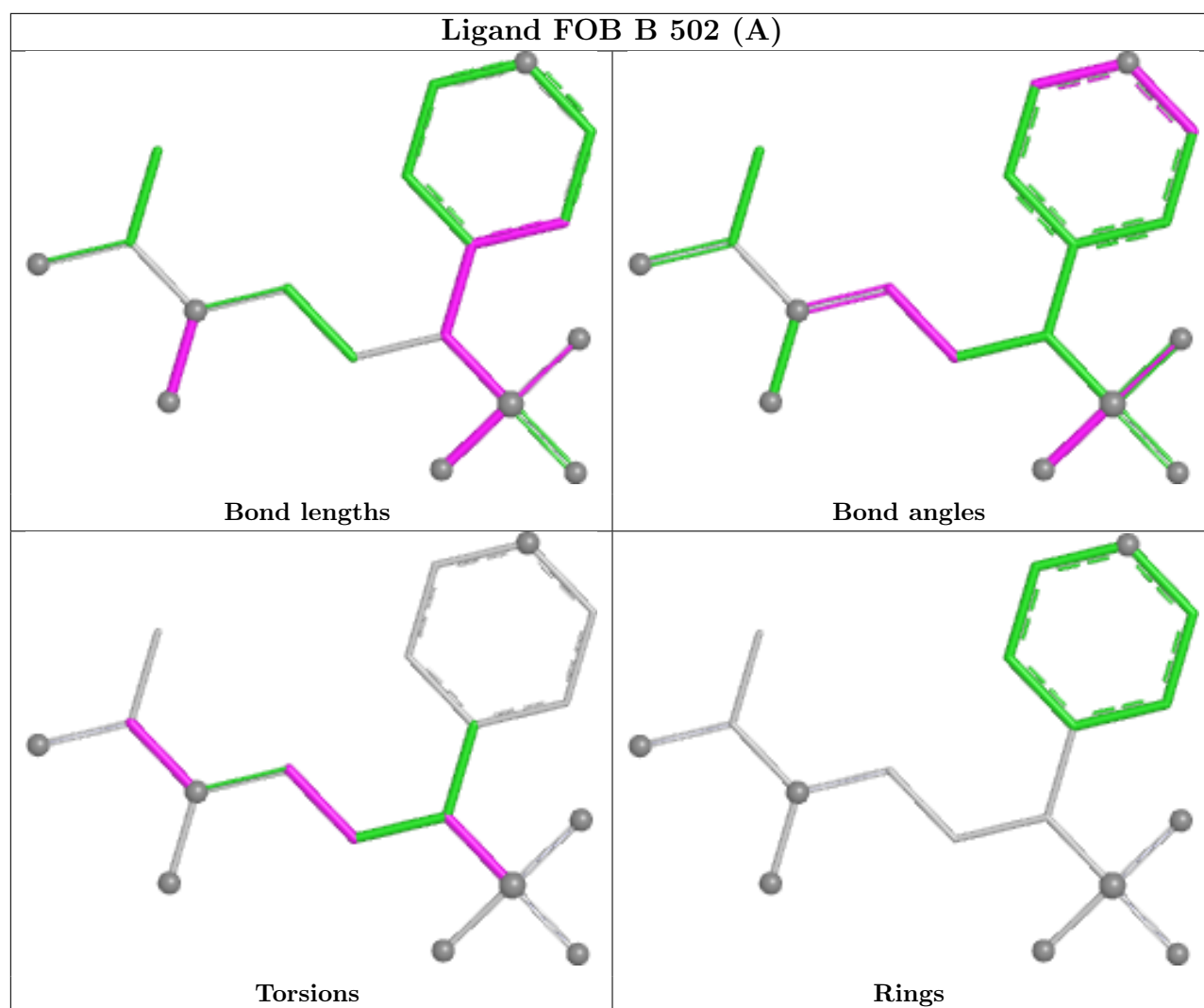


Ligand FOQ B 503 (B)



Ligand FOQ A 503 (B)





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	416/426 (97%)	1.30	97 (23%) 2 2	21, 36, 71, 104	1 (0%)
1	B	410/426 (96%)	0.99	66 (16%) 4 5	18, 30, 54, 98	0
All	All	826/852 (96%)	1.14	163 (19%) 3 3	18, 33, 65, 104	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	LYS	11.1
1	B	291	LEU	10.0
1	A	132	TYR	8.2
1	A	214	PHE	7.2
1	B	294	PRO	7.1
1	A	157	ILE	6.9
1	B	142	GLU	6.9
1	B	158	ILE	6.6
1	A	293	HIS	6.4
1	A	184	PHE	6.2
1	A	158	ILE	6.2
1	B	78	ILE	6.1
1	A	291	LEU	6.1
1	B	274	PHE	5.8
1	B	356	TYR	5.7
1	A	414	PHE	5.6
1	B	79	ASN	5.6
1	A	296	TRP	5.5
1	A	295	LYS	5.3
1	B	277	LEU	5.2
1	A	105	ASN	5.1
1	A	326	ASP	5.1
1	B	295	LYS	5.0
1	B	486	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	173	SER	4.8
1	B	293	HIS	4.8
1	A	77	PRO	4.7
1	A	294	PRO	4.7
1	A	177	ILE	4.6
1	A	408	ALA	4.5
1	B	174	ILE	4.5
1	A	471	HIS	4.5
1	B	296	TRP	4.4
1	B	300	LYS	4.3
1	B	453	SER	4.3
1	A	103	ILE	4.2
1	A	334	VAL	4.2
1	A	269	SER	4.1
1	B	292	LYS	4.1
1	A	119	ASN	4.1
1	B	472	SER	4.0
1	B	475	LYS	4.0
1	A	409	GLY	4.0
1	A	192	TYR	4.0
1	A	133	LEU	3.8
1	A	148	VAL	3.8
1	A	229	PRO	3.8
1	A	82	ILE	3.7
1	B	463	LEU	3.7
1	B	150	ASN	3.7
1	A	111	ALA	3.6
1	A	481	ILE	3.6
1	A	71	HIS	3.6
1	A	144	LEU	3.5
1	A	168	ILE	3.5
1	B	160	CYS	3.5
1	A	279	MET	3.4
1	A	213	PHE	3.4
1	B	184	PHE	3.4
1	B	351	VAL	3.3
1	A	83	PHE	3.3
1	A	465	LYS	3.3
1	A	332	VAL	3.3
1	B	77	PRO	3.3
1	B	345	GLU	3.2
1	A	378	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	ILE	3.2
1	A	375	LYS	3.2
1	A	149	LYS	3.1
1	A	410	ILE	3.1
1	A	140	VAL	3.1
1	B	290	ALA	3.1
1	A	436	LYS	3.1
1	B	233	GLU	3.1
1	A	109	VAL	3.1
1	B	140	VAL	3.1
1	A	143	GLU	3.0
1	A	391	PHE	3.0
1	A	195	MET	3.0
1	A	74	SER	3.0
1	A	146	GLU	2.9
1	A	221	ILE	2.9
1	A	108	ASN	2.9
1	B	359	ASP	2.9
1	A	73	GLY	2.8
1	B	314	LEU	2.8
1	A	128	PHE	2.8
1	A	235	SER	2.8
1	A	331	GLU	2.7
1	B	104	GLU	2.7
1	B	482	TYR	2.7
1	A	116	LYS	2.7
1	A	399	PHE	2.6
1	B	165	MET	2.6
1	A	78	ILE	2.6
1	B	420	ASN	2.6
1	B	250	LYS	2.6
1	B	297	LYS	2.6
1	B	459	ASN	2.5
1	A	286	THR	2.5
1	A	303	THR	2.5
1	A	455	LYS	2.5
1	B	106	VAL	2.5
1	B	193	ALA	2.5
1	A	266	PHE	2.5
1	A	302	ILE	2.5
1	A	112	LEU	2.5
1	A	155	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.5
1	A	418	VAL	2.5
1	A	237	ILE	2.4
1	A	333	ILE	2.4
1	A	188	TYR	2.4
1	B	480	ASP	2.4
1	B	103	ILE	2.4
1	B	418	VAL	2.4
1	A	252	LEU	2.4
1	A	131	GLU	2.4
1	A	151	ILE	2.4
1	B	485	HIS	2.4
1	A	290	ALA	2.4
1	A	313	GLY	2.4
1	A	343	CYS	2.3
1	B	118	VAL	2.3
1	B	471	HIS	2.3
1	A	162	ASP	2.3
1	B	92	ASN	2.3
1	A	85	SER	2.3
1	A	80	VAL	2.3
1	B	161	GLY	2.3
1	A	147	LEU	2.3
1	B	133	LEU	2.3
1	B	149	LYS	2.3
1	B	188	TYR	2.2
1	B	385	GLN	2.2
1	B	276	ASN	2.2
1	B	169	CYS	2.2
1	A	152	LYS	2.2
1	A	278	THR	2.2
1	A	141	TYR	2.2
1	A	208	ILE	2.2
1	B	402	ILE	2.2
1	A	72	HIS	2.2
1	B	111	ALA	2.2
1	A	179	ILE	2.2
1	A	202	LEU	2.2
1	B	96	ILE	2.2
1	A	230	VAL	2.2
1	B	272	GLY	2.2
1	B	147	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	180	GLY	2.1
1	A	97	ILE	2.1
1	A	205	LYS	2.1
1	B	484	LYS	2.1
1	A	239	GLN	2.1
1	B	97	ILE	2.1
1	B	242	ASP	2.1
1	A	124	GLN	2.1
1	A	212	GLY	2.1
1	B	299	GLY	2.1
1	A	106	VAL	2.1
1	B	358	PRO	2.0
1	B	166	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	A	507	4/4	0.43	0.42	78,79,80,80	0
8	EDO	B	509	4/4	0.49	0.34	78,79,79,79	0
7	ACT	B	507	4/4	0.52	0.36	65,67,67,67	0
8	EDO	B	508	4/4	0.66	0.26	64,65,65,65	0
7	ACT	A	506	4/4	0.72	0.28	93,93,94,94	0
3	FOB	A	502[A]	18/18	0.90	0.11	28,35,38,39	18
2	NDP	A	501	48/48	0.90	0.10	30,38,42,42	0
4	FOQ	A	503[B]	18/18	0.91	0.11	26,33,36,37	18
2	NDP	B	501	48/48	0.94	0.08	22,28,30,32	0
3	FOB	B	502[A]	18/18	0.94	0.10	26,30,36,36	18

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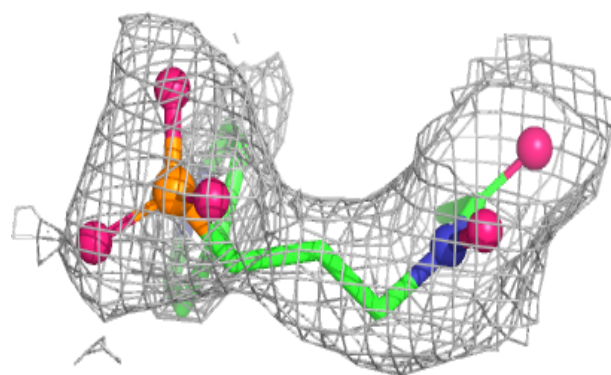
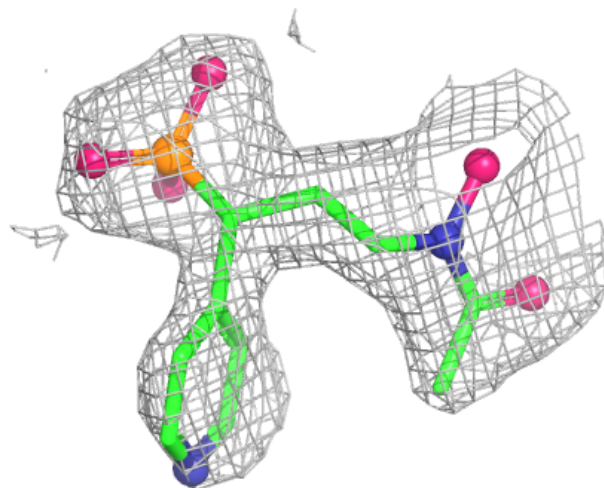
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MN	B	506	1/1	0.95	0.04	49,49,49,49	0
4	FOQ	B	503[B]	18/18	0.95	0.09	20,24,31,31	18
6	CL	A	505	1/1	0.96	0.09	45,45,45,45	0
5	MN	B	505	1/1	0.97	0.04	40,40,40,40	0
5	MN	A	504	1/1	0.99	0.07	26,26,26,26	0
5	MN	B	504	1/1	0.99	0.02	24,24,24,24	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.

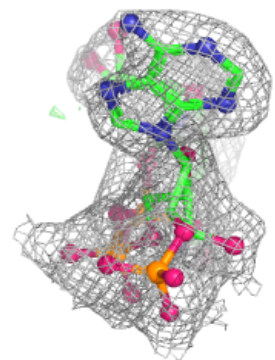
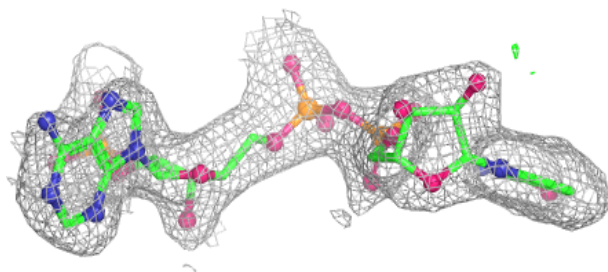
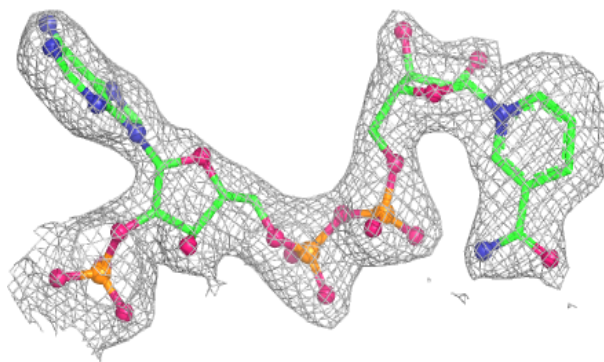
Electron density around FOB A 502 (A):

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



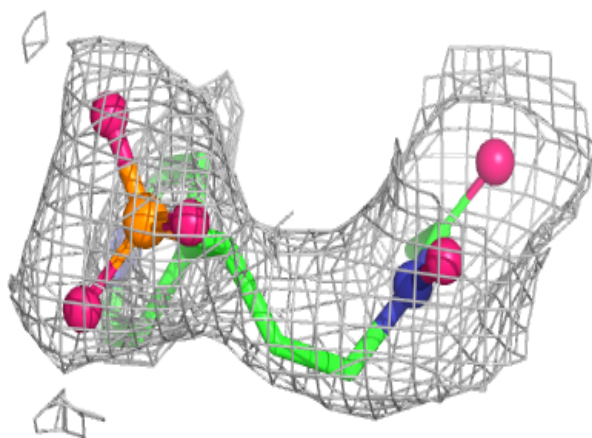
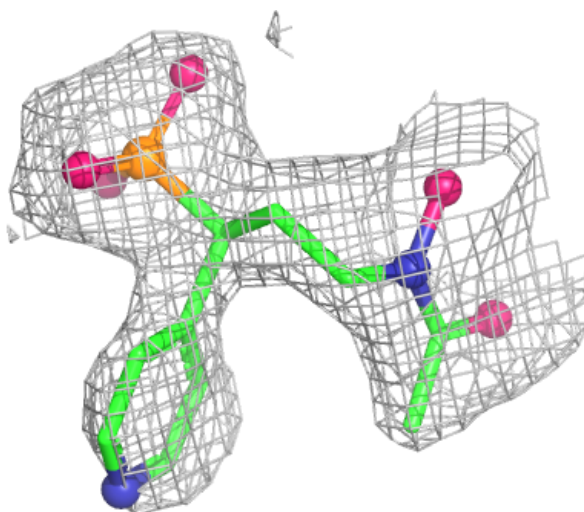
Electron density around NDP A 501:

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



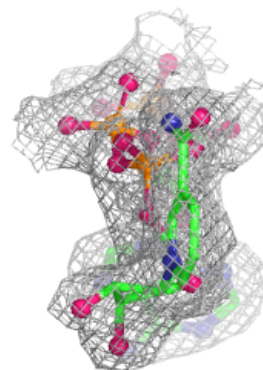
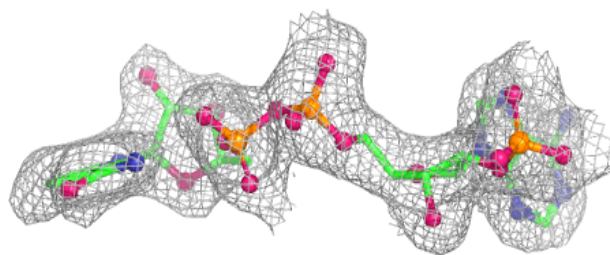
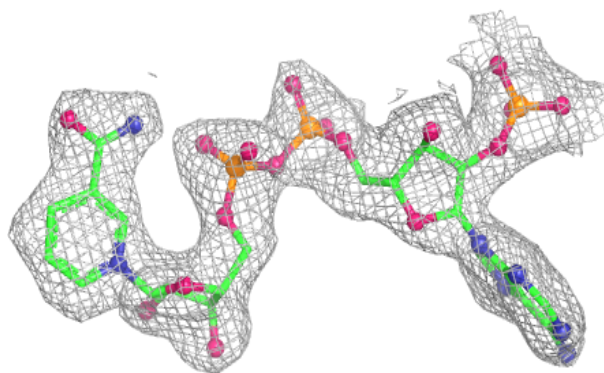
Electron density around FOQ A 503 (B):

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



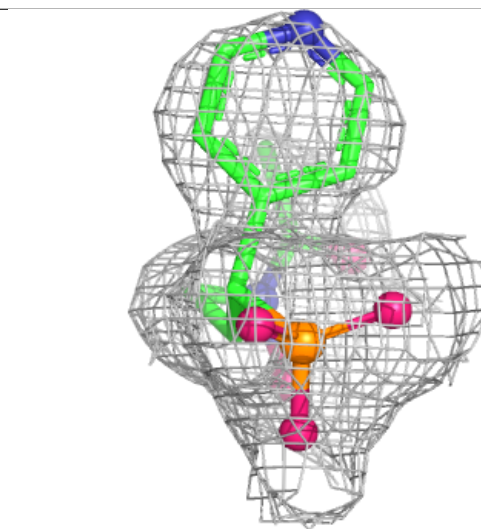
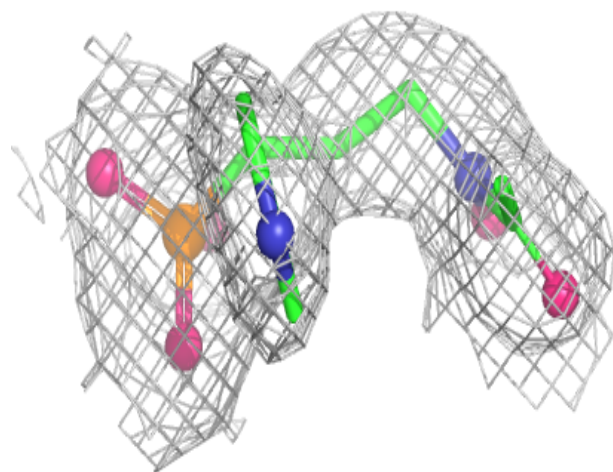
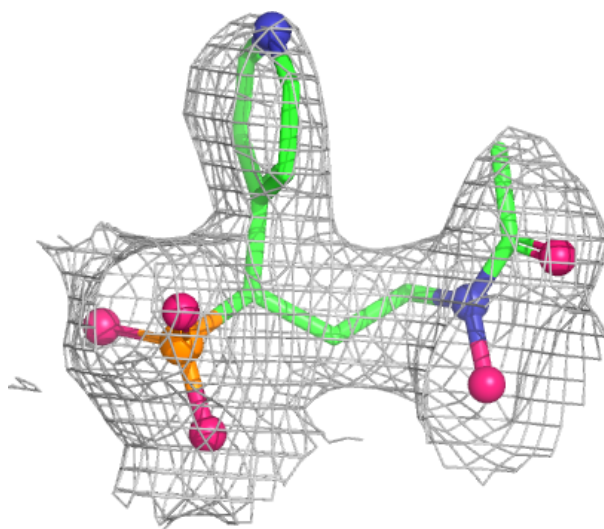
Electron density around NDP B 501:

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



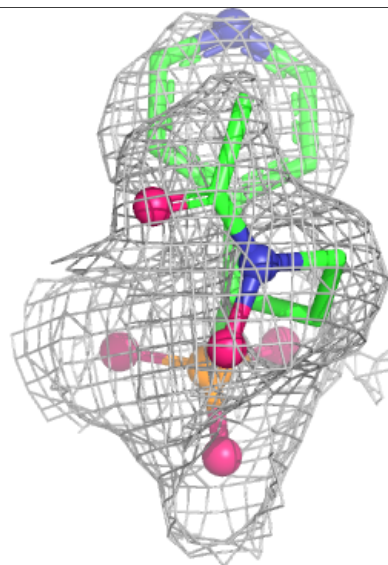
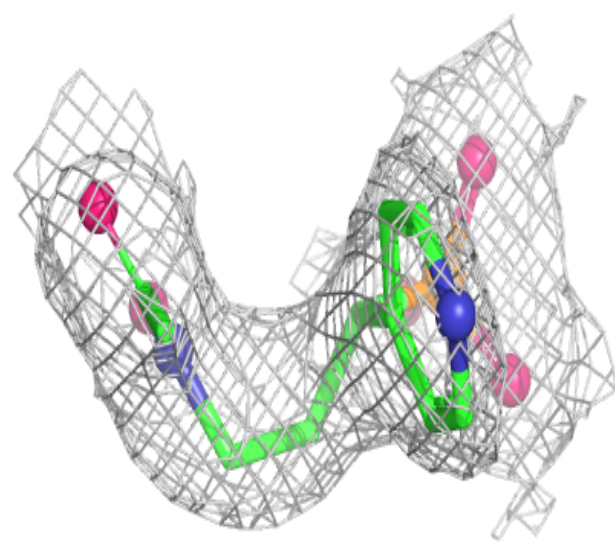
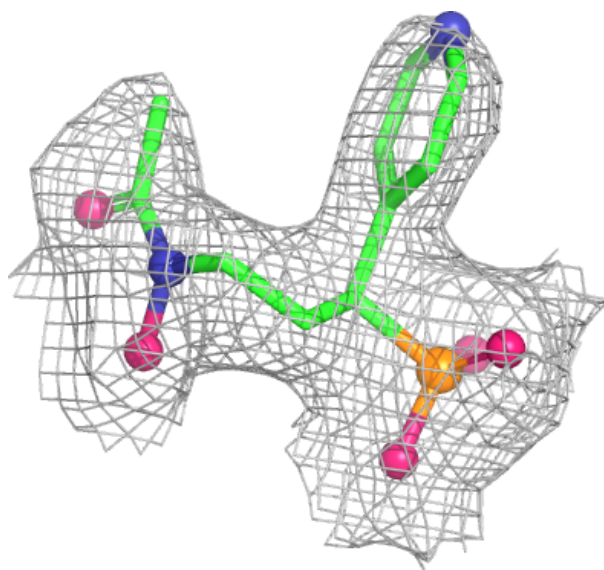
Electron density around FOB B 502 (A):

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



Electron density around FOQ B 503 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.