



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:26 pm BST

PDB ID : 4GAE
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

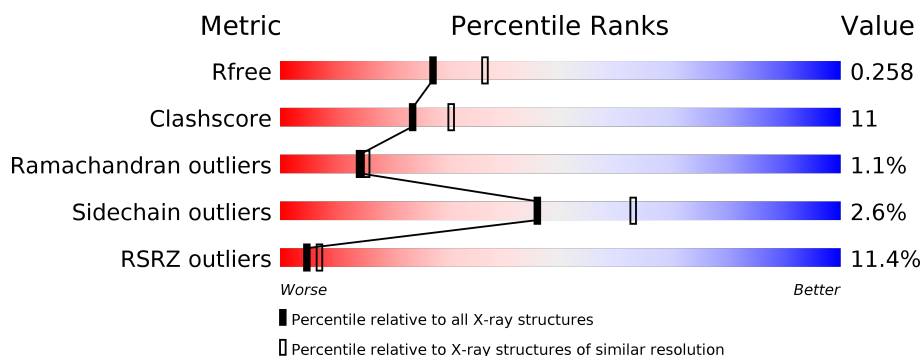
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on 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	<div> <div>13%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	B	426	<div> <div>9%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition [i](#)

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:

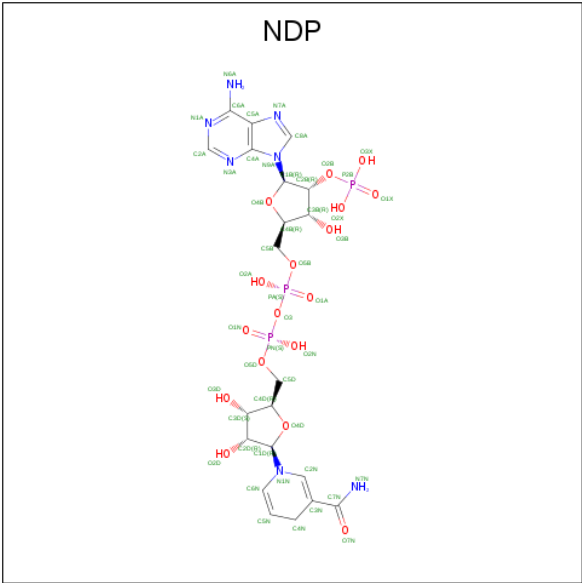
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	EXPRESSION TAG	UNP O96693
A	64	ARG	-	EXPRESSION TAG	UNP O96693
A	65	GLY	-	EXPRESSION TAG	UNP O96693
A	66	SER	-	EXPRESSION TAG	UNP O96693
A	67	HIS	-	EXPRESSION TAG	UNP O96693
A	68	HIS	-	EXPRESSION TAG	UNP O96693
A	69	HIS	-	EXPRESSION TAG	UNP O96693
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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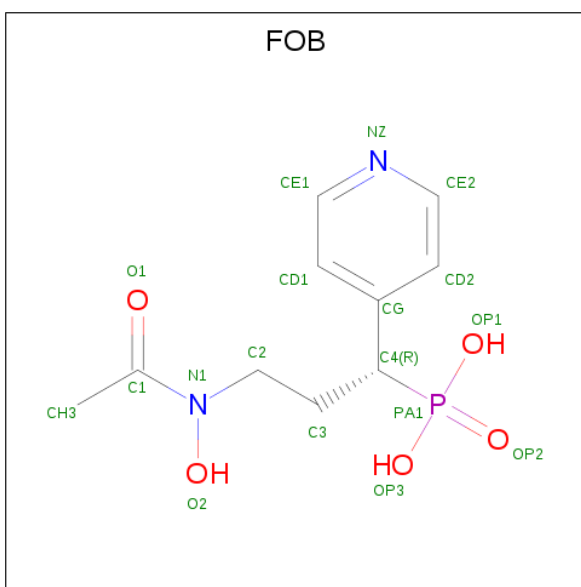
Chain	Residue	Modelled	Actual	Comment	Reference
B	247	ILE	LEU	ENGINEERED MUTATION	UNP O96693

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



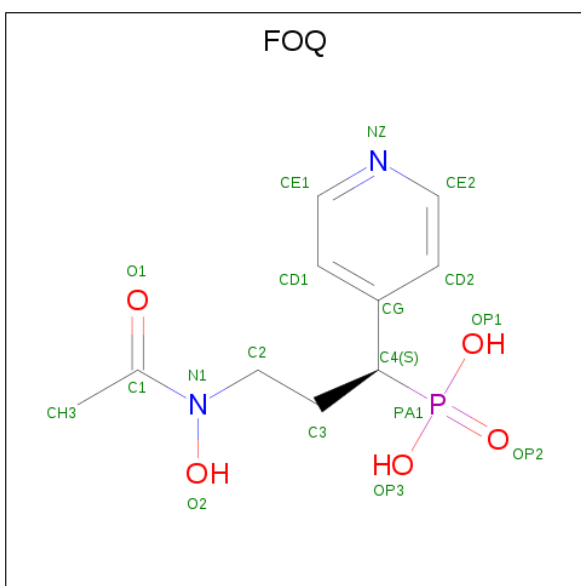
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is [(1R)-3-[acetyl(hydroxy)amino]-1-(pyridin-4-yl)propyl]phosphonic acid (three-letter code: FOB) (formula: C₁₀H₁₅N₂O₅P).



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 (three-letter code: 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		

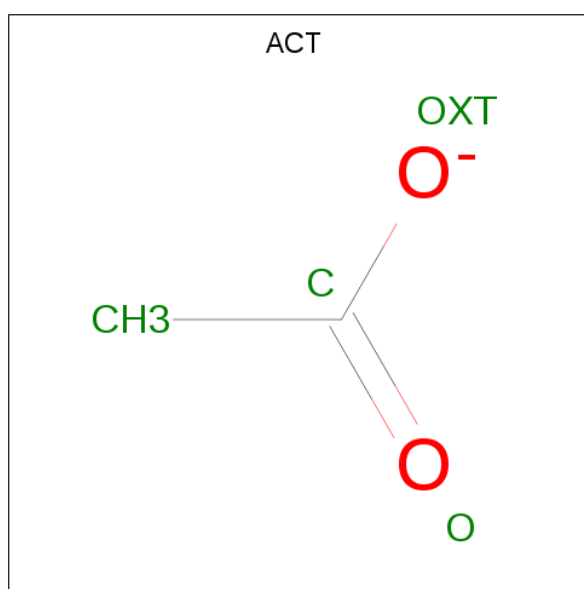
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is ACETATE ION (three-letter code: 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 (three-letter code: 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		

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 0.210 , 0.258	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)	0.31 , 30.2	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	0.87	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: FOQ, CL, MN, EDO, FOB, ACT, 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	0.35	0/3389	0.60	0/4575
1	B	0.38	0/3339	0.61	0/4509
All	All	0.37	0/6728	0.60	0/9084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	88	0
1	B	3276	0	3322	67	0
2	A	48	0	26	2	0
2	B	48	0	26	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	153	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 11.

All (153) 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: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:B:283:LYS:HB2	1:B:283:LYS:NZ	1.98	0.77
1:B:269:SER:CB	1:B:312:LYS:HE3	2.16	0.76
1:B:485:HIS:O	1:B:486:ASN:C	2.28	0.72
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: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:HZ2	1:B:283:LYS:HB2	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: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:A:165:MET:HE2	1:A:169:CYS:SG	2.37	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:A:202:LEU:HD23	1:A:208:ILE:HD11	1.80	0.62
1:B:292:LYS:HG2	1:B:292:LYS:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:HZ3	1:A:205:LYS:HB3	1.66	0.60
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:425:ILE:O	1:A:429:LEU:HD13	2.04	0.57
1:A:71:HIS:HB3	1:B:258:LYS:NZ	2.19	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: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
1:B:421:ALA:HB1	1:B:475:LYS:HG3	1.88	0.55
1:A:205:LYS:NZ	1:A:231:ASP:OD2	2.39	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:483:ASN:C	1:B:485:HIS:H	2.09	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: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: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:A:310:MET:HE2	1:A:314:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:141:TYR:HE1	1:A:158:ILE:HG22	1.75	0.50
1:A:109:VAL:O	1:A:109:VAL:HG23	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:165:MET:HE3	1:B:192:TYR:HB2	1.93	0.49
1:B:296:TRP:HE1	1:B:298:MET:HG2	1.77	0.49
1:B:348:ASP:O	1:B:349:LYS:HB2	2.12	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
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:A:245:LYS:NZ	6:A:505:CL:CL	2.82	0.47
1:A:296:TRP:CZ3	2:A:501:NDP:O7N	2.67	0.47
1:A:93:ALA:O	1:A:96:ILE:HG22	2.14	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: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:B:250:LYS:HG2	9:B:660:HOH:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:GLU:HA	1:B:146:GLU:OE2	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
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:HG23	1:A:135:ILE:O	2.19	0.42
1:A:158:ILE:N	1:A:158:ILE:CD1	2.80	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:A:75:LYS:C	1:A:76:LYS:HD2	2.40	0.42
1:B:206:GLU:HG3	1:B:420:ASN:HD21	1.84	0.42
1:A:289:ASN:HD22	1:A:289:ASN:N	2.18	0.41
1:A:296:TRP:N	1:A:296:TRP:CD1	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: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: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:A:164:GLY:O	1:A:168:ILE:HG13	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	13	14
1	B	408/426 (96%)	386 (95%)	18 (4%)	4 (1%)	15	17
All	All	822/852 (96%)	771 (94%)	42 (5%)	9 (1%)	14	15

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%)	371 (97%)	11 (3%)	42	58
1	B	377/391 (96%)	368 (98%)	9 (2%)	49	66
All	All	759/782 (97%)	739 (97%)	20 (3%)	46	63

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	99	GLU
1	A	139	SER
1	A	165	MET
1	A	176	LYS
1	A	205	LYS
1	A	213	PHE
1	A	252	LEU
1	A	264	LYS
1	A	296	TRP
1	A	372	ASP
1	B	92	ASN
1	B	110	LYS
1	B	163	GLU
1	B	165	MET
1	B	217	LYS
1	B	252	LEU
1	B	264	LYS
1	B	284	ASN
1	B	292	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	136	HIS
1	A	172	ASN
1	A	255	ASN
1	A	289	ASN
1	A	341	HIS
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	433	ASN
1	A	459	ASN
1	B	92	ASN
1	B	136	HIS
1	B	150	ASN
1	B	185	GLN
1	B	197	ASN
1	B	255	ASN
1	B	289	ASN
1	B	385	GLN
1	B	420	ASN
1	B	433	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	FOQ	A	503[B]	5	16,18,18	2.21	7 (43%)	17,25,25	1.79	5 (29%)

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	2.27	5 (31%)	17,25,25	2.63	5 (29%)
2	NDP	B	501	-	45,52,52	1.61	5 (11%)	53,80,80	1.44	5 (9%)
4	FOQ	B	503[B]	5	16,18,18	2.28	7 (43%)	17,25,25	1.64	3 (17%)
3	FOB	B	502[A]	5	16,18,18	2.25	6 (37%)	17,25,25	2.60	3 (17%)
8	EDO	B	509	-	3,3,3	0.57	0	2,2,2	0.27	0
7	ACT	A	506	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
8	EDO	A	507	-	3,3,3	0.52	0	2,2,2	0.32	0
2	NDP	A	501	-	45,52,52	1.54	5 (11%)	53,80,80	1.39	4 (7%)
8	EDO	B	508	-	3,3,3	0.52	0	2,2,2	0.31	0
7	ACT	B	507	-	1,3,3	2.13	1 (100%)	0,3,3	0.00	-

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	FOQ	A	503[B]	5	-	4/19/19/19	0/1/1/1
3	FOB	A	502[A]	5	-	4/19/19/19	0/1/1/1
2	NDP	B	501	-	-	4/30/77/77	0/5/5/5
4	FOQ	B	503[B]	5	-	3/19/19/19	0/1/1/1
3	FOB	B	502[A]	5	-	8/19/19/19	0/1/1/1
8	EDO	B	509	-	-	0/1/1/1	-
8	EDO	A	507	-	-	0/1/1/1	-
2	NDP	A	501	-	-	4/30/77/77	0/5/5/5
8	EDO	B	508	-	-	1/1/1/1	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	FOB	PA1-C4	-6.38	1.73	1.82
2	B	501	NDP	O7N-C7N	6.01	1.38	1.24
4	B	503[B]	FOQ	PA1-C4	-5.87	1.73	1.82
3	B	502[A]	FOB	PA1-C4	-5.71	1.74	1.82
4	A	503[B]	FOQ	PA1-C4	-5.65	1.74	1.82
2	A	501	NDP	O7N-C7N	5.61	1.37	1.24
2	B	501	NDP	C2A-N3A	4.40	1.39	1.32
2	A	501	NDP	C6N-C5N	4.36	1.41	1.33
2	A	501	NDP	C2A-N3A	4.24	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	C6N-C5N	4.24	1.40	1.33
2	B	501	NDP	C2A-N1A	3.50	1.40	1.33
4	A	503[B]	FOQ	PA1-OP1	-3.47	1.49	1.54
3	A	502[A]	FOB	PA1-OP1	-3.36	1.49	1.54
3	B	502[A]	FOB	O2-N1	3.36	1.42	1.40
3	B	502[A]	FOB	PA1-OP3	-3.30	1.49	1.54
4	B	503[B]	FOQ	O2-N1	3.26	1.42	1.40
2	A	501	NDP	C2A-N1A	3.15	1.39	1.33
4	A	503[B]	FOQ	CG-C4	2.91	1.57	1.52
3	A	502[A]	FOB	CG-C4	2.87	1.56	1.52
4	B	503[B]	FOQ	PA1-OP3	-2.87	1.50	1.54
3	B	502[A]	FOB	CG-C4	2.87	1.56	1.52
4	B	503[B]	FOQ	CG-C4	2.73	1.56	1.52
3	A	502[A]	FOB	CD2-CG	2.67	1.43	1.39
4	A	503[B]	FOQ	PA1-OP3	-2.59	1.50	1.54
3	A	502[A]	FOB	PA1-OP3	-2.58	1.50	1.54
3	B	502[A]	FOB	CD2-CG	2.51	1.43	1.39
2	A	501	NDP	C4N-C3N	2.48	1.54	1.49
4	B	503[B]	FOQ	CD1-CG	2.48	1.43	1.39
4	A	503[B]	FOQ	CD1-CG	2.34	1.42	1.39
2	B	501	NDP	C4N-C3N	2.33	1.54	1.49
7	A	506	ACT	CH3-C	2.24	1.51	1.48
4	A	503[B]	FOQ	C3-C2	2.23	1.57	1.52
4	B	503[B]	FOQ	PA1-OP1	-2.15	1.51	1.54
4	B	503[B]	FOQ	C3-C2	2.14	1.57	1.52
4	A	503[B]	FOQ	CD2-CG	2.13	1.42	1.39
7	B	507	ACT	CH3-C	2.13	1.51	1.48
3	B	502[A]	FOB	PA1-OP1	-2.11	1.51	1.54

All (25) 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	-6.60	118.37	128.68
2	A	501	NDP	N3A-C2A-N1A	-6.59	118.38	128.68
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	B	501	NDP	C1B-N9A-C4A	-3.39	120.69	126.64
2	B	501	NDP	C3N-C7N-N7N	3.13	123.23	117.67
4	A	503[B]	FOQ	OP2-PA1-C4	-3.04	104.85	113.35
2	A	501	NDP	C3N-C7N-N7N	2.97	122.95	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NDP	O7N-C7N-C3N	-2.94	115.36	120.90
3	A	502[A]	FOB	OP2-PA1-C4	-2.94	105.13	113.35
2	B	501	NDP	O7N-C7N-C3N	-2.93	115.39	120.90
2	A	501	NDP	C1B-N9A-C4A	-2.82	121.68	126.64
4	B	503[B]	FOQ	CE2-NZ-CE1	2.54	122.83	116.85
3	B	502[A]	FOB	CE2-NZ-CE1	2.52	122.79	116.85
4	A	503[B]	FOQ	CE2-NZ-CE1	2.47	122.67	116.85
3	A	502[A]	FOB	CE2-NZ-CE1	2.47	122.66	116.85
3	A	502[A]	FOB	OP3-PA1-OP1	2.20	113.54	107.64
4	A	503[B]	FOQ	OP3-PA1-OP1	2.16	113.44	107.64
4	A	503[B]	FOQ	O2-N1-C2	2.15	118.96	113.59
4	B	503[B]	FOQ	O2-N1-C2	2.04	118.69	113.59
3	A	502[A]	FOB	CD2-CE2-NZ	-2.03	120.08	123.62
3	B	502[A]	FOB	OP3-PA1-OP1	2.02	113.06	107.64
2	B	501	NDP	O3D-C3D-C4D	-2.02	105.22	111.05

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[A]	FOB	N1-C2-C3-C4
8	B	508	EDO	O1-C1-C2-O2
2	A	501	NDP	O4D-C1D-N1N-C6N
3	A	502[A]	FOB	N1-C2-C3-C4
4	A	503[B]	FOQ	C3-C2-N1-C1
3	B	502[A]	FOB	CG-C4-PA1-OP1
3	B	502[A]	FOB	CG-C4-PA1-OP3
2	B	501	NDP	O4D-C1D-N1N-C6N
3	B	502[A]	FOB	CG-C4-PA1-OP2
3	A	502[A]	FOB	C3-C4-PA1-OP2
3	B	502[A]	FOB	C3-C4-PA1-OP2
2	A	501	NDP	PN-O3-PA-O1A
2	B	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	PN-O3-PA-O1A
2	A	501	NDP	O4B-C4B-C5B-O5B
4	A	503[B]	FOQ	C3-C2-N1-O2
4	B	503[B]	FOQ	C3-C2-N1-C1
3	B	502[A]	FOB	C3-C2-N1-C1
4	A	503[B]	FOQ	CH3-C1-N1-O2
3	A	502[A]	FOB	CH3-C1-N1-O2
4	B	503[B]	FOQ	CH3-C1-N1-O2
3	B	502[A]	FOB	CH3-C1-N1-O2

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Mol	Chain	Res	Type	Atoms
4	A	503[B]	FOQ	O1-C1-N1-O2
3	A	502[A]	FOB	O1-C1-N1-O2
4	B	503[B]	FOQ	O1-C1-N1-O2
3	B	502[A]	FOB	O1-C1-N1-O2
2	B	501	NDP	C2N-C3N-C7N-N7N
2	A	501	NDP	C2N-C3N-C7N-N7N

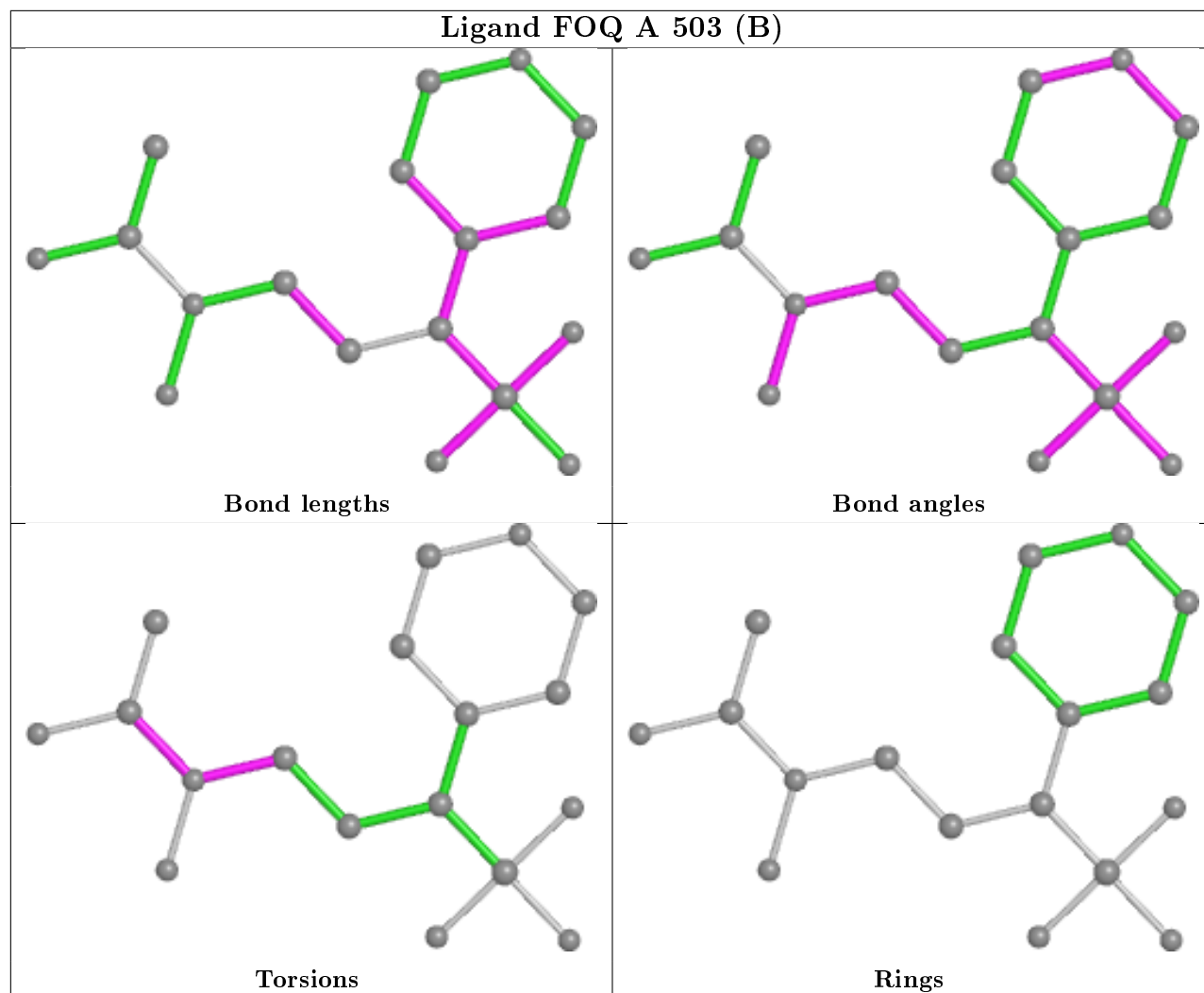
There are no ring outliers.

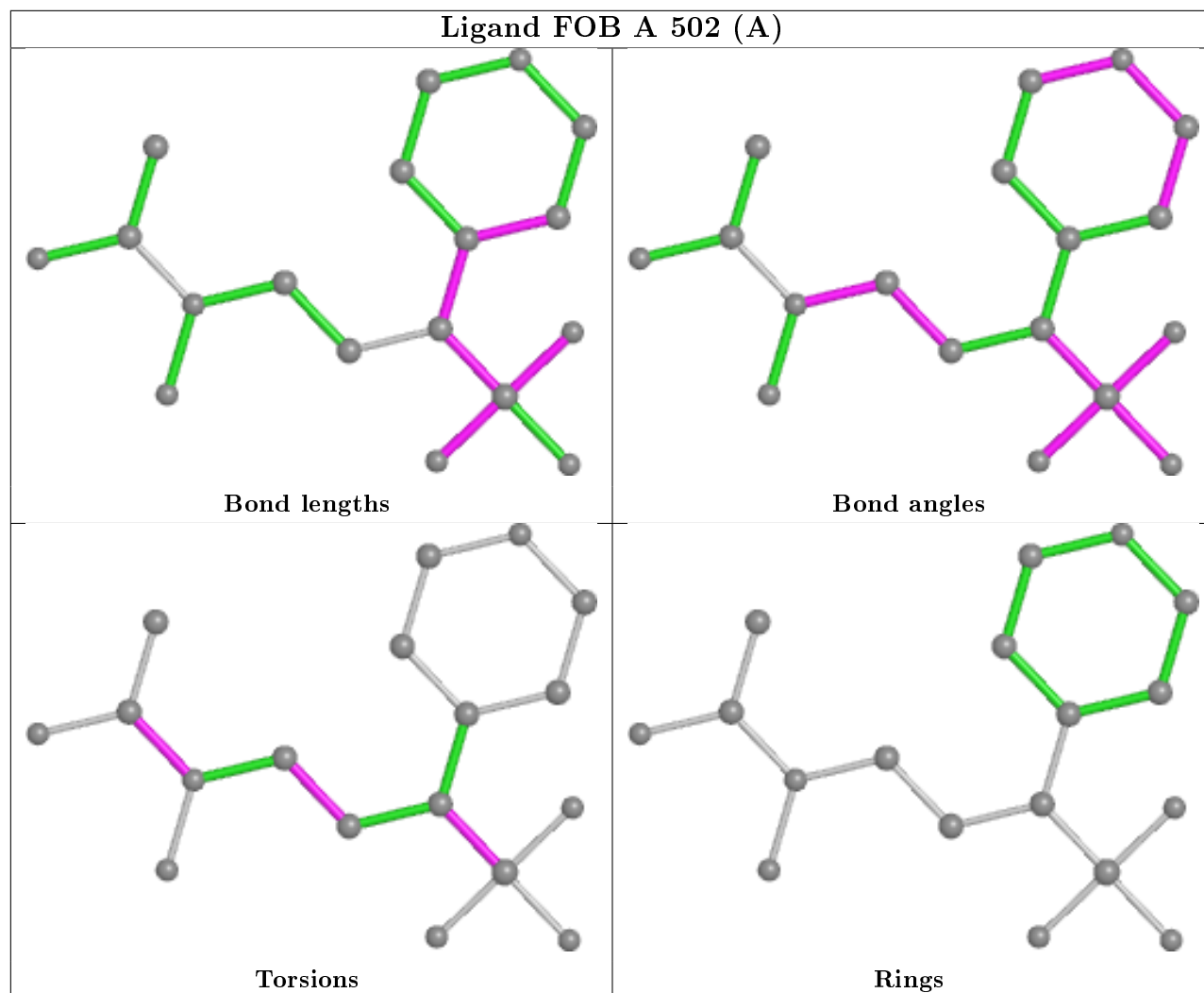
2 monomers are involved in 3 short contacts:

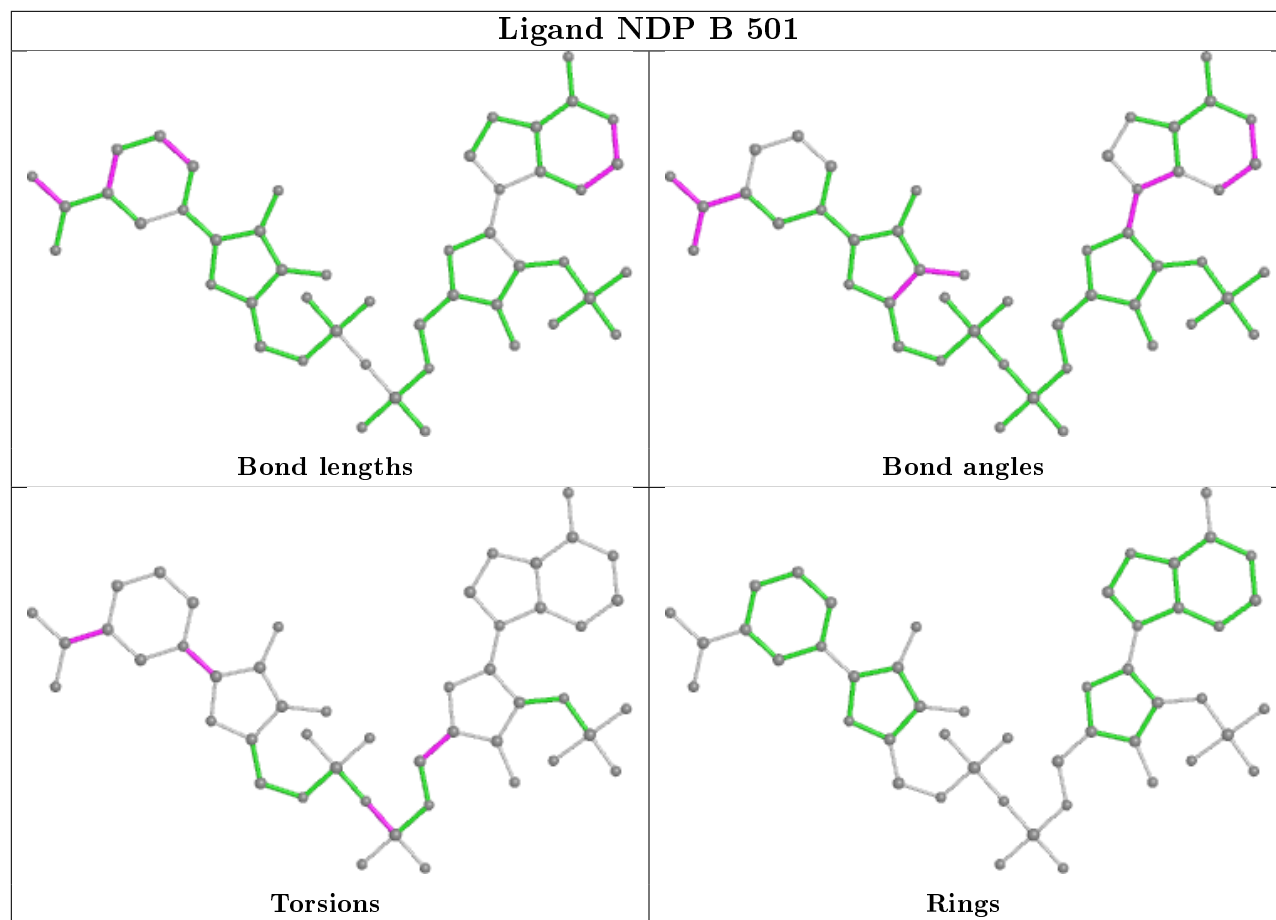
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[A]	FOB	1	0
2	A	501	NDP	2	0

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.

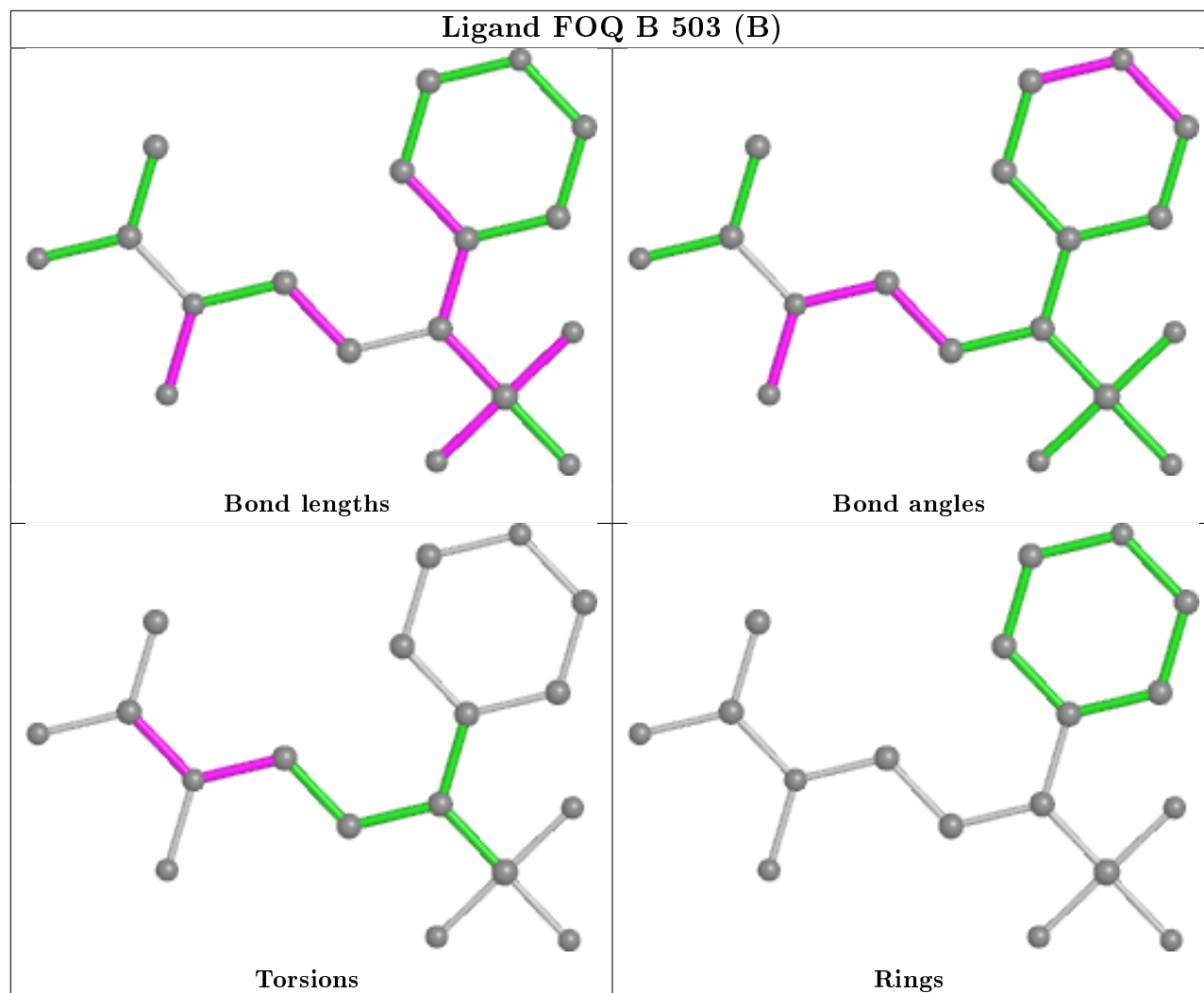
Ligand FOQ A 503 (B)

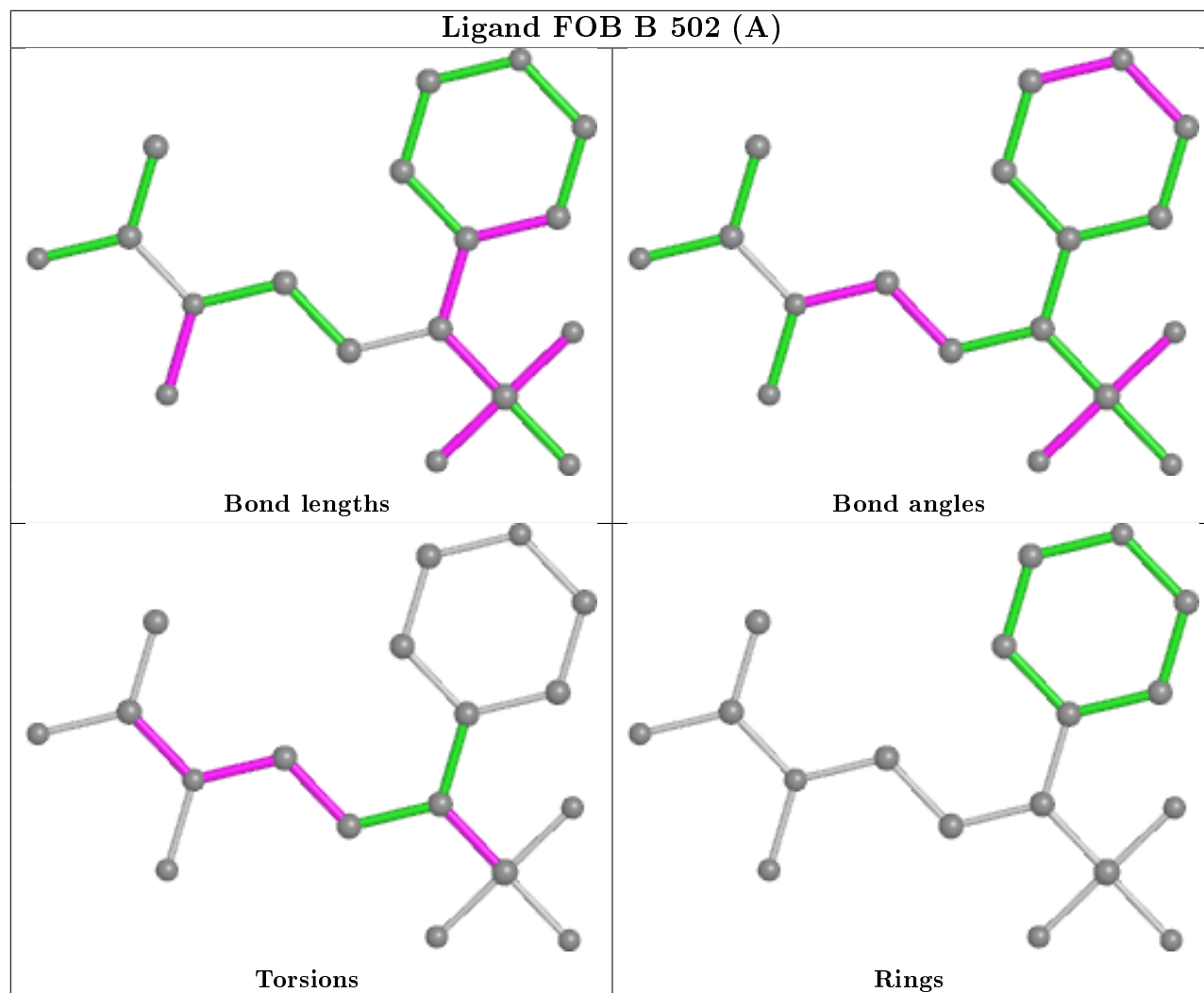


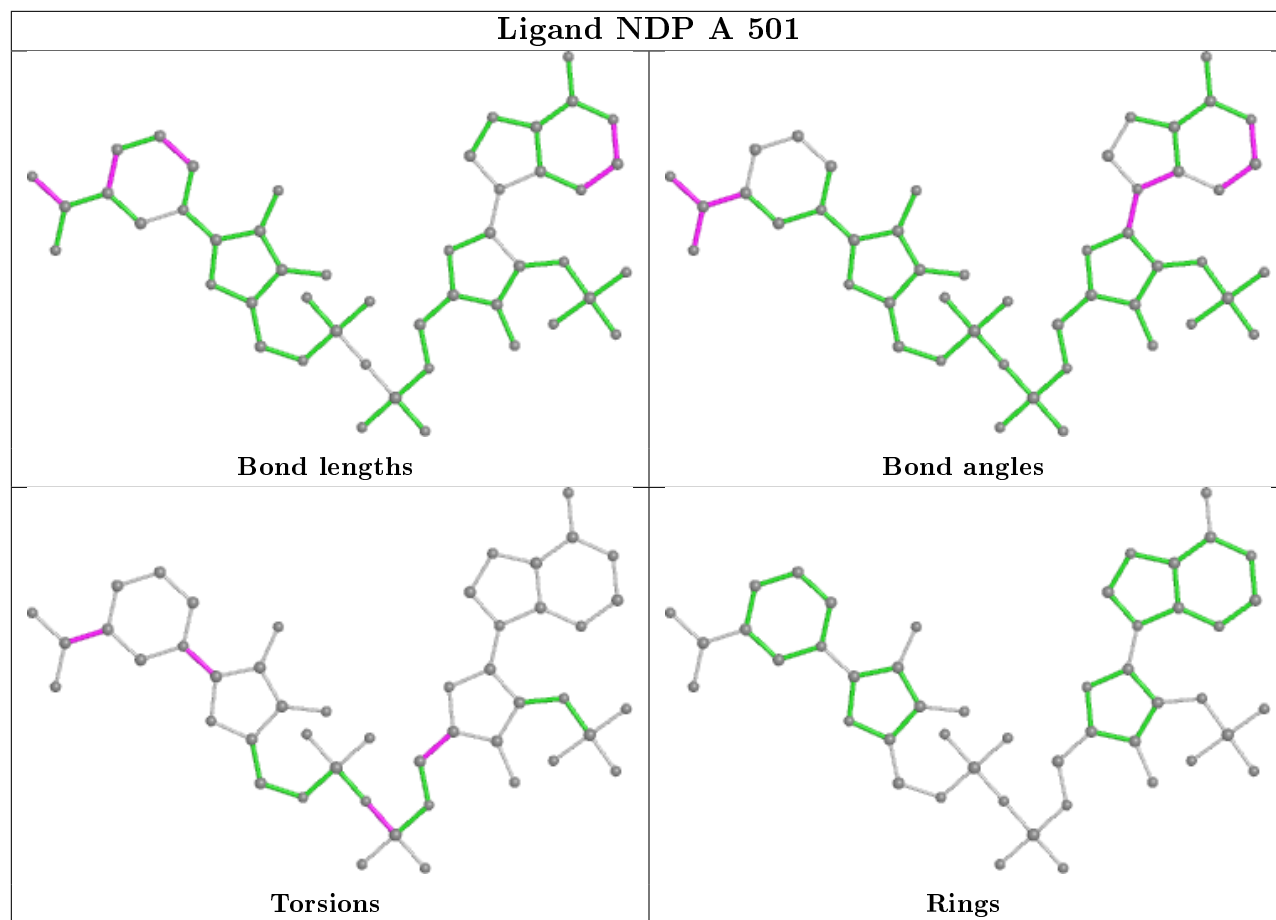




Ligand FOQ B 503 (B)







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%)	0.69	57 (13%) 3 4	21, 36, 71, 104	1 (0%)
1	B	410/426 (96%)	0.44	37 (9%) 9 12	18, 30, 54, 98	0
All	All	826/852 (96%)	0.57	94 (11%) 5 7	18, 33, 65, 104	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	PRO	16.9
1	B	291	LEU	11.2
1	A	292	LYS	10.4
1	A	295	LYS	9.4
1	A	132	TYR	9.4
1	B	295	LYS	8.3
1	B	158	ILE	7.9
1	A	158	ILE	7.1
1	A	105	ASN	6.8
1	A	214	PHE	6.4
1	A	157	ILE	6.1
1	B	292	LYS	6.1
1	A	296	TRP	6.0
1	A	177	ILE	6.0
1	B	274	PHE	5.8
1	A	184	PHE	5.8
1	B	300	LYS	5.5
1	B	293	HIS	5.4
1	A	146	GLU	5.3
1	A	414	PHE	5.2
1	A	74	SER	5.1
1	B	174	ILE	4.9
1	B	78	ILE	4.8
1	B	142	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	149	LYS	4.5
1	A	436	LYS	4.4
1	B	351	VAL	4.3
1	A	147	LEU	4.1
1	B	296	TRP	4.1
1	A	128	PHE	4.0
1	B	356	TYR	3.9
1	B	277	LEU	3.8
1	A	192	TYR	3.8
1	A	75	LYS	3.5
1	B	149	LYS	3.5
1	B	150	ASN	3.4
1	B	314	LEU	3.4
1	A	408	ALA	3.4
1	A	73	GLY	3.4
1	A	279	MET	3.4
1	A	103	ILE	3.4
1	A	471	HIS	3.3
1	A	109	VAL	3.3
1	A	119	ASN	3.3
1	B	453	SER	3.2
1	A	83	PHE	3.2
1	B	173	SER	3.2
1	A	168	ILE	3.1
1	A	293	HIS	3.1
1	A	195	MET	3.1
1	A	221	ILE	3.0
1	B	79	ASN	3.0
1	A	410	ILE	2.9
1	B	472	SER	2.8
1	A	455	LYS	2.8
1	B	482	TYR	2.8
1	A	334	VAL	2.7
1	B	475	LYS	2.7
1	A	229	PRO	2.7
1	B	184	PHE	2.6
1	B	192	TYR	2.6
1	A	237	ILE	2.6
1	A	465	LYS	2.6
1	A	399	PHE	2.5
1	A	266	PHE	2.5
1	A	481	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	138	LYS	2.4
1	B	104	GLU	2.4
1	A	375	LYS	2.4
1	A	106	VAL	2.4
1	A	378	LEU	2.4
1	A	162	ASP	2.4
1	A	409	GLY	2.4
1	B	486	ASN	2.3
1	A	276	ASN	2.3
1	A	240	CYS	2.3
1	A	104	GLU	2.3
1	A	113	TYR	2.2
1	B	250	LYS	2.2
1	B	352	ILE	2.2
1	B	106	VAL	2.2
1	B	406	TYR	2.2
1	A	135	ILE	2.2
1	A	291	LEU	2.2
1	B	249	THR	2.2
1	B	96	ILE	2.2
1	A	121	LEU	2.2
1	A	94	LEU	2.1
1	A	188	TYR	2.1
1	B	165	MET	2.1
1	B	111	ALA	2.1
1	A	131	GLU	2.0
1	A	140	VAL	2.0
1	B	188	TYR	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 carbohydrates 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,

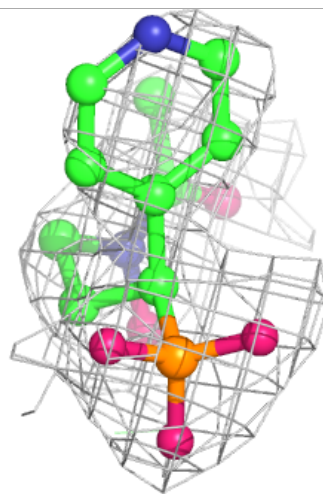
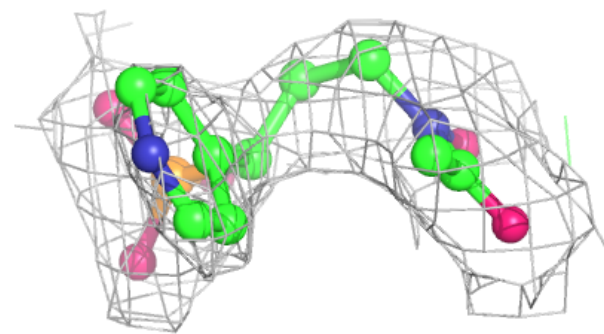
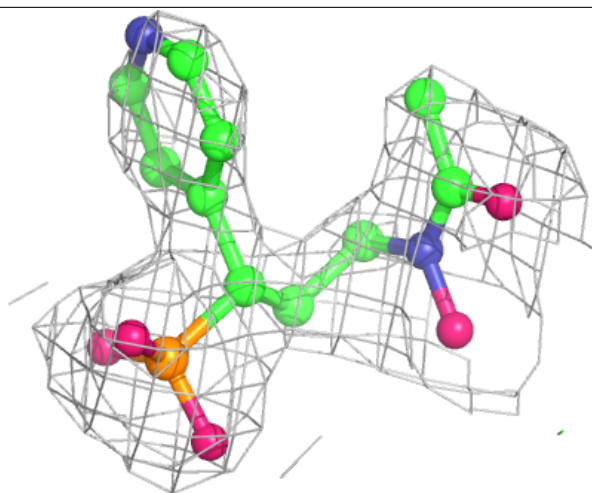
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ACT	A	506	4/4	0.74	0.32	93,93,94,94	0
8	EDO	A	507	4/4	0.80	0.35	78,79,80,80	0
8	EDO	B	509	4/4	0.81	0.37	78,79,79,79	0
8	EDO	B	508	4/4	0.81	0.16	64,65,65,65	0
4	FOQ	A	503[B]	18/18	0.90	0.19	26,33,36,37	18
7	ACT	B	507	4/4	0.90	0.28	65,67,67,67	0
3	FOB	A	502[A]	18/18	0.91	0.20	28,35,38,39	18
2	NDP	A	501	48/48	0.92	0.12	30,38,42,42	0
5	MN	B	506	1/1	0.93	0.04	49,49,49,49	0
3	FOB	B	502[A]	18/18	0.94	0.16	26,30,36,36	18
4	FOQ	B	503[B]	18/18	0.94	0.15	20,24,31,31	18
2	NDP	B	501	48/48	0.95	0.10	22,28,30,32	0
5	MN	B	505	1/1	0.98	0.05	40,40,40,40	0
5	MN	B	504	1/1	0.99	0.04	24,24,24,24	0
6	CL	A	505	1/1	0.99	0.06	45,45,45,45	0
5	MN	A	504	1/1	1.00	0.14	26,26,26,26	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.

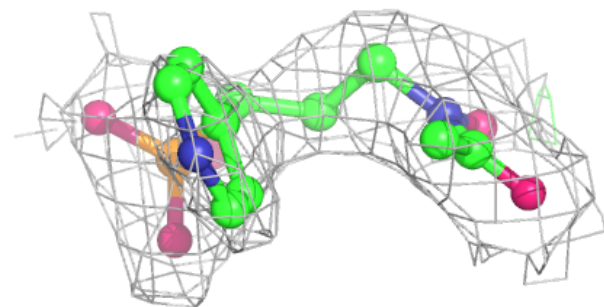
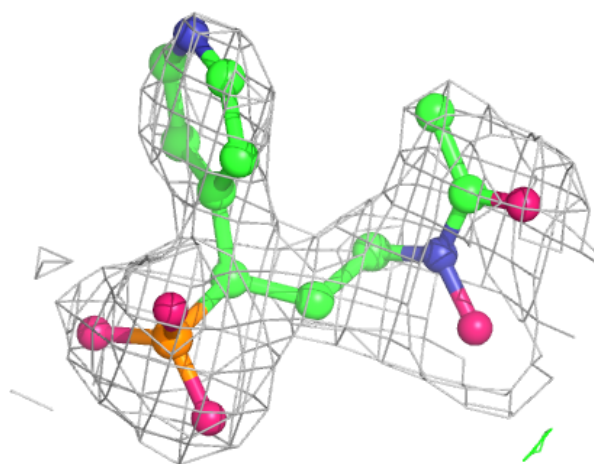
Electron density around FOQ A 503 (B):

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



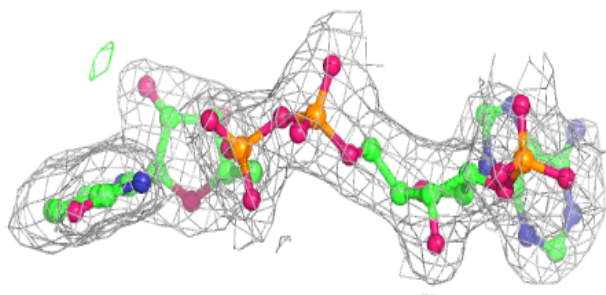
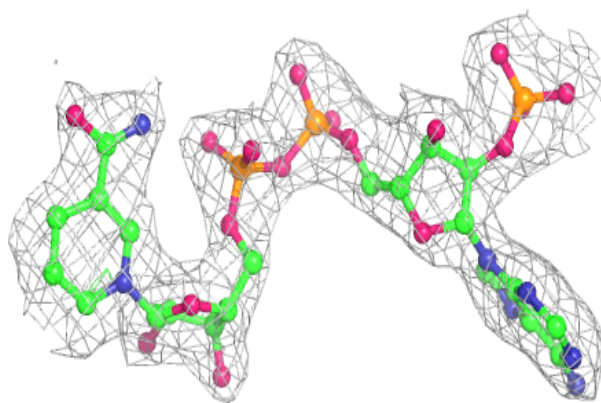
Electron density around FOB A 502 (A):

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



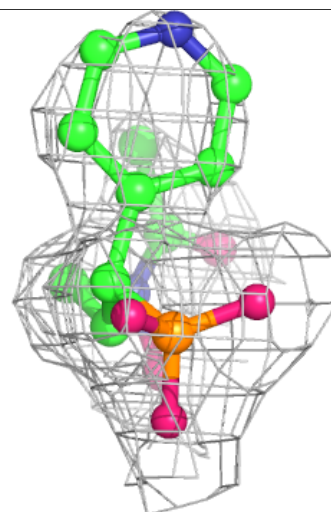
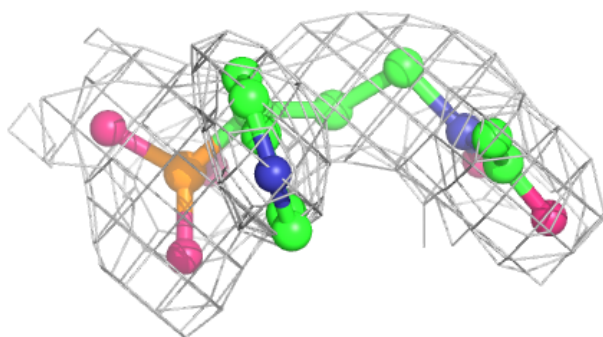
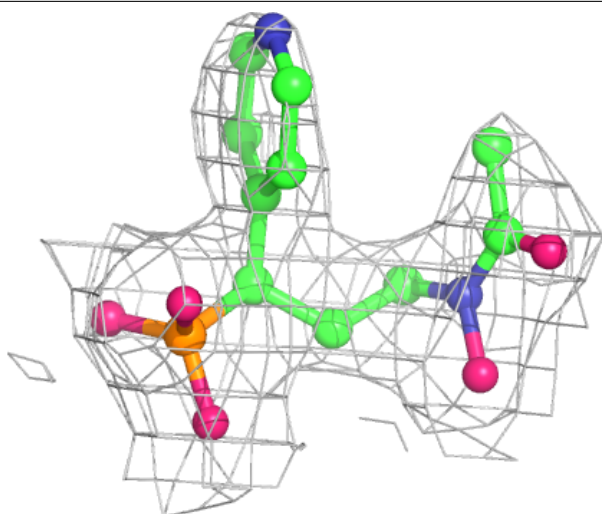
Electron density around NDP A 501:

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



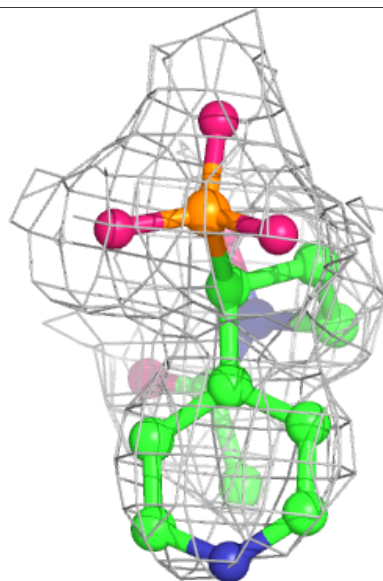
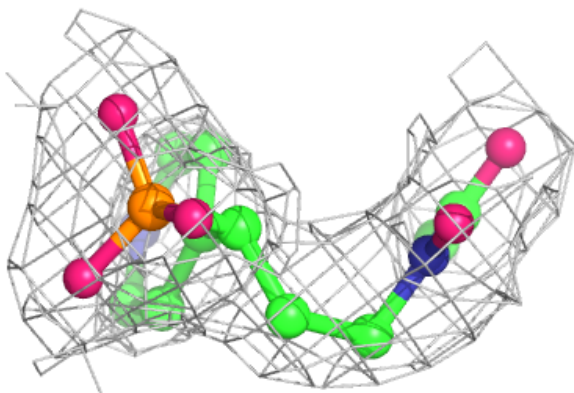
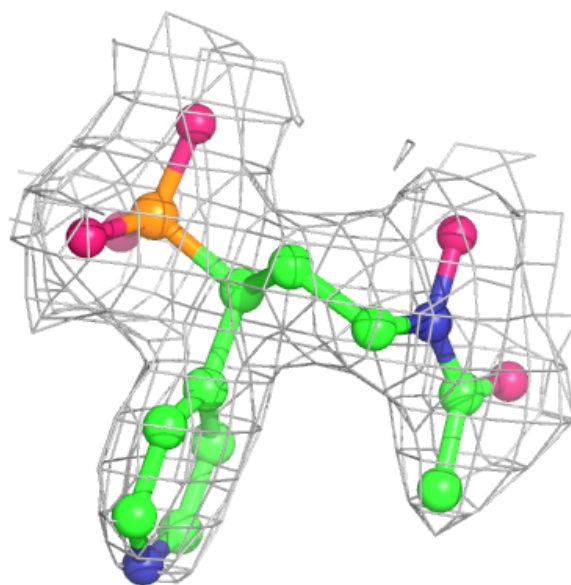
Electron density around FOB B 502 (A):

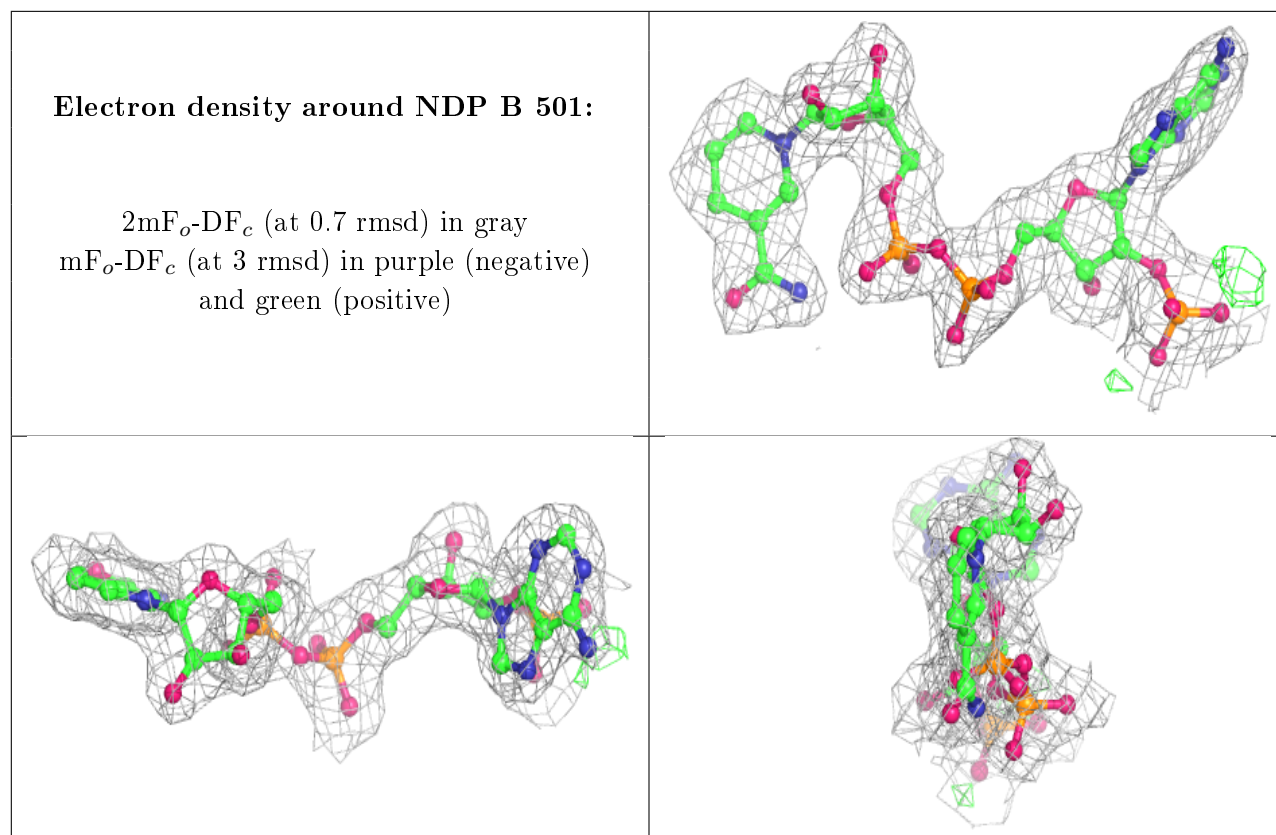
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.