



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2019 – 05:00 PM EST

PDB ID : 6D3Q
Title : Crystal structure of Escherichia coli enolase complexed with a natural inhibitor SF2312.
Authors : Erlandsen, H.; Krucinska, J.; Hazeen, A.; Wright, D.
Deposited on : 2018-04-16
Resolution : 2.24 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

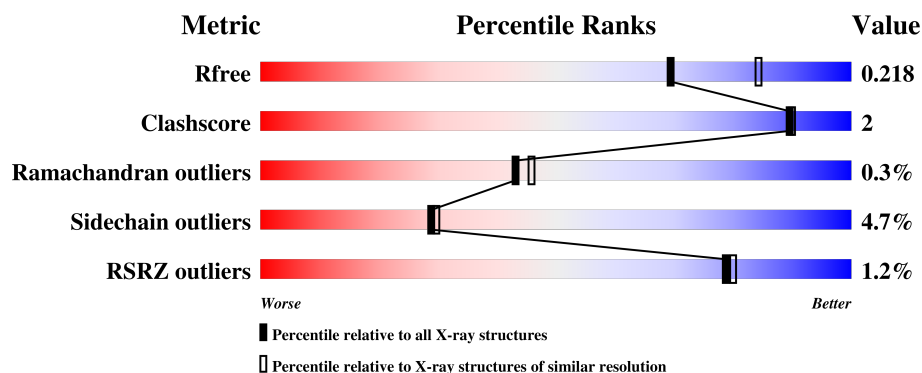
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	111664	2027 (2.26-2.22)
Clashscore	122126	2170 (2.26-2.22)
Ramachandran outliers	120053	2129 (2.26-2.22)
Sidechain outliers	120020	2130 (2.26-2.22)
RSRZ outliers	108989	1991 (2.26-2.22)

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. 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	439	<div> <div>92%</div> <div>7%</div> </div>
1	B	439	<div> <div>91%</div> <div>8%</div> </div>
1	C	439	<div> <div>2%</div> <div>88%</div> <div>10%</div> </div>
1	D	439	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
1	E	439	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	439	<div> <div></div> <div>%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	C	504	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20194 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	C	437	Total	C	N	O	S	0	0	0
			3240	2027	556	642	15			
1	B	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	E	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	F	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	D	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			

There are 42 discrepancies between the modelled and reference sequences:

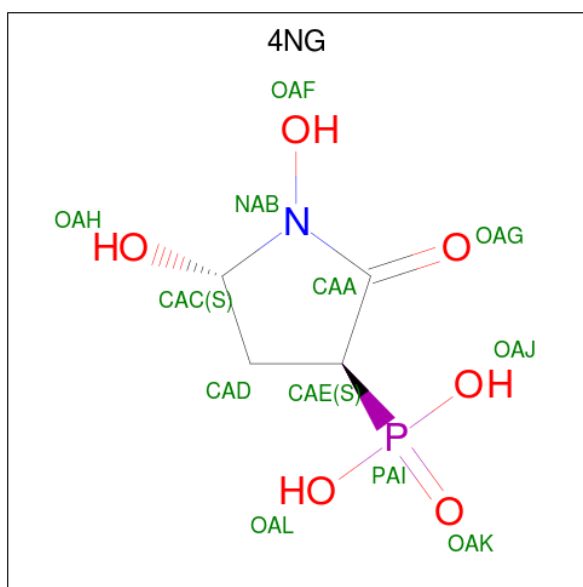
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLN	-	expression tag	UNP B7MLA0
A	-6	GLN	-	expression tag	UNP B7MLA0
A	-5	MET	-	expression tag	UNP B7MLA0
A	-4	GLY	-	expression tag	UNP B7MLA0
A	-3	ARG	-	expression tag	UNP B7MLA0
A	-2	GLY	-	expression tag	UNP B7MLA0
A	-1	SER	-	expression tag	UNP B7MLA0
C	-7	GLN	-	expression tag	UNP B7MLA0
C	-6	GLN	-	expression tag	UNP B7MLA0
C	-5	MET	-	expression tag	UNP B7MLA0
C	-4	GLY	-	expression tag	UNP B7MLA0
C	-3	ARG	-	expression tag	UNP B7MLA0
C	-2	GLY	-	expression tag	UNP B7MLA0
C	-1	SER	-	expression tag	UNP B7MLA0
B	-7	GLN	-	expression tag	UNP B7MLA0
B	-6	GLN	-	expression tag	UNP B7MLA0
B	-5	MET	-	expression tag	UNP B7MLA0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP B7MLA0
B	-3	ARG	-	expression tag	UNP B7MLA0
B	-2	GLY	-	expression tag	UNP B7MLA0
B	-1	SER	-	expression tag	UNP B7MLA0
E	-7	GLN	-	expression tag	UNP B7MLA0
E	-6	GLN	-	expression tag	UNP B7MLA0
E	-5	MET	-	expression tag	UNP B7MLA0
E	-4	GLY	-	expression tag	UNP B7MLA0
E	-3	ARG	-	expression tag	UNP B7MLA0
E	-2	GLY	-	expression tag	UNP B7MLA0
E	-1	SER	-	expression tag	UNP B7MLA0
F	-7	GLN	-	expression tag	UNP B7MLA0
F	-6	GLN	-	expression tag	UNP B7MLA0
F	-5	MET	-	expression tag	UNP B7MLA0
F	-4	GLY	-	expression tag	UNP B7MLA0
F	-3	ARG	-	expression tag	UNP B7MLA0
F	-2	GLY	-	expression tag	UNP B7MLA0
F	-1	SER	-	expression tag	UNP B7MLA0
D	-7	GLN	-	expression tag	UNP B7MLA0
D	-6	GLN	-	expression tag	UNP B7MLA0
D	-5	MET	-	expression tag	UNP B7MLA0
D	-4	GLY	-	expression tag	UNP B7MLA0
D	-3	ARG	-	expression tag	UNP B7MLA0
D	-2	GLY	-	expression tag	UNP B7MLA0
D	-1	SER	-	expression tag	UNP B7MLA0

- Molecule 2 is [(3S,5S)-1,5-dihydroxy-2-oxopyrrolidin-3-yl]phosphonic acid (three-letter code: 4NG) (formula: C₄H₈NO₆P) (labeled as "Ligand of Interest" by author).

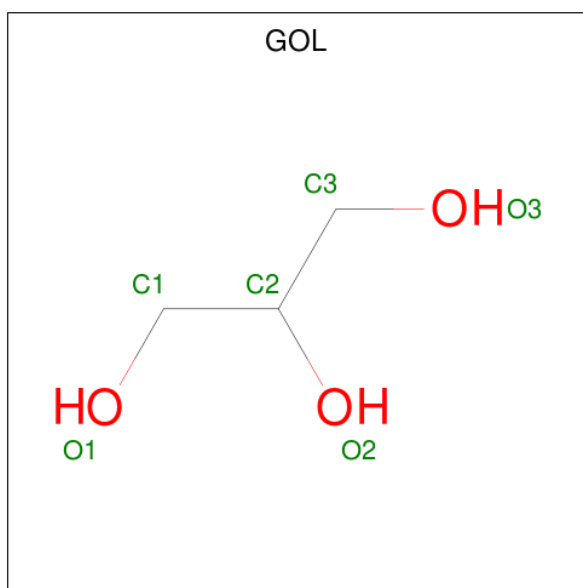


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			12	4	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			12	4	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			12	4	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			12	4	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			12	4	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			12	4	1	6	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

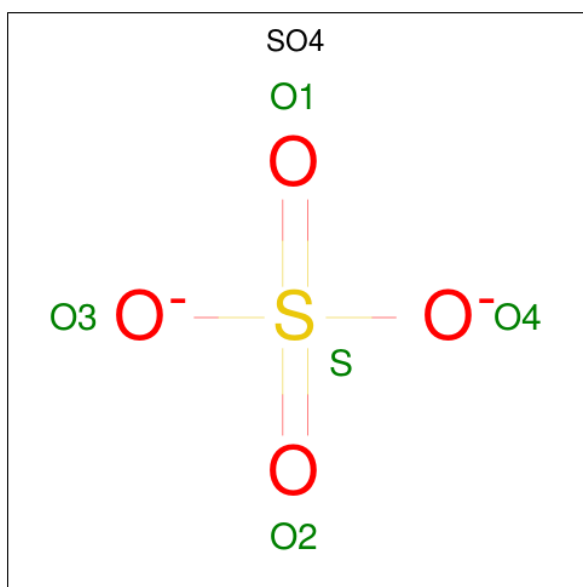
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

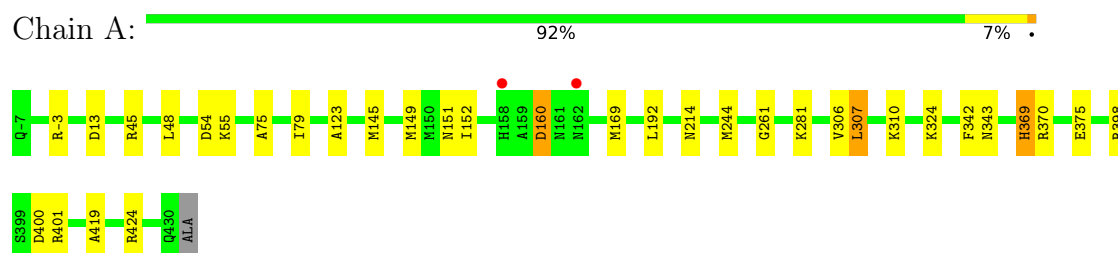
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	C	39	Total 39	O 39	0	0
6	B	119	Total 119	O 119	0	0
6	E	101	Total 101	O 101	0	0
6	F	80	Total 80	O 80	0	0
6	D	70	Total 70	O 70	0	0

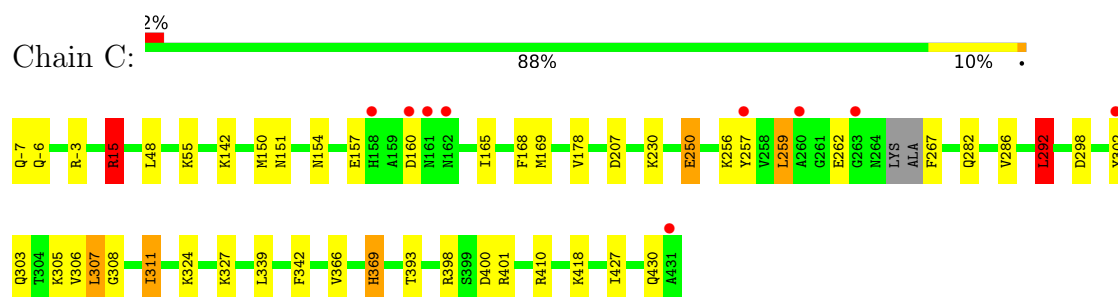
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

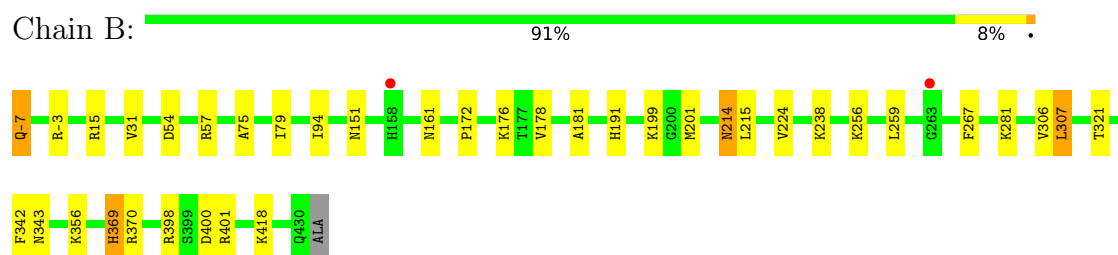
• Molecule 1: Enolase



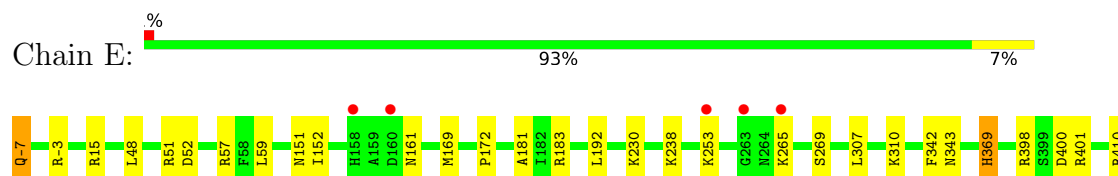
• Molecule 1: Enolase



• Molecule 1: Enolase

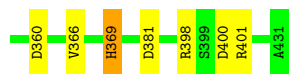
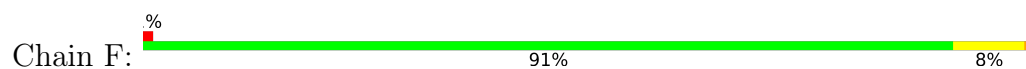


• Molecule 1: Enolase

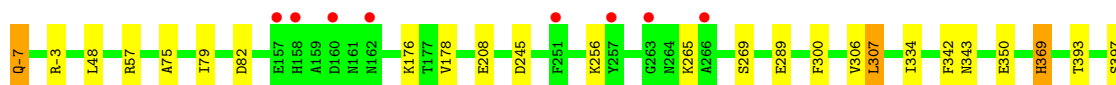
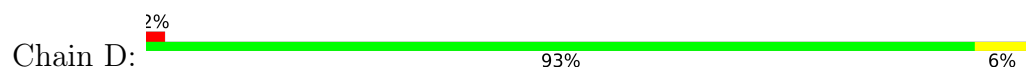




• Molecule 1: Enolase



• Molecule 1: Enolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.75Å 142.07Å 207.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	207.28 – 2.24 93.49 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.7 (207.28-2.24) 99.8 (93.49-2.24)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.80 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.163 , 0.216 0.172 , 0.218	Depositor DCC
R_{free} test set	7420 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20194	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: GOL, MG, SO4, 4NG

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	0.91	1/3291 (0.0%)	0.94	7/4428 (0.2%)
1	B	0.91	0/3291	0.92	6/4428 (0.1%)
1	C	0.85	0/3281	0.90	5/4414 (0.1%)
1	D	0.86	0/3296	0.88	2/4435 (0.0%)
1	E	0.86	0/3296	0.91	8/4435 (0.2%)
1	F	0.87	0/3296	0.91	7/4435 (0.2%)
All	All	0.88	1/19751 (0.0%)	0.91	35/26575 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	GLU	CG-CD	5.39	1.60	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	15	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	13	ASP	CB-CG-OD1	7.72	125.25	118.30
1	E	57	ARG	NE-CZ-NH1	7.49	124.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	51	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	C	292	LEU	CA-CB-CG	6.61	130.50	115.30
1	F	9	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	410	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	15	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	82	ASP	CB-CG-OD1	6.10	123.79	118.30
1	E	410	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	F	360	ASP	CB-CG-OD1	5.77	123.49	118.30
1	F	13	ASP	CB-CG-OD1	5.71	123.44	118.30
1	F	381	ASP	CB-CG-OD2	5.71	123.44	118.30
1	F	244	MET	CG-SD-CE	-5.65	91.15	100.20
1	F	57	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	E	52	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	C	15	ARG	CG-CD-NE	5.52	123.39	111.80
1	B	54	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	F	51	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	149	MET	CG-SD-CE	5.38	108.81	100.20
1	A	45	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	15	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	370	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	54	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	-3	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	57	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	410	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	15	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	-3	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	E	183	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	E	52	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	424	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	244	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	F	159	ALA	Peptide

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	3249	0	3273	9	0
1	B	3249	0	3274	16	0
1	C	3240	0	3259	22	0
1	D	3254	0	3278	10	0
1	E	3254	0	3278	8	0
1	F	3254	0	3278	12	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
2	C	12	0	0	0	0
2	D	12	0	0	0	0
2	E	12	0	0	0	0
2	F	12	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	1	0
5	B	10	0	0	0	0
5	C	10	0	0	2	0
5	D	15	0	0	1	0
5	E	10	0	0	0	0
5	F	15	0	0	1	0
6	A	111	0	0	0	0
6	B	119	0	0	1	0
6	C	39	0	0	1	0
6	D	70	0	0	2	0
6	E	101	0	0	1	0
6	F	80	0	0	1	0
All	All	20194	0	19680	77	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 2.

All (77) 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)
5:F:505:SO4:O2	6:F:601:HOH:O	1.77	1.02
5:D:505:SO4:O2	6:D:601:HOH:O	1.81	0.97
5:C:504:SO4:O4	6:C:601:HOH:O	1.87	0.91
1:F:151:ASN:HD21	1:F:154:ASN:HD21	1.38	0.71
1:C:369:HIS:CD2	1:C:401:ARG:HH11	2.11	0.69
1:A:369:HIS:CD2	1:A:401:ARG:HH11	2.12	0.68
1:C:151:ASN:HD21	1:C:154:ASN:HD21	1.42	0.65
1:B:369:HIS:CD2	1:B:401:ARG:HH11	2.15	0.64
1:B:306:VAL:HG12	1:B:307:LEU:HD13	1.79	0.64
1:D:-7:GLN:HA	1:D:-7:GLN:HE21	1.65	0.61
1:E:369:HIS:CD2	1:E:401:ARG:HH11	2.19	0.61
1:F:369:HIS:CD2	1:F:401:ARG:HH11	2.22	0.57
1:D:369:HIS:CD2	1:D:401:ARG:HH11	2.24	0.56
1:C:15:ARG:HD2	1:C:207:ASP:OD2	2.06	0.56
1:A:75:ALA:O	1:A:79:ILE:HG12	2.05	0.56
1:B:94:ILE:HG23	4:B:504:GOL:H12	1.88	0.55
1:D:350:GLU:OE2	4:D:504:GOL:O2	2.20	0.55
1:E:172:PRO:HG2	1:E:181:ALA:HB1	1.89	0.54
1:B:259:LEU:HD12	1:B:267:PHE:CE1	2.43	0.54
1:B:75:ALA:O	1:B:79:ILE:HG12	2.09	0.53
1:C:339:LEU:HD12	1:C:366:VAL:HB	1.91	0.53
1:B:306:VAL:HG12	1:B:307:LEU:CD1	2.38	0.53
1:C:307:LEU:HG	1:C:311:ILE:HD11	1.92	0.52
1:C:259:LEU:HD13	1:C:267:PHE:CE1	2.45	0.51
1:C:151:ASN:ND2	1:C:154:ASN:HD21	2.06	0.50
1:D:306:VAL:HG12	1:D:307:LEU:HD13	1.92	0.50
1:A:-3:ARG:HE	1:C:-6:GLN:HE22	1.60	0.50
1:E:424:ARG:HD2	6:E:686:HOH:O	2.12	0.50
1:F:172:PRO:HG2	1:F:181:ALA:HB1	1.94	0.49
1:D:75:ALA:O	1:D:79:ILE:HG12	2.13	0.49
1:C:151:ASN:HD21	1:C:154:ASN:ND2	2.10	0.49
1:E:152:ILE:HD12	1:E:192:LEU:HD22	1.95	0.49
1:C:257:TYR:CE2	1:C:292:LEU:HD12	2.48	0.49
1:D:369:HIS:CD2	1:D:393:THR:HA	2.48	0.49
1:C:259:LEU:HD22	1:C:262:GLU:HB2	1.96	0.48
1:C:286:VAL:HG13	1:C:430:GLN:NE2	2.29	0.48
1:B:-7:GLN:HE21	1:B:-7:GLN:HA	1.78	0.47
1:A:151:ASN:HA	1:A:169:MET:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:VAL:HG12	1:C:427:ILE:HG21	1.95	0.47
1:D:-7:GLN:HA	1:D:-7:GLN:NE2	2.29	0.47
1:F:94:ILE:HG23	4:F:504:GOL:H12	1.95	0.47
1:F:339:LEU:HD12	1:F:366:VAL:HB	1.97	0.47
1:A:145:MET:HG2	1:A:419:ALA:O	2.16	0.46
1:F:260:ALA:HA	1:F:264:ASN:HD22	1.80	0.46
1:B:191:HIS:HE1	6:B:713:HOH:O	1.97	0.46
1:B:151:ASN:OD1	1:B:151:ASN:C	2.55	0.46
1:B:172:PRO:HG2	1:B:181:ALA:HB1	1.98	0.45
1:E:-7:GLN:HA	1:E:-7:GLN:HE21	1.81	0.45
1:C:165:ILE:HB	1:C:168:PHE:CZ	2.52	0.45
1:E:59:LEU:HD12	1:E:59:LEU:N	2.32	0.45
1:B:199:LYS:HE3	1:B:224:VAL:HG12	1.98	0.45
1:A:160:ASP:N	1:A:160:ASP:OD1	2.51	0.45
1:C:157:GLU:HG3	1:C:250:GLU:HG2	1.99	0.44
1:C:165:ILE:HB	1:C:168:PHE:CE1	2.52	0.44
1:D:300:PHE:HB3	1:D:334:ILE:HG23	1.99	0.44
1:A:306:VAL:HG12	1:A:307:LEU:HD13	1.98	0.44
1:B:161:ASN:HB3	1:B:214:ASN:HA	1.99	0.44
1:B:201:MET:CE	1:B:215:LEU:HD23	2.48	0.44
1:F:321:THR:O	1:F:321:THR:HG22	2.18	0.43
1:A:123:ALA:HB2	1:C:-7:GLN:HB3	2.01	0.43
5:C:504:SO4:O1	1:B:-3:ARG:NH2	2.52	0.43
1:C:292:LEU:HD22	1:C:303:GLN:OE1	2.18	0.43
1:C:303:GLN:HG3	1:C:307:LEU:HD22	2.01	0.43
1:F:306:VAL:HG12	1:F:307:LEU:HD13	2.00	0.43
1:D:245:ASP:HA	1:D:289:GLU:HB3	2.01	0.42
1:F:-7:GLN:HE21	1:F:-7:GLN:HA	1.84	0.42
1:C:302:TYR:O	1:C:306:VAL:HG23	2.19	0.42
1:D:178:VAL:HG12	1:D:412:GLU:CD	2.40	0.42
1:E:-3:ARG:NH2	6:D:601:HOH:O	2.53	0.42
1:F:151:ASN:HD21	1:F:154:ASN:ND2	2.12	0.42
1:B:321:THR:HG22	1:B:321:THR:O	2.20	0.42
1:E:151:ASN:HA	1:E:169:MET:HG2	2.01	0.41
1:C:150:MET:O	1:C:169:MET:HA	2.20	0.41
1:B:31:VAL:O	1:F:-7:GLN:NE2	2.52	0.40
1:A:152:ILE:HD12	1:A:192:LEU:HD22	2.04	0.40
1:F:225:ILE:O	1:F:229:VAL:HG23	2.22	0.40
1:C:369:HIS:CD2	1:C:393:THR:C	2.95	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	436/439 (99%)	424 (97%)	11 (2%)	1 (0%)	49	55
1	B	436/439 (99%)	422 (97%)	13 (3%)	1 (0%)	49	55
1	C	433/439 (99%)	412 (95%)	19 (4%)	2 (0%)	31	30
1	D	437/439 (100%)	424 (97%)	12 (3%)	1 (0%)	49	55
1	E	437/439 (100%)	421 (96%)	15 (3%)	1 (0%)	49	55
1	F	437/439 (100%)	419 (96%)	16 (4%)	2 (0%)	31	30
All	All	2616/2634 (99%)	2522 (96%)	86 (3%)	8 (0%)	43	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	308	GLY
1	C	398	ARG
1	A	398	ARG
1	B	398	ARG
1	E	398	ARG
1	F	260	ALA
1	F	398	ARG
1	D	398	ARG

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	319 (96%)	12 (4%)	38	43
1	B	331/331 (100%)	317 (96%)	14 (4%)	32	35
1	C	330/331 (100%)	308 (93%)	22 (7%)	18	15
1	D	331/331 (100%)	316 (96%)	15 (4%)	30	32
1	E	331/331 (100%)	317 (96%)	14 (4%)	32	35
1	F	331/331 (100%)	314 (95%)	17 (5%)	26	25
All	All	1985/1986 (100%)	1891 (95%)	94 (5%)	29	30

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	55	LYS
1	A	160	ASP
1	A	214	ASN
1	A	281	LYS
1	A	307	LEU
1	A	310	LYS
1	A	324	LYS
1	A	342	PHE
1	A	343	ASN
1	A	369	HIS
1	A	400	ASP
1	C	15	ARG
1	C	48	LEU
1	C	55	LYS
1	C	142	LYS
1	C	160	ASP
1	C	178	VAL
1	C	230	LYS
1	C	250	GLU
1	C	256	LYS
1	C	259	LEU
1	C	282	GLN
1	C	292	LEU
1	C	298	ASP
1	C	305	LYS
1	C	307	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	311	ILE
1	C	324	LYS
1	C	327	LYS
1	C	342	PHE
1	C	369	HIS
1	C	400	ASP
1	C	418	LYS
1	B	-7	GLN
1	B	176	LYS
1	B	178	VAL
1	B	214	ASN
1	B	238	LYS
1	B	256	LYS
1	B	281	LYS
1	B	307	LEU
1	B	342	PHE
1	B	343	ASN
1	B	356	LYS
1	B	369	HIS
1	B	400	ASP
1	B	418	LYS
1	E	-7	GLN
1	E	48	LEU
1	E	161	ASN
1	E	230	LYS
1	E	238	LYS
1	E	253	LYS
1	E	265	LYS
1	E	269	SER
1	E	307	LEU
1	E	310	LYS
1	E	342	PHE
1	E	343	ASN
1	E	369	HIS
1	E	400	ASP
1	F	-7	GLN
1	F	48	LEU
1	F	55	LYS
1	F	157	GLU
1	F	158	HIS
1	F	178	VAL
1	F	197	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	230	LYS
1	F	253	LYS
1	F	264	ASN
1	F	265	LYS
1	F	307	LEU
1	F	310	LYS
1	F	342	PHE
1	F	343	ASN
1	F	369	HIS
1	F	400	ASP
1	D	-7	GLN
1	D	48	LEU
1	D	57	ARG
1	D	176	LYS
1	D	208	GLU
1	D	256	LYS
1	D	265	LYS
1	D	269	SER
1	D	307	LEU
1	D	342	PHE
1	D	343	ASN
1	D	369	HIS
1	D	397	SER
1	D	400	ASP
1	D	424	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-7	GLN
1	A	137	ASN
1	A	171	GLN
1	A	214	ASN
1	A	303	GLN
1	A	369	HIS
1	C	-6	GLN
1	C	154	ASN
1	C	166	GLN
1	C	171	GLN
1	C	191	HIS
1	C	202	ASN
1	C	369	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	430	GLN
1	B	-7	GLN
1	B	162	ASN
1	B	171	GLN
1	B	191	HIS
1	B	214	ASN
1	B	264	ASN
1	B	303	GLN
1	B	369	HIS
1	E	-7	GLN
1	E	101	ASN
1	E	161	ASN
1	E	166	GLN
1	E	171	GLN
1	E	282	GLN
1	E	303	GLN
1	E	369	HIS
1	F	-7	GLN
1	F	154	ASN
1	F	166	GLN
1	F	171	GLN
1	F	214	ASN
1	F	264	ASN
1	F	303	GLN
1	F	369	HIS
1	D	-7	GLN
1	D	137	ASN
1	D	154	ASN
1	D	166	GLN
1	D	171	GLN
1	D	369	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 12 are monoatomic - leaving 23 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	4NG	A	501	3	9,12,12	1.68	2 (22%)	7,19,19	2.20	2 (28%)
4	GOL	A	504	-	5,5,5	0.63	0	5,5,5	0.97	0
2	4NG	B	501	3	9,12,12	1.69	3 (33%)	7,19,19	1.21	1 (14%)
4	GOL	B	504	-	5,5,5	0.38	0	5,5,5	1.19	0
5	SO4	B	505	-	4,4,4	0.80	0	6,6,6	0.63	0
5	SO4	B	506	-	4,4,4	0.85	0	6,6,6	0.22	0
2	4NG	C	501	3	9,12,12	1.69	2 (22%)	7,19,19	1.97	2 (28%)
5	SO4	C	504	-	4,4,4	0.39	0	6,6,6	0.43	0
5	SO4	C	505	-	4,4,4	0.65	0	6,6,6	0.71	0
2	4NG	D	501	3	9,12,12	1.24	1 (11%)	7,19,19	1.85	1 (14%)
4	GOL	D	504	-	5,5,5	0.64	0	5,5,5	1.05	0
5	SO4	D	505	-	4,4,4	0.63	0	6,6,6	0.47	0
5	SO4	D	506	-	4,4,4	0.59	0	6,6,6	0.36	0
5	SO4	D	507	-	4,4,4	0.52	0	6,6,6	0.60	0
2	4NG	E	501	3	9,12,12	1.85	3 (33%)	7,19,19	1.15	1 (14%)
4	GOL	E	504	-	5,5,5	0.49	0	5,5,5	0.66	0
5	SO4	E	505	-	4,4,4	0.72	0	6,6,6	0.21	0
5	SO4	E	506	-	4,4,4	0.70	0	6,6,6	0.54	0
2	4NG	F	501	3	9,12,12	1.15	1 (11%)	7,19,19	2.18	2 (28%)
4	GOL	F	504	-	5,5,5	0.38	0	5,5,5	0.64	0
5	SO4	F	505	-	4,4,4	0.64	0	6,6,6	0.69	0
5	SO4	F	506	-	4,4,4	0.82	0	6,6,6	0.45	0
5	SO4	F	507	-	4,4,4	0.49	0	6,6,6	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
2	4NG	A	501	3	-	0/6/22/22	0/1/1/1
4	GOL	A	504	-	-	2/4/4/4	-
2	4NG	B	501	3	-	0/6/22/22	0/1/1/1
4	GOL	B	504	-	-	1/4/4/4	-
2	4NG	C	501	3	-	0/6/22/22	0/1/1/1
2	4NG	D	501	3	-	0/6/22/22	0/1/1/1
4	GOL	D	504	-	-	2/4/4/4	-
2	4NG	E	501	3	-	1/6/22/22	0/1/1/1
4	GOL	E	504	-	-	0/4/4/4	-
2	4NG	F	501	3	-	0/6/22/22	0/1/1/1
4	GOL	F	504	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4NG	PAI-OAL	-3.95	1.48	1.54
2	E	501	4NG	PAI-OAL	-3.56	1.49	1.54
2	C	501	4NG	PAI-OAK	3.43	1.55	1.49
2	B	501	4NG	PAI-OAL	-3.28	1.49	1.54
2	D	501	4NG	PAI-OAL	-3.10	1.49	1.54
2	E	501	4NG	CAD-CAE	-2.72	1.51	1.55
2	E	501	4NG	PAI-OAK	-2.52	1.45	1.49
2	B	501	4NG	OAF-NAB	2.50	1.44	1.40
2	F	501	4NG	PAI-OAJ	-2.44	1.50	1.54
2	A	501	4NG	PAI-OAJ	-2.20	1.51	1.54
2	B	501	4NG	CAD-CAE	-2.20	1.52	1.55
2	C	501	4NG	PAI-OAL	-2.13	1.51	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	4NG	PAI-CAE-CAA	-4.53	105.23	114.55
2	D	501	4NG	PAI-CAE-CAA	-4.40	105.49	114.55
2	A	501	4NG	PAI-CAE-CAA	-4.06	106.19	114.55
2	A	501	4NG	OAK-PAI-CAE	-3.81	102.04	113.22
2	C	501	4NG	OAK-PAI-CAE	-3.41	103.21	113.22
2	C	501	4NG	PAI-CAE-CAA	-3.31	107.74	114.55
2	F	501	4NG	OAL-PAI-OAK	-2.47	107.15	113.43
2	E	501	4NG	PAI-CAE-CAA	-2.32	109.78	114.55
2	B	501	4NG	PAI-CAE-CAA	-2.09	110.26	114.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

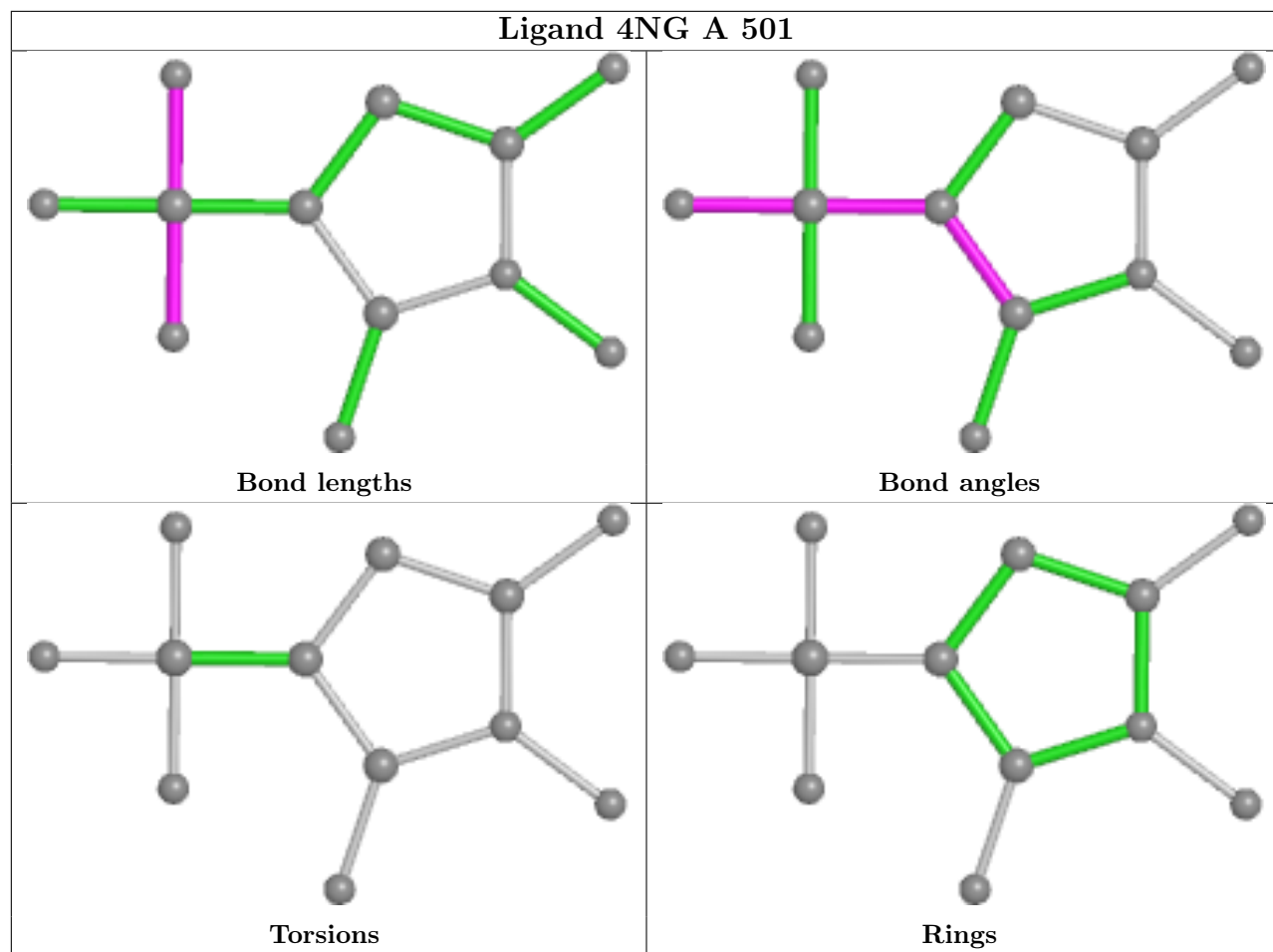
Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
4	D	504	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-O2
4	D	504	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-O2
2	E	501	4NG	CAA-CAE-PAI-OAJ

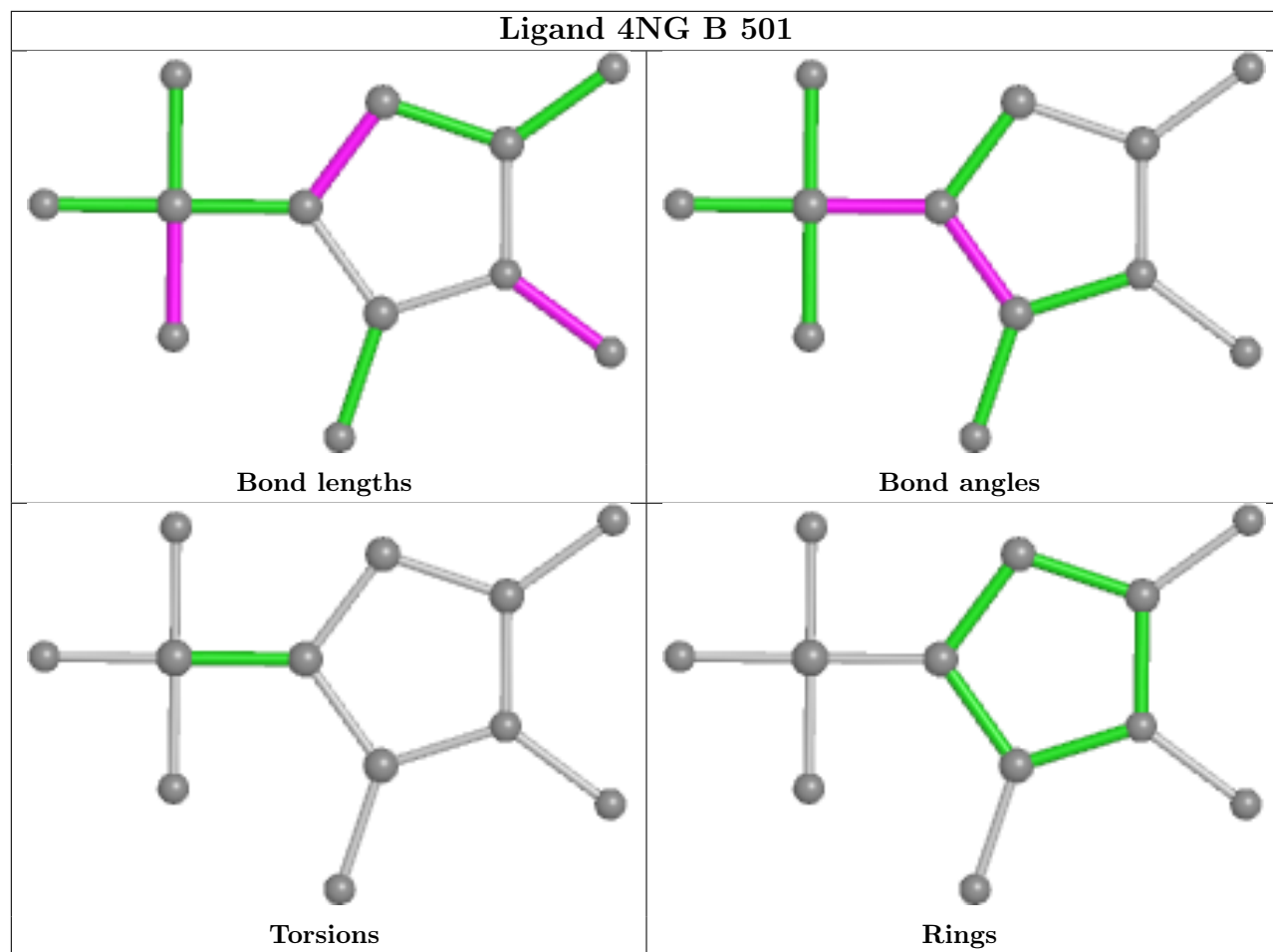
There are no ring outliers.

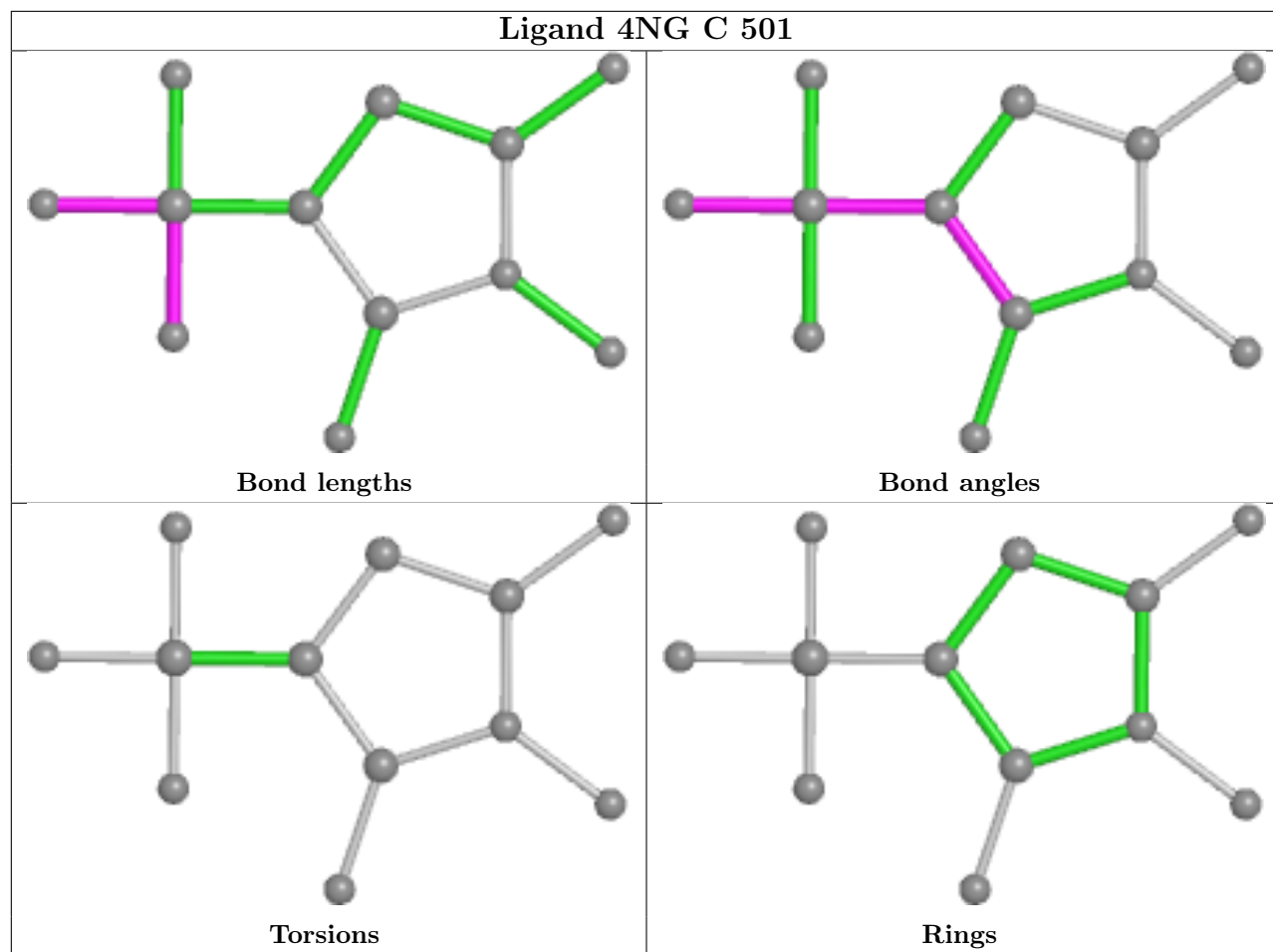
3 monomers are involved in 3 short contacts:

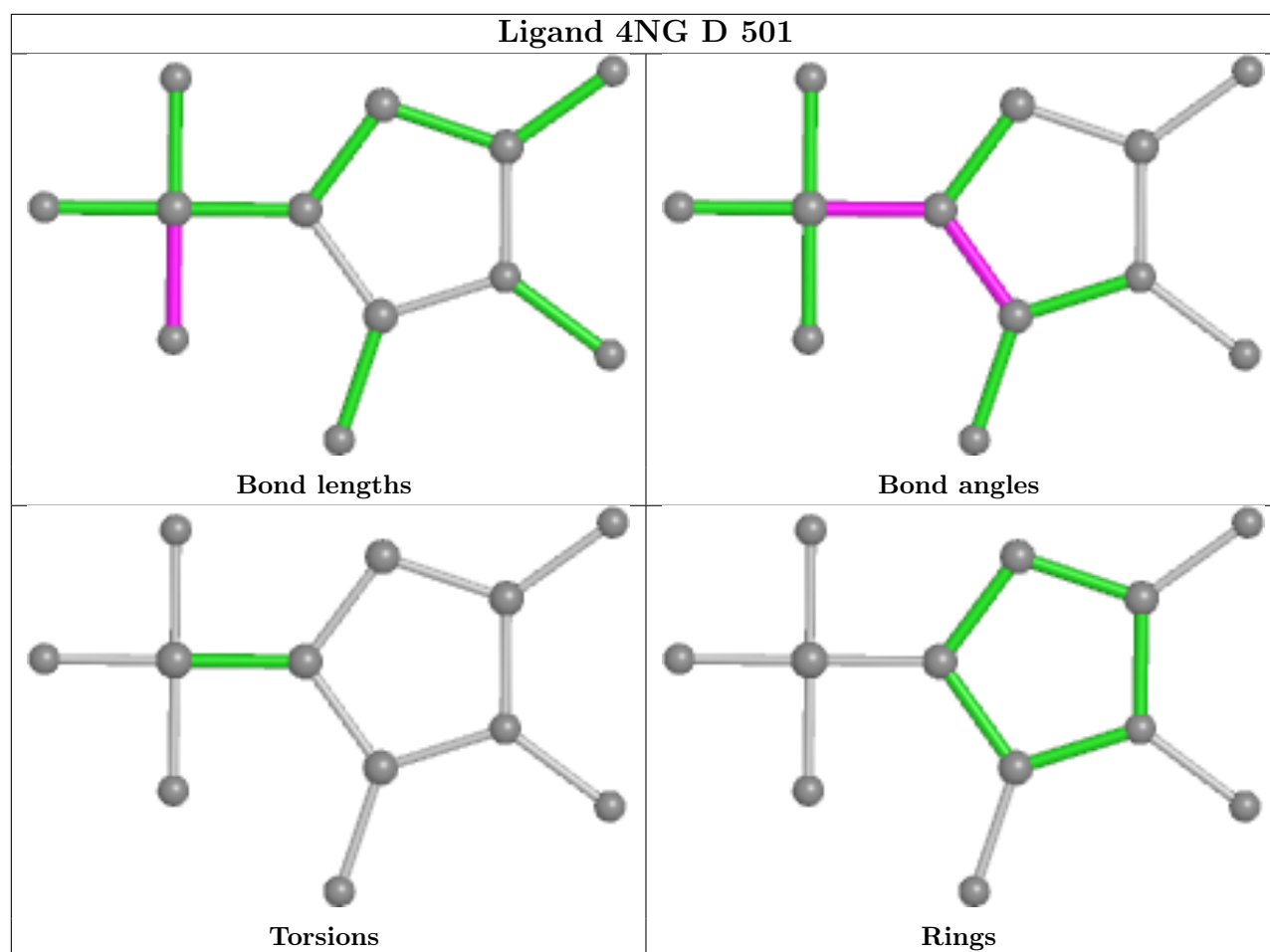
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	GOL	1	0
4	D	504	GOL	1	0
4	F	504	GOL	1	0

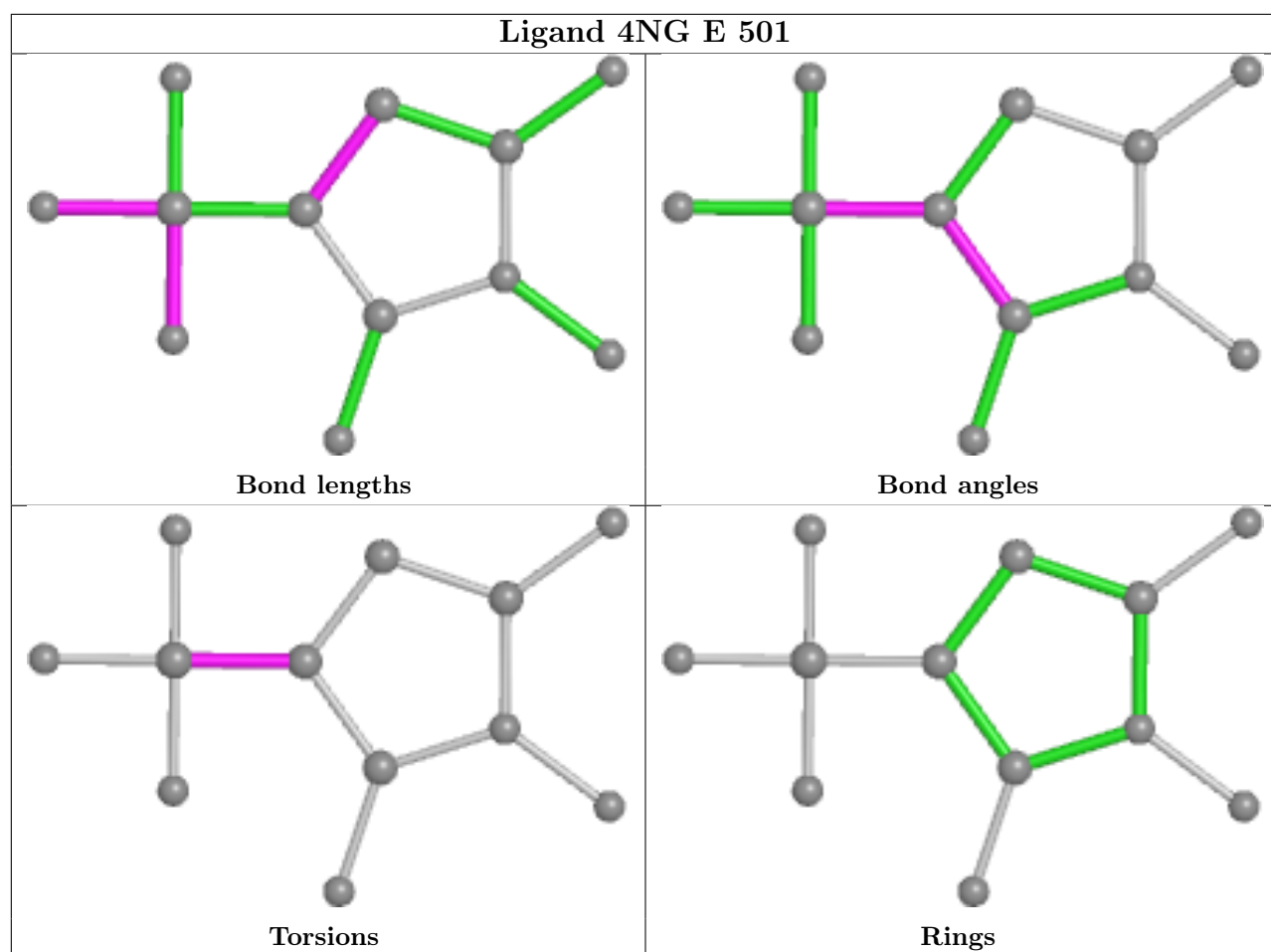
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

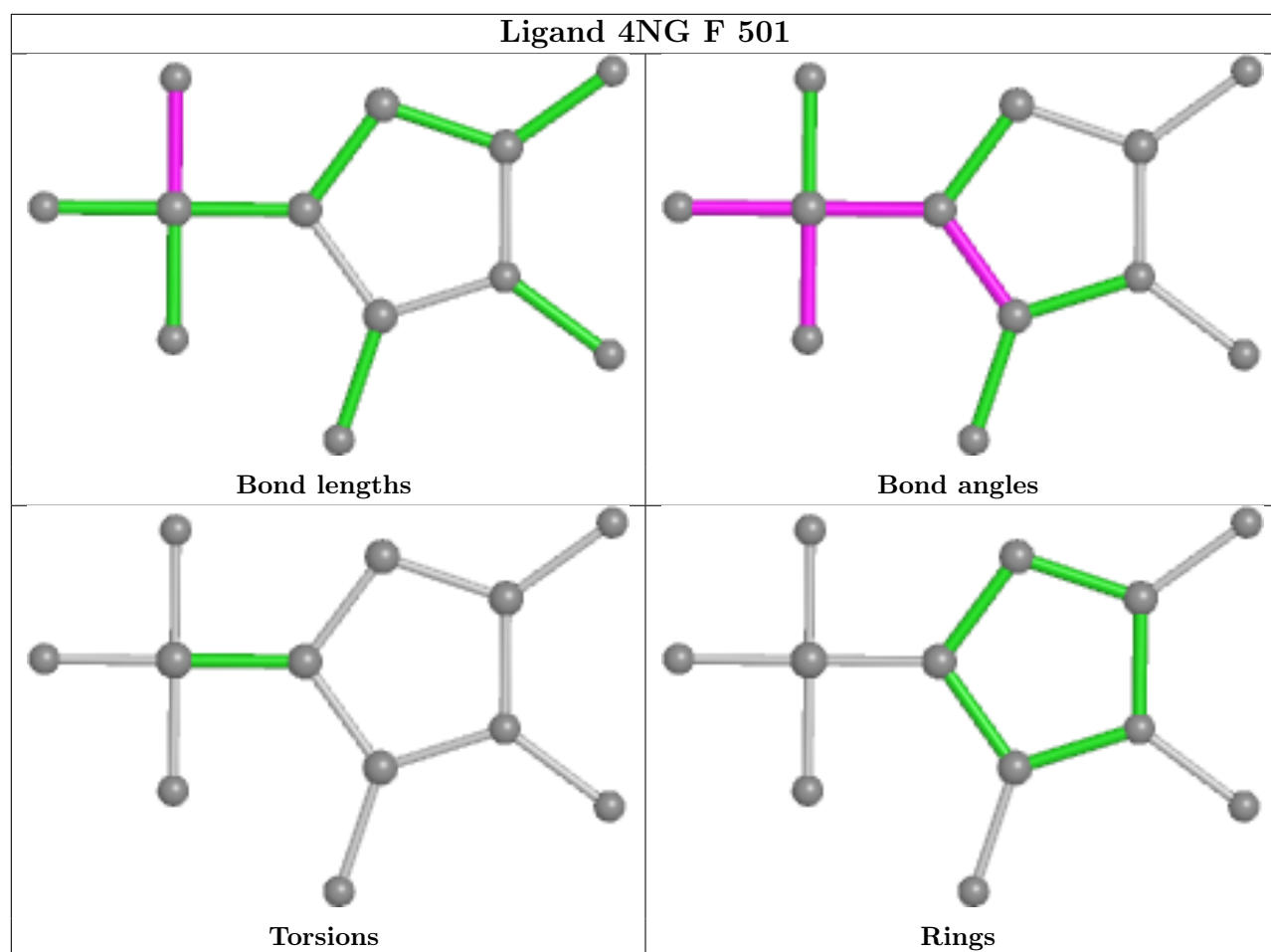












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/439 (99%)	-0.39	2 (0%) 90 91	18, 29, 54, 109	0
1	B	438/439 (99%)	-0.40	2 (0%) 90 91	19, 31, 61, 117	0
1	C	437/439 (99%)	-0.02	9 (2%) 63 65	23, 45, 84, 119	0
1	D	439/439 (100%)	-0.27	8 (1%) 68 70	24, 38, 70, 115	0
1	E	439/439 (100%)	-0.50	5 (1%) 80 81	21, 30, 59, 114	0
1	F	439/439 (100%)	-0.40	5 (1%) 80 81	20, 32, 58, 110	0
All	All	2630/2634 (99%)	-0.33	31 (1%) 79 80	18, 34, 70, 119	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	HIS	5.2
1	C	260	ALA	5.2
1	E	158	HIS	4.3
1	B	263	GLY	4.2
1	C	431	ALA	4.1
1	F	159	ALA	4.1
1	F	158	HIS	4.1
1	C	162	ASN	3.7
1	A	162	ASN	3.5
1	D	157	GLU	3.5
1	D	158	HIS	3.4
1	B	158	HIS	3.2
1	D	160	ASP	3.0
1	F	157	GLU	2.9
1	E	160	ASP	2.8
1	C	160	ASP	2.8
1	D	162	ASN	2.7
1	A	158	HIS	2.7
1	F	162	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	257	TYR	2.6
1	C	302	TYR	2.4
1	C	263	GLY	2.4
1	E	253	LYS	2.3
1	D	266	ALA	2.3
1	E	263	GLY	2.3
1	D	257	TYR	2.3
1	F	263	GLY	2.2
1	C	161	ASN	2.2
1	D	263	GLY	2.2
1	E	265	LYS	2.1
1	D	251	PHE	2.1

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
5	SO4	D	506	5/5	0.90	0.17	82,85,86,94	0
5	SO4	C	504	5/5	0.92	0.15	67,76,86,86	0
5	SO4	D	507	5/5	0.92	0.19	71,74,78,83	0
5	SO4	D	505	5/5	0.93	0.18	47,73,81,95	0
5	SO4	F	505	5/5	0.94	0.20	72,75,90,91	0
4	GOL	E	504	6/6	0.94	0.13	35,36,41,43	0
5	SO4	E	505	5/5	0.94	0.10	60,62,73,81	0
5	SO4	C	505	5/5	0.95	0.10	59,67,71,75	0
4	GOL	D	504	6/6	0.95	0.16	38,46,51,52	0
4	GOL	F	504	6/6	0.96	0.11	36,41,45,46	0
2	4NG	C	501	12/12	0.96	0.09	39,44,49,50	0

Continued on next page...

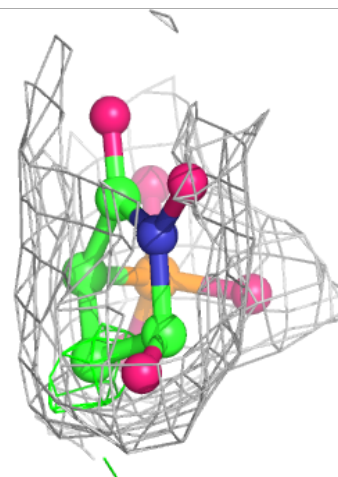
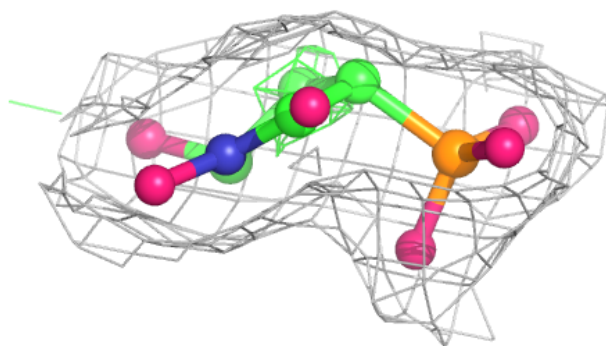
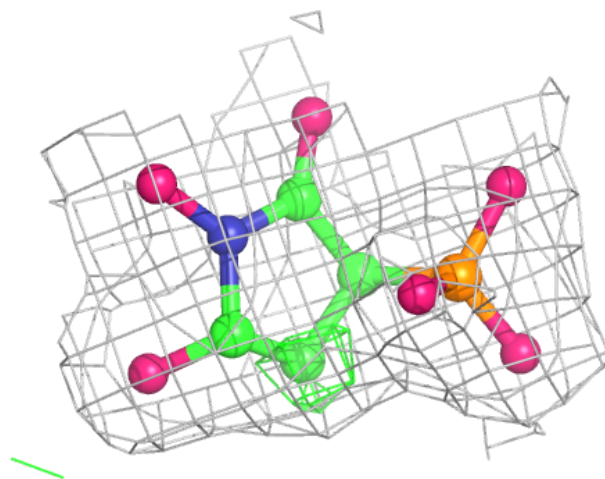
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	503	1/1	0.96	0.05	34,34,34,34	0
4	GOL	B	504	6/6	0.96	0.09	29,39,44,45	0
5	SO4	B	506	5/5	0.96	0.09	52,55,69,71	0
4	GOL	A	504	6/6	0.96	0.13	32,44,46,50	0
5	SO4	E	506	5/5	0.96	0.19	59,65,71,71	0
5	SO4	F	507	5/5	0.97	0.16	62,69,71,78	0
5	SO4	B	505	5/5	0.97	0.10	52,52,59,62	0
5	SO4	F	506	5/5	0.97	0.08	50,54,55,70	0
3	MG	E	502	1/1	0.98	0.07	24,24,24,24	0
2	4NG	B	501	12/12	0.98	0.10	26,29,30,34	0
3	MG	C	502	1/1	0.98	0.12	41,41,41,41	0
3	MG	F	502	1/1	0.99	0.09	33,33,33,33	0
2	4NG	A	501	12/12	0.99	0.10	24,27,29,29	0
2	4NG	E	501	12/12	0.99	0.09	25,28,30,30	0
3	MG	E	503	1/1	0.99	0.04	26,26,26,26	0
3	MG	A	503	1/1	0.99	0.04	29,29,29,29	0
2	4NG	D	501	12/12	0.99	0.09	33,37,42,42	0
3	MG	F	503	1/1	0.99	0.03	31,31,31,31	0
3	MG	D	502	1/1	0.99	0.04	34,34,34,34	0
3	MG	A	502	1/1	0.99	0.04	26,26,26,26	0
3	MG	C	503	1/1	0.99	0.07	35,35,35,35	0
2	4NG	F	501	12/12	0.99	0.07	28,31,33,34	0
3	MG	B	502	1/1	0.99	0.09	26,26,26,26	0
3	MG	D	503	1/1	0.99	0.02	38,38,38,38	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.

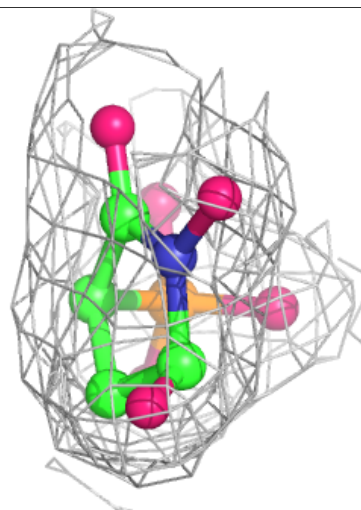
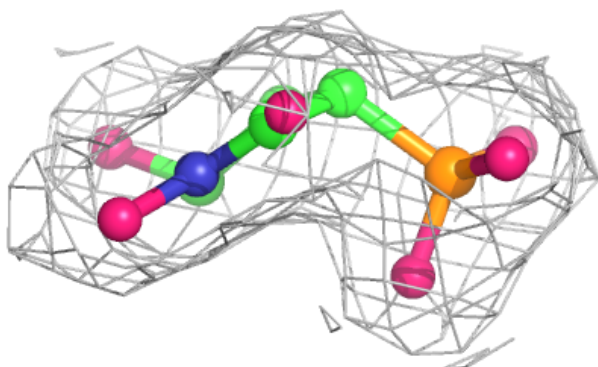
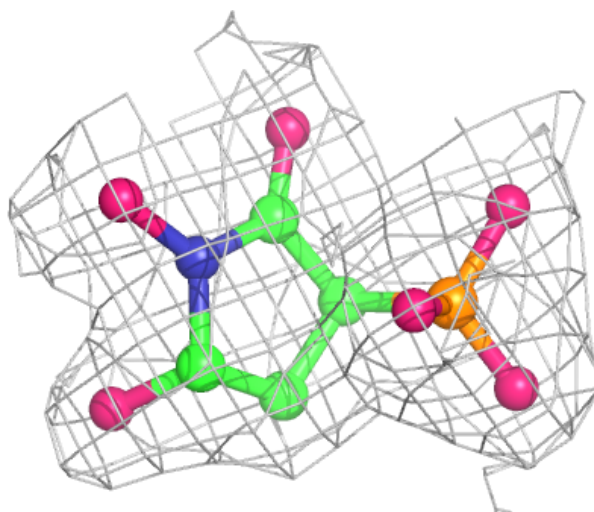
Electron density around 4NG C 501:

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



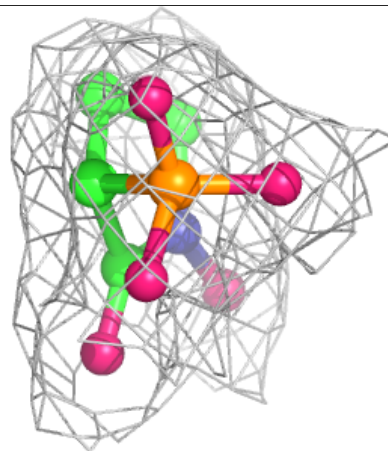
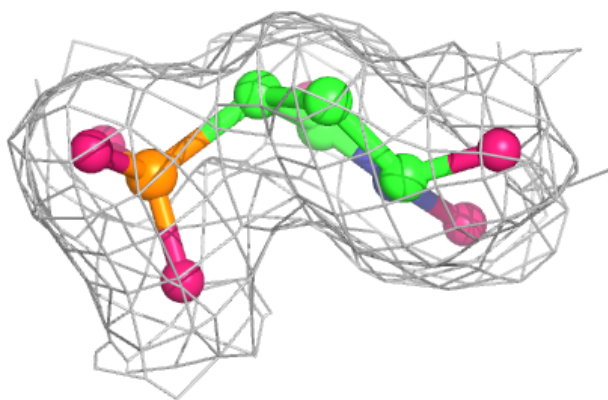
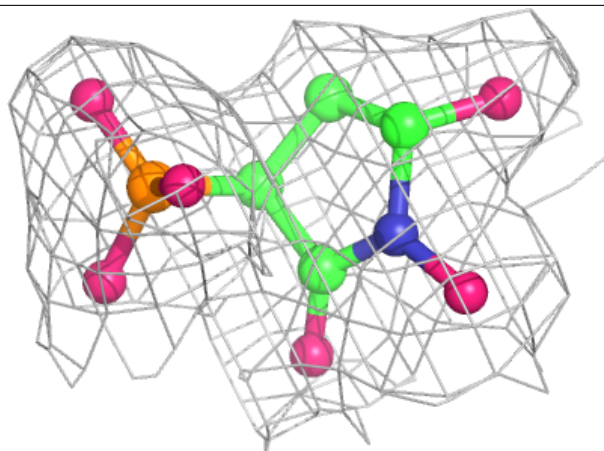
Electron density around 4NG B 501:

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



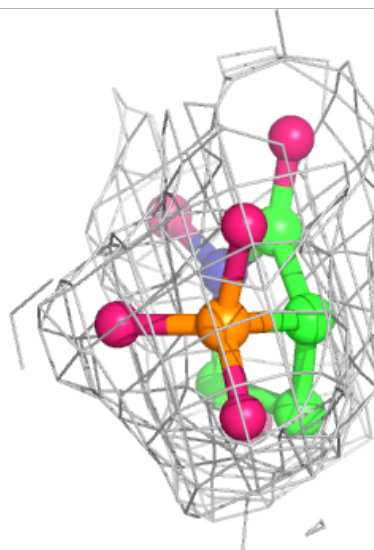
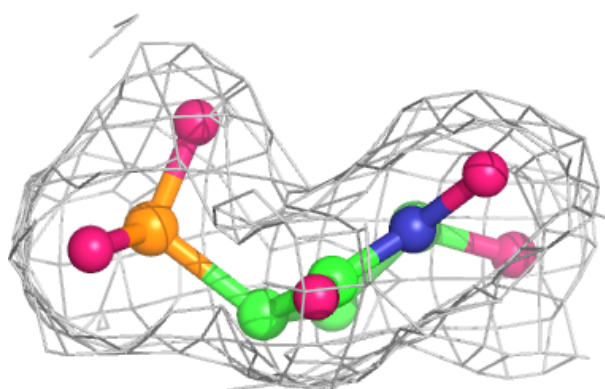
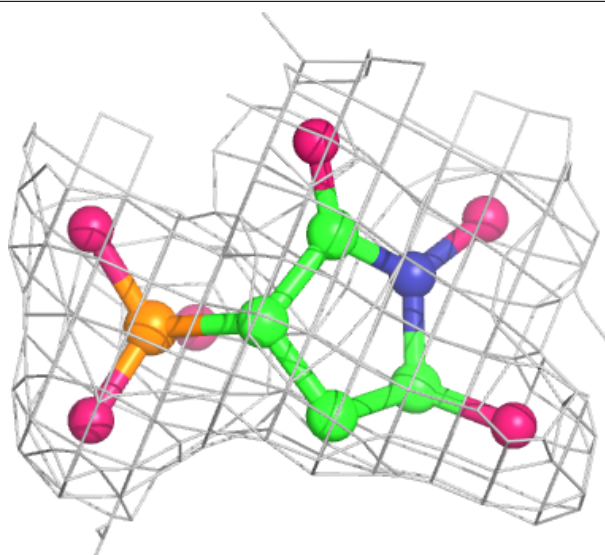
Electron density around 4NG A 501:

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



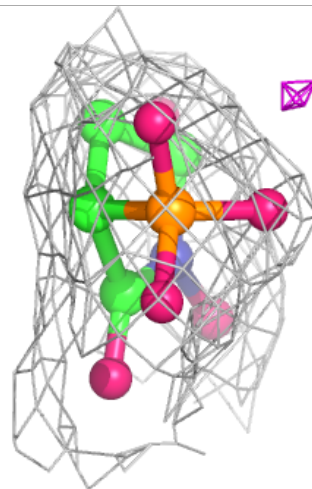
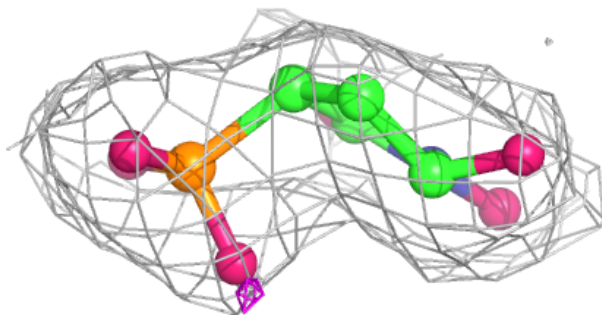
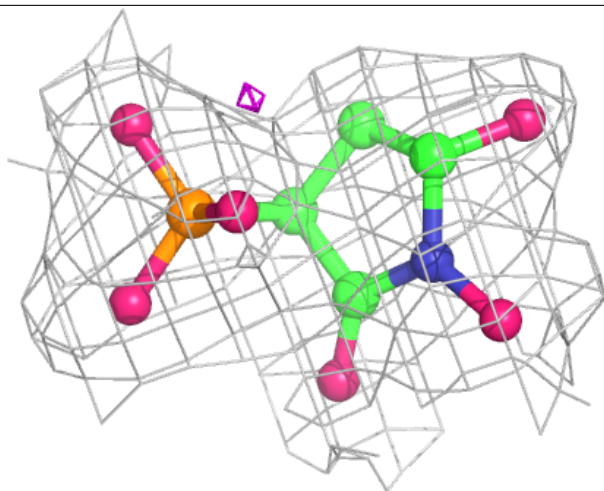
Electron density around 4NG E 501:

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



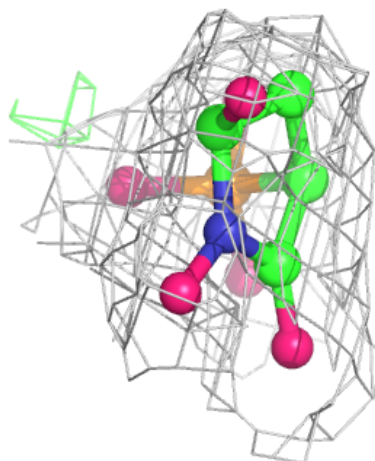
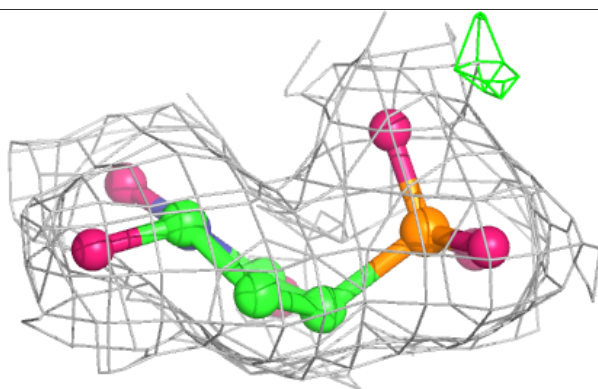
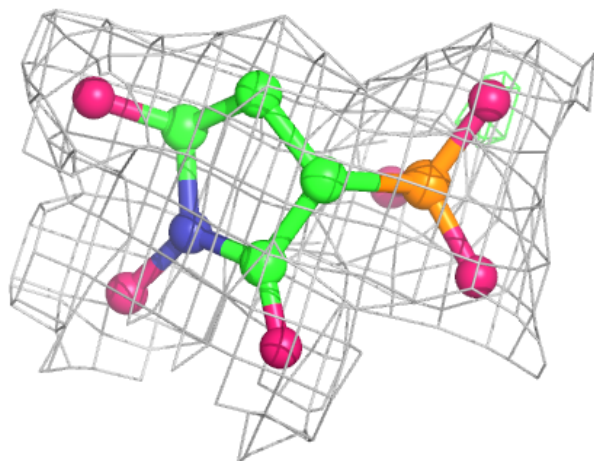
Electron density around 4NG D 501:

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



Electron density around 4NG F 501:

$2mF_o-DF_c$ (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.