



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:34 PM UTC

PDB ID : 1VA6 / pdb_00001va6
Title : Crystal structure of Gamma-glutamylcysteine synthetase from Escherichia Coli B complexed with Transition-state analogue
Authors : Hibi, T.; Nii, H.; Nakatsu, T.; Kato, H.; Hiratake, J.; Oda, J.
Deposited on : 2004-02-12
Resolution : 2.10 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

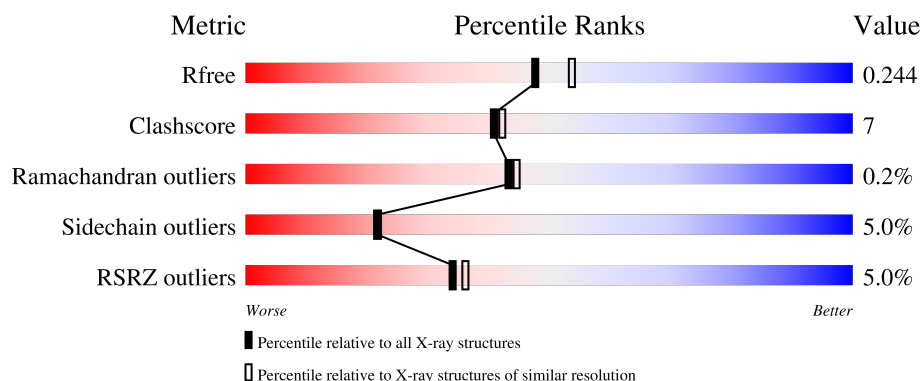
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	518	 3% 81% 16% ..
1	B	518	 7% 82% 14% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8486 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4017	2549	685	765	18			
1	B	503	Total	C	N	O	S	0	0	0
			3981	2528	679	756	18			

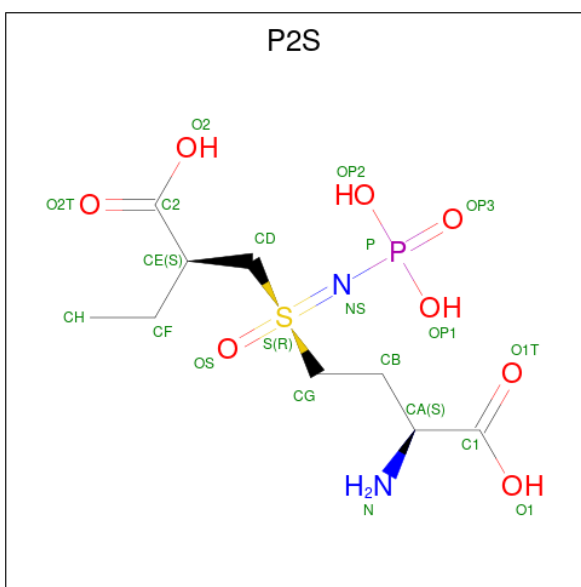
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	CYS	engineered mutation	UNP P0A6W9
A	164	SER	CYS	engineered mutation	UNP P0A6W9
A	205	SER	CYS	engineered mutation	UNP P0A6W9
A	223	SER	CYS	engineered mutation	UNP P0A6W9
B	106	SER	CYS	engineered mutation	UNP P0A6W9
B	164	SER	CYS	engineered mutation	UNP P0A6W9
B	205	SER	CYS	engineered mutation	UNP P0A6W9
B	223	SER	CYS	engineered mutation	UNP P0A6W9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

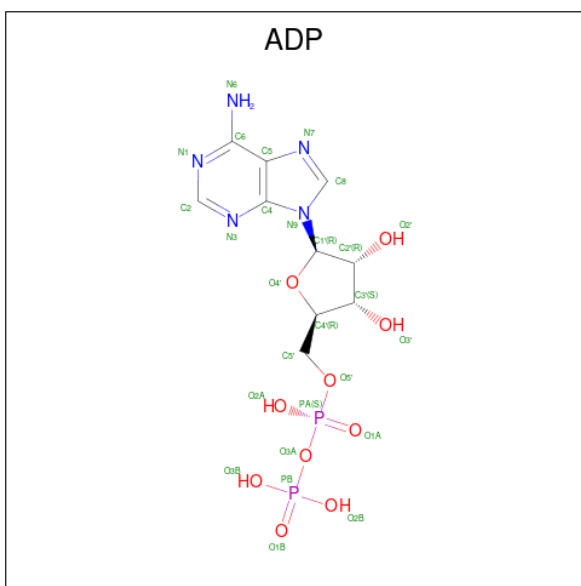
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		
2	B	4	Total	Mg	0	0
			4	4		

- Molecule 3 is (2S)-2-AMINO-4-[[[(2R)-2-CARBOXYBUTYL](PHOSPHONO)SULFONIMIDOYL]BUTANOIC ACID (CCD ID: P2S) (formula: C₉H₁₉N₂O₈PS).



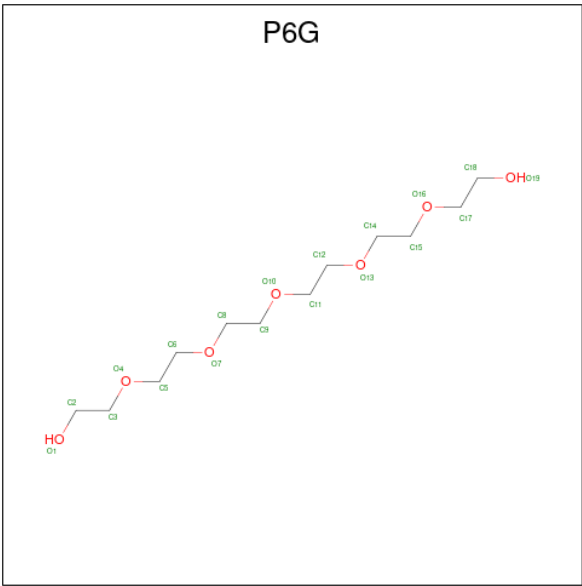
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	N 2	O 8	P 1	S 1	0	0
3	B	1	Total 21	C 9	N 2	O 8	P 1	S 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	B	1	Total	C	O	0	0
			19	12	7		

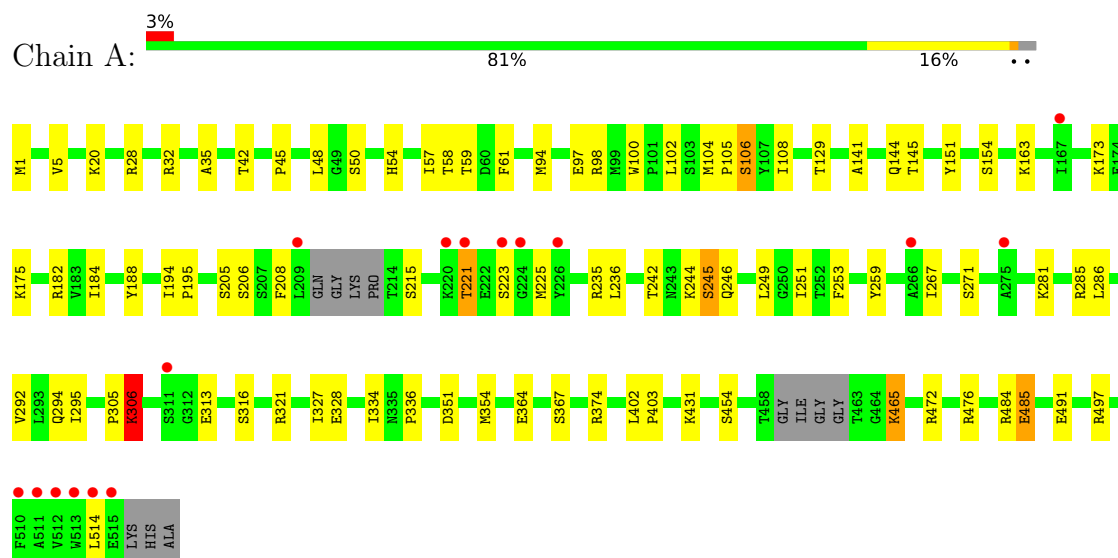
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total	O	0	0
			194	194		
6	B	152	Total	O	0	0
			152	152		

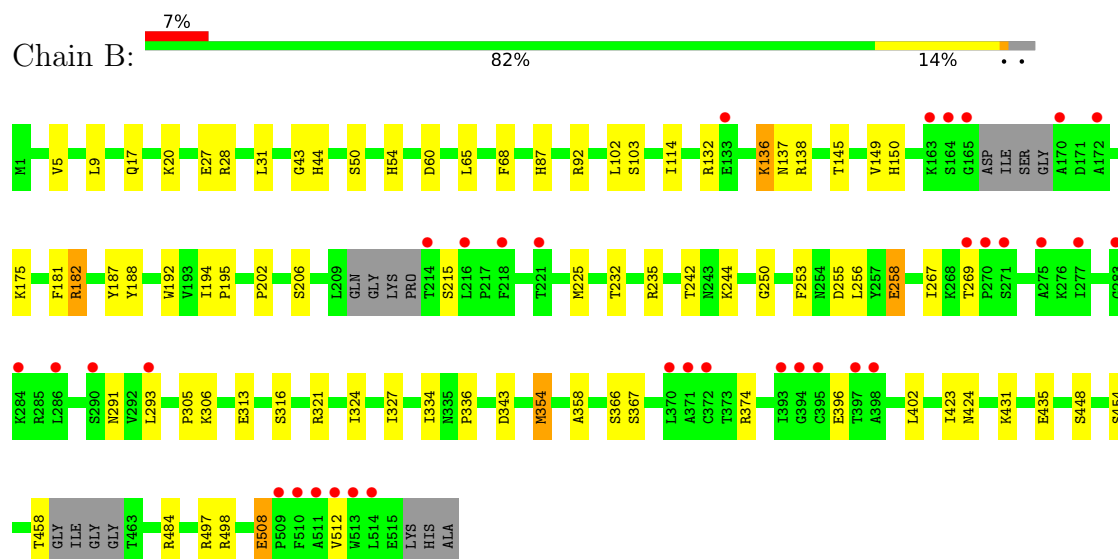
3 Residue-property plots [i](#)

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

• Molecule 1: Glutamate–cysteine ligase



• Molecule 1: Glutamate–cysteine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.47Å 97.36Å 102.19Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.10) 97.0 (40.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.225 0.225 , 0.244	Depositor DCC
R_{free} test set	3702 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: P2S, P6G, MG, ADP

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	1.08	0/4103	0.98	2/5555 (0.0%)
1	B	0.99	1/4066 (0.0%)	0.96	3/5506 (0.1%)
All	All	1.04	1/8169 (0.0%)	0.97	5/11061 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	ASP	CA-C	13.24	1.60	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	ILE	CB-CA-C	-6.09	104.05	112.02
1	B	269	THR	N-CA-C	5.33	117.28	109.71
1	A	294	GLN	N-CA-C	-5.16	105.34	111.69
1	B	306	LYS	N-CA-C	5.13	116.88	109.07
1	A	306	LYS	N-CA-C	5.03	116.71	108.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4017	0	3935	59	0
1	B	3981	0	3889	45	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	21	0	15	0	0
3	B	21	0	15	0	0
4	A	27	0	12	1	0
4	B	27	0	12	0	0
5	A	19	0	26	5	0
5	B	19	0	26	7	0
6	A	194	0	0	6	0
6	B	152	0	0	4	0
All	All	8486	0	7930	105	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 7.

All (105) 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:431:LYS:HE2	1:B:435:GLU:OE2	1.79	0.82
1:A:242:THR:HG22	1:A:244:LYS:H	1.47	0.77
1:B:225:MET:HA	1:B:225:MET:HE2	1.68	0.74
1:A:188:TYR:HE1	5:A:526:P6G:H152	1.54	0.72
1:A:485:GLU:HG2	6:A:678:HOH:O	1.90	0.70
1:B:188:TYR:HE1	5:B:1526:P6G:H152	1.57	0.69
1:B:508:GLU:HG2	6:B:1674:HOH:O	1.92	0.69
1:A:225:MET:HE2	1:A:225:MET:HA	1.75	0.68
1:A:305:PRO:O	1:A:306:LYS:HG2	1.94	0.68
1:B:192:TRP:O	1:B:195:PRO:HD2	1.93	0.67
1:A:5:VAL:O	1:A:5:VAL:HG12	1.97	0.65
1:A:497:ARG:HD2	6:A:677:HOH:O	1.97	0.65
1:B:27:GLU:HB2	1:B:150:HIS:HB2	1.80	0.64
1:A:236:LEU:CD2	5:A:526:P6G:H32	2.28	0.63
1:B:192:TRP:C	1:B:195:PRO:HD2	2.24	0.63
1:A:221:THR:HG23	1:A:223:SER:H	1.63	0.63
1:A:1:MET:HE3	6:A:577:HOH:O	1.98	0.63
1:A:100:TRP:CZ2	1:A:106:SER:HB2	2.34	0.62
1:B:242:THR:HG22	1:B:244:LYS:H	1.64	0.62
1:A:285:ARG:NH1	1:A:514:LEU:HD12	2.16	0.60
1:B:194:ILE:HB	1:B:195:PRO:HD3	1.84	0.60
1:B:374:ARG:HD2	5:B:1526:P6G:H141	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HE2	6:A:643:HOH:O	2.02	0.58
1:B:114:ILE:HD13	1:B:145:THR:HG21	1.84	0.58
1:B:374:ARG:HB2	5:B:1526:P6G:H142	1.85	0.58
1:A:334:ILE:O	1:A:336:PRO:HD3	2.03	0.58
1:A:259:TYR:CZ	1:A:305:PRO:HG2	2.40	0.57
1:B:267:ILE:HD13	1:B:293:LEU:HB2	1.86	0.57
1:B:235:ARG:NH2	5:B:1526:P6G:H22	2.19	0.56
5:B:1526:P6G:H32	6:B:1633:HOH:O	2.04	0.56
1:A:281:LYS:HB3	1:A:286:LEU:HD11	1.87	0.56
1:A:141:ALA:O	1:A:145:THR:HG23	2.06	0.55
1:A:105:PRO:HD2	1:A:208:PHE:CZ	2.42	0.55
1:A:151:TYR:OH	1:A:351:ASP:OD1	2.23	0.55
1:B:188:TYR:CE1	5:B:1526:P6G:H152	2.40	0.54
1:A:54:HIS:HB3	1:A:57:ILE:O	2.09	0.53
1:B:68:PHE:CD2	1:B:87:HIS:CE1	2.97	0.52
1:A:32:ARG:HG2	1:A:94:MET:CE	2.39	0.52
1:B:402:LEU:C	1:B:402:LEU:HD23	2.35	0.52
1:B:242:THR:HG22	1:B:244:LYS:N	2.25	0.52
1:A:259:TYR:CE2	1:A:305:PRO:HG2	2.45	0.52
1:A:244:LYS:C	1:A:246:GLN:H	2.19	0.51
1:A:45:PRO:HD2	1:A:48:LEU:HD12	1.90	0.51
1:B:305:PRO:HB3	1:B:324:ILE:HD13	1.92	0.51
1:A:313:GLU:OE1	1:A:321:ARG:NH1	2.43	0.51
1:B:431:LYS:HE2	1:B:435:GLU:CD	2.35	0.50
1:A:364:GLU:HG3	6:A:691:HOH:O	2.11	0.50
1:B:17:GLN:HB2	6:B:1672:HOH:O	2.11	0.50
1:B:181:PHE:CE2	1:B:256:LEU:HA	2.47	0.50
1:A:267:ILE:HD12	1:A:295:ILE:HA	1.95	0.49
1:B:454:SER:O	1:B:458:THR:HG23	2.13	0.49
1:B:334:ILE:O	1:B:336:PRO:HD3	2.13	0.48
1:A:50:SER:O	1:A:54:HIS:HB2	2.14	0.48
1:A:306:LYS:NZ	1:A:328:GLU:OE1	2.42	0.48
1:B:202:PRO:HD2	6:B:1601:HOH:O	2.13	0.47
1:A:244:LYS:C	1:A:246:GLN:N	2.70	0.47
1:A:259:TYR:OH	1:A:305:PRO:HD2	2.15	0.47
1:A:154:SER:OG	4:A:521:ADP:N1	2.48	0.47
1:B:374:ARG:HD2	5:B:1526:P6G:C14	2.45	0.47
1:A:205:SER:CB	1:A:225:MET:HE1	2.45	0.47
1:B:313:GLU:OE1	1:B:321:ARG:NH1	2.48	0.47
1:A:472:ARG:O	1:A:476:ARG:HG3	2.15	0.47
1:B:132:ARG:HH11	1:B:132:ARG:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CG	1:A:144:GLN:HB3	2.49	0.46
1:A:102:LEU:HD23	1:A:336:PRO:HB3	1.98	0.46
1:B:181:PHE:HE2	1:B:256:LEU:HA	1.81	0.46
1:A:402:LEU:C	1:A:402:LEU:HD23	2.41	0.46
1:B:255:ASP:HB3	1:B:258:GLU:HB2	1.98	0.45
1:A:188:TYR:CE1	5:A:526:P6G:H152	2.44	0.45
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.00	0.44
1:B:138:ARG:NH2	1:B:291:ASN:O	2.43	0.44
1:A:184:ILE:HG21	1:A:253:PHE:CD1	2.52	0.44
1:B:5:VAL:HB	1:B:9:LEU:HD12	1.99	0.44
1:A:305:PRO:O	1:A:306:LYS:CG	2.64	0.44
1:A:105:PRO:HD2	1:A:208:PHE:HZ	1.83	0.44
1:A:105:PRO:HB3	1:A:108:ILE:HD12	1.99	0.44
1:A:182:ARG:NH1	6:A:666:HOH:O	2.51	0.44
1:A:54:HIS:NE2	1:A:491:GLU:HG3	2.33	0.43
1:B:50:SER:O	1:B:54:HIS:HB2	2.18	0.43
1:A:465:LYS:HB3	1:A:465:LYS:HE2	1.78	0.43
1:A:42:THR:OG1	1:A:97:GLU:OE2	2.30	0.43
1:B:149:VAL:HG23	1:B:334:ILE:HD13	2.00	0.43
1:A:249:LEU:HD21	1:A:292:VAL:HG11	2.01	0.42
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.91	0.42
1:A:35:ALA:HA	1:A:98:ARG:HD3	2.01	0.42
1:B:232:THR:HA	1:B:448:SER:CB	2.49	0.42
1:B:250:GLY:HA2	1:B:367:SER:OG	2.19	0.42
1:A:194:ILE:HB	1:A:195:PRO:CD	2.50	0.42
1:A:194:ILE:HB	1:A:195:PRO:HD3	2.02	0.42
1:B:187:TYR:HD2	1:B:354:MET:HE1	1.85	0.42
1:A:402:LEU:N	1:A:403:PRO:CD	2.83	0.42
1:A:104:MET:HE1	1:A:235:ARG:HA	2.01	0.41
1:B:31:LEU:CD2	1:B:65:LEU:HD13	2.51	0.41
1:A:104:MET:CE	1:A:235:ARG:HA	2.50	0.41
1:A:374:ARG:HG3	5:A:526:P6G:H121	2.03	0.41
1:B:343:ASP:OD1	1:B:343:ASP:C	2.63	0.41
1:B:43:GLY:O	1:B:44:HIS:C	2.63	0.41
1:A:236:LEU:HD23	5:A:526:P6G:H32	2.03	0.41
1:B:136:LYS:HG2	1:B:137:ASN:N	2.36	0.41
1:B:188:TYR:CE2	1:B:253:PHE:CE2	3.09	0.41
1:B:182:ARG:HH11	1:B:182:ARG:HD2	1.76	0.40
1:B:182:ARG:HD3	1:B:358:ALA:O	2.20	0.40
1:A:244:LYS:O	1:A:246:GLN:N	2.55	0.40
1:A:58:THR:OG1	1:A:59:THR:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:SER:HA	1:A:225:MET:CE	2.51	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	501/518 (97%)	489 (98%)	11 (2%)	1 (0%)	43	44
1	B	495/518 (96%)	480 (97%)	14 (3%)	1 (0%)	43	44
All	All	996/1036 (96%)	969 (97%)	25 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLU
1	A	245	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/434 (98%)	402 (95%)	22 (5%)	21	20
1	B	418/434 (96%)	398 (95%)	20 (5%)	23	23
All	All	842/868 (97%)	800 (95%)	42 (5%)	22	22

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	28	ARG
1	A	106	SER
1	A	129	THR
1	A	173	LYS
1	A	175	LYS
1	A	206	SER
1	A	215	SER
1	A	221	THR
1	A	245	SER
1	A	251	ILE
1	A	271	SER
1	A	306	LYS
1	A	316	SER
1	A	327	ILE
1	A	354	MET
1	A	367	SER
1	A	431	LYS
1	A	454	SER
1	A	465	LYS
1	A	484	ARG
1	A	485	GLU
1	B	20	LYS
1	B	28	ARG
1	B	92	ARG
1	B	103	SER
1	B	136	LYS
1	B	175	LYS
1	B	182	ARG
1	B	206	SER
1	B	215	SER
1	B	258	GLU
1	B	316	SER
1	B	327	ILE
1	B	354	MET
1	B	366	SER
1	B	424	ASN
1	B	484	ARG
1	B	497	ARG
1	B	498	ARG
1	B	508	GLU
1	B	512	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	424	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	ADP	A	521	2	28,29,29	1.27	4 (14%)	43,45,45	1.99	15 (34%)
3	P2S	A	520	2	15,20,20	3.88	9 (60%)	13,29,29	1.57	3 (23%)
3	P2S	B	1520	2	15,20,20	3.88	9 (60%)	13,29,29	1.76	4 (30%)
4	ADP	B	1521	2	28,29,29	1.12	2 (7%)	43,45,45	1.94	12 (27%)
5	P6G	B	1526	-	18,18,18	0.64	0	17,17,17	0.84	0
5	P6G	A	526	-	18,18,18	0.58	0	17,17,17	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	521	2	-	4/16/32/32	0/3/3/3
3	P2S	A	520	2	-	4/19/27/27	-
3	P2S	B	1520	2	-	4/19/27/27	-
4	ADP	B	1521	2	-	3/16/32/32	0/3/3/3
5	P6G	B	1526	-	-	8/16/16/16	-
5	P6G	A	526	-	-	10/16/16/16	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1520	P2S	CB-CG	-10.10	1.43	1.52
3	A	520	P2S	CB-CG	-8.53	1.44	1.52
3	A	520	P2S	P-OP3	6.61	1.56	1.46
3	B	1520	P2S	P-OP3	6.27	1.56	1.46
3	A	520	P2S	P-OP2	5.76	1.66	1.54
3	B	1520	P2S	CE-C2	-5.03	1.42	1.51
3	A	520	P2S	CE-C2	-4.82	1.42	1.51
3	A	520	P2S	CB-CA	-4.45	1.43	1.53
3	B	1520	P2S	CB-CA	-3.96	1.44	1.53
3	B	1520	P2S	P-NS	3.16	1.70	1.58
4	A	521	ADP	O4'-C4'	-2.80	1.38	1.45
3	B	1520	P2S	P-OP2	2.59	1.60	1.54
4	B	1521	ADP	O4'-C4'	-2.59	1.39	1.45
3	B	1520	P2S	O2T-C2	2.52	1.29	1.22
4	A	521	ADP	PA-O3A	2.51	1.62	1.59
3	A	520	P2S	O2T-C2	2.43	1.29	1.22
3	A	520	P2S	CA-N	-2.40	1.36	1.48
3	A	520	P2S	OS-S	2.36	1.58	1.45
3	B	1520	P2S	CA-N	-2.33	1.36	1.48
4	B	1521	ADP	C8-N7	2.31	1.36	1.31
3	A	520	P2S	O1T-C1	2.21	1.28	1.22
4	A	521	ADP	PB-O1B	-2.20	1.43	1.50
3	B	1520	P2S	O1T-C1	2.12	1.28	1.22
4	A	521	ADP	PB-O3B	2.08	1.62	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	521	ADP	N3-C2-N1	-5.05	120.93	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1521	ADP	N3-C2-N1	-4.96	121.07	128.58
4	B	1521	ADP	N9-C8-N7	-4.87	107.03	113.94
4	A	521	ADP	C5-C4-N3	-4.38	120.69	126.72
4	A	521	ADP	N9-C8-N7	-4.27	107.88	113.94
4	B	1521	ADP	C5-N7-C8	3.72	109.29	103.45
4	A	521	ADP	C2'-C3'-C4'	3.59	109.54	102.61
4	B	1521	ADP	C5-C4-N3	-3.50	121.89	126.72
4	A	521	ADP	C4-N9-C8	3.39	109.30	105.74
4	B	1521	ADP	C2'-C3'-C4'	3.38	109.13	102.61
3	B	1520	P2S	O1-C1-O1T	-3.16	116.90	124.08
4	A	521	ADP	N3-C4-N9	2.97	132.22	127.17
4	A	521	ADP	C2-N3-C4	2.96	119.05	111.83
3	B	1520	P2S	O2-C2-CE	2.84	121.53	114.16
3	B	1520	P2S	OP2-P-OP3	-2.81	107.90	113.77
3	B	1520	P2S	O2-C2-O2T	-2.80	117.74	124.08
4	A	521	ADP	O4'-C1'-N9	2.79	113.45	108.09
4	B	1521	ADP	O4'-C4'-C5'	2.78	118.23	109.33
4	A	521	ADP	C5-N7-C8	2.72	107.73	103.45
4	B	1521	ADP	O3B-PB-O3A	2.72	113.76	104.64
4	B	1521	ADP	C2-N3-C4	2.69	118.39	111.83
4	A	521	ADP	O3B-PB-O3A	2.63	113.47	104.64
4	B	1521	ADP	C5'-C4'-C3'	-2.60	105.85	115.21
4	B	1521	ADP	O2A-PA-O3A	2.54	114.13	107.27
3	A	520	P2S	OP1-P-OP3	-2.52	108.52	113.77
4	B	1521	ADP	O4'-C1'-N9	2.47	112.83	108.09
4	B	1521	ADP	O3'-C3'-C4'	-2.28	104.53	111.08
4	A	521	ADP	C4-C5-N7	-2.27	107.99	110.58
4	A	521	ADP	C6-C5-C4	2.25	120.25	117.18
4	A	521	ADP	O4'-C4'-C5'	2.18	116.32	109.33
4	A	521	ADP	O2'-C2'-C1'	2.17	117.57	110.10
3	A	520	P2S	O2-C2-O2T	-2.15	119.21	124.08
4	A	521	ADP	C5'-C4'-C3'	-2.09	107.70	115.21
3	A	520	P2S	O2-C2-CE	2.02	119.40	114.16

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	520	P2S	S-CD-CE-C2
3	A	520	P2S	S-CD-CE-CF
3	B	1520	P2S	S-CD-CE-C2
3	B	1520	P2S	S-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
5	B	1526	P6G	O13-C14-C15-O16
5	A	526	P6G	O13-C14-C15-O16
5	B	1526	P6G	O1-C2-C3-O4
5	A	526	P6G	O4-C5-C6-O7
4	A	521	ADP	C3'-C4'-C5'-O5'
5	A	526	P6G	C18-C17-O16-C15
5	B	1526	P6G	O7-C8-C9-O10
5	A	526	P6G	O10-C11-C12-O13
4	A	521	ADP	O4'-C4'-C5'-O5'
5	A	526	P6G	C12-C11-O10-C9
5	B	1526	P6G	C18-C17-O16-C15
5	B	1526	P6G	C2-C3-O4-C5
5	A	526	P6G	C6-C5-O4-C3
5	B	1526	P6G	C12-C11-O10-C9
4	B	1521	ADP	O4'-C4'-C5'-O5'
4	B	1521	ADP	PB-O3A-PA-O2A
3	A	520	P2S	O1T-C1-CA-CB
5	B	1526	P6G	C5-C6-O7-C8
5	B	1526	P6G	O16-C17-C18-O19
5	A	526	P6G	C5-C6-O7-C8
3	A	520	P2S	O1-C1-CA-CB
4	A	521	ADP	PB-O3A-PA-O2A
4	B	1521	ADP	C3'-C4'-C5'-O5'
5	A	526	P6G	C9-C8-O7-C6
4	A	521	ADP	PB-O3A-PA-O1A
3	B	1520	P2S	O1-C1-CA-CB
5	A	526	P6G	O1-C2-C3-O4
5	A	526	P6G	C11-C12-O13-C14
3	B	1520	P2S	O1T-C1-CA-CB

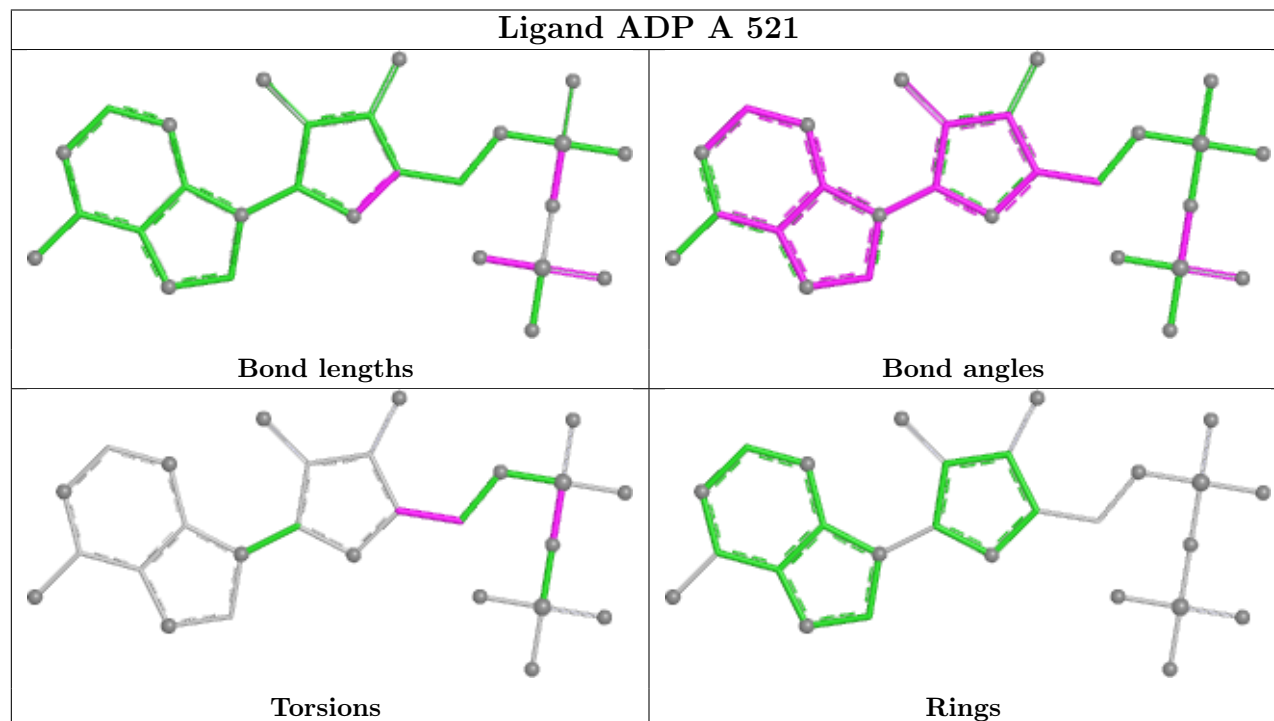
There are no ring outliers.

3 monomers are involved in 13 short contacts:

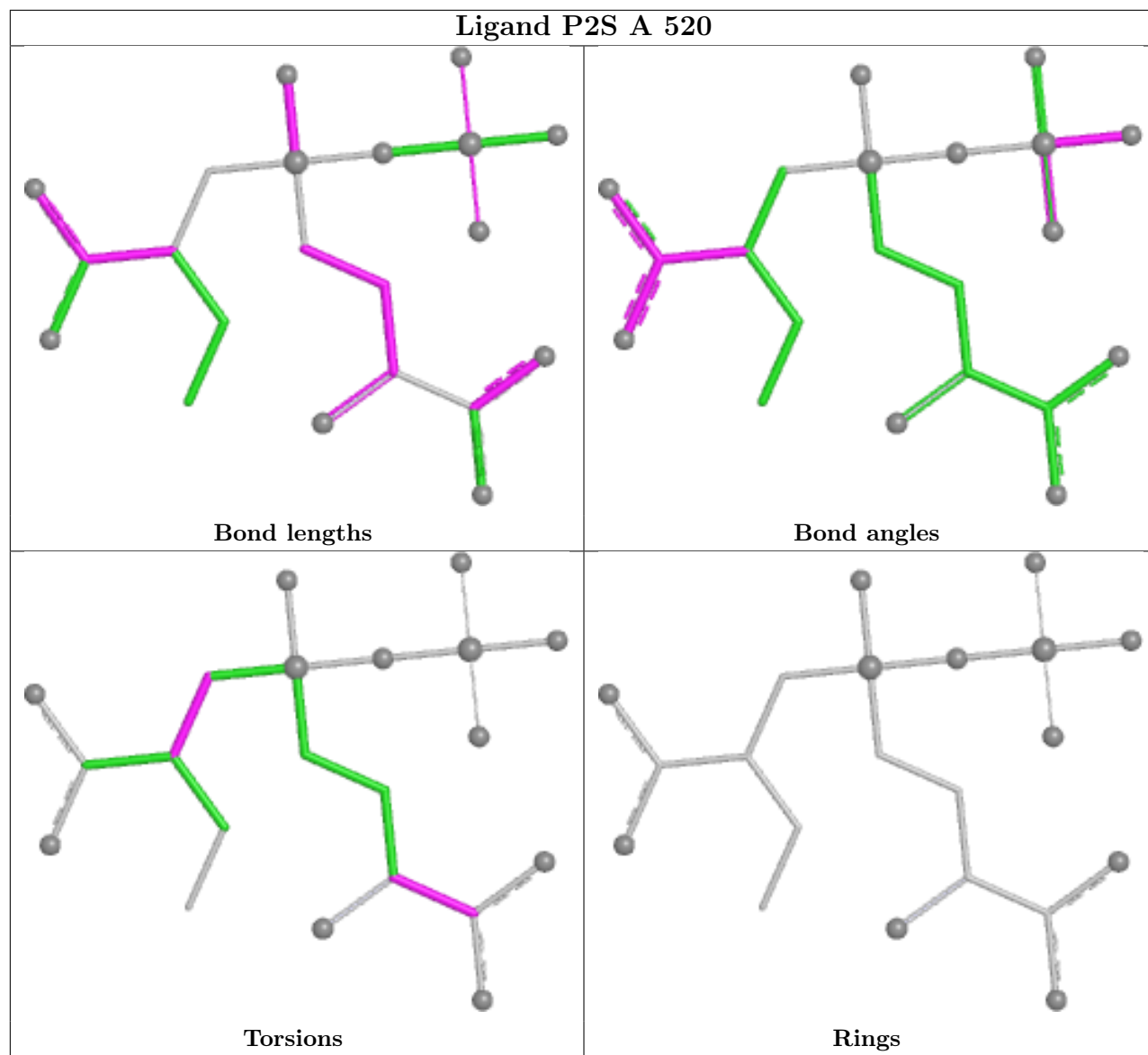
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	521	ADP	1	0
5	B	1526	P6G	7	0
5	A	526	P6G	5	0

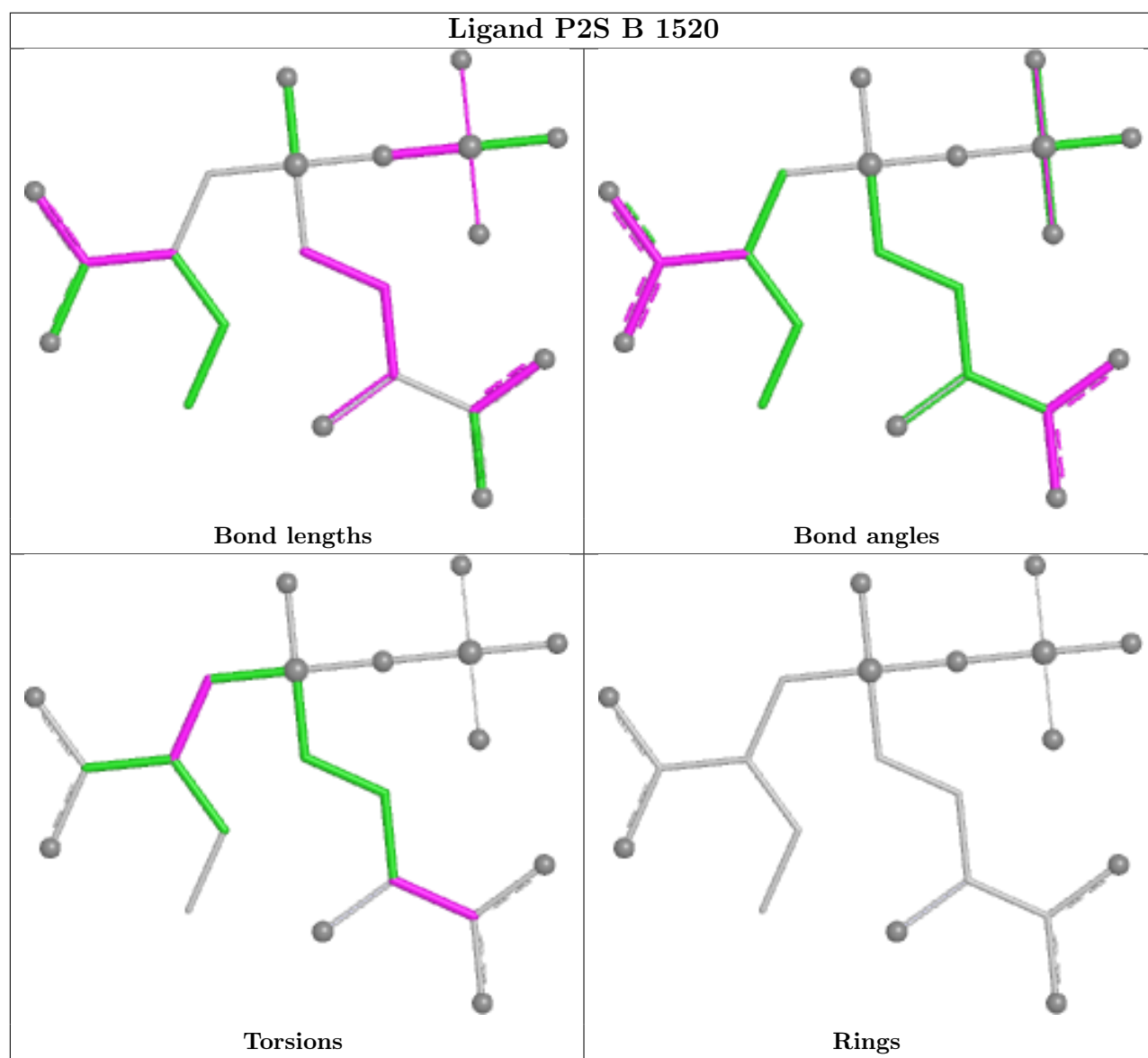
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

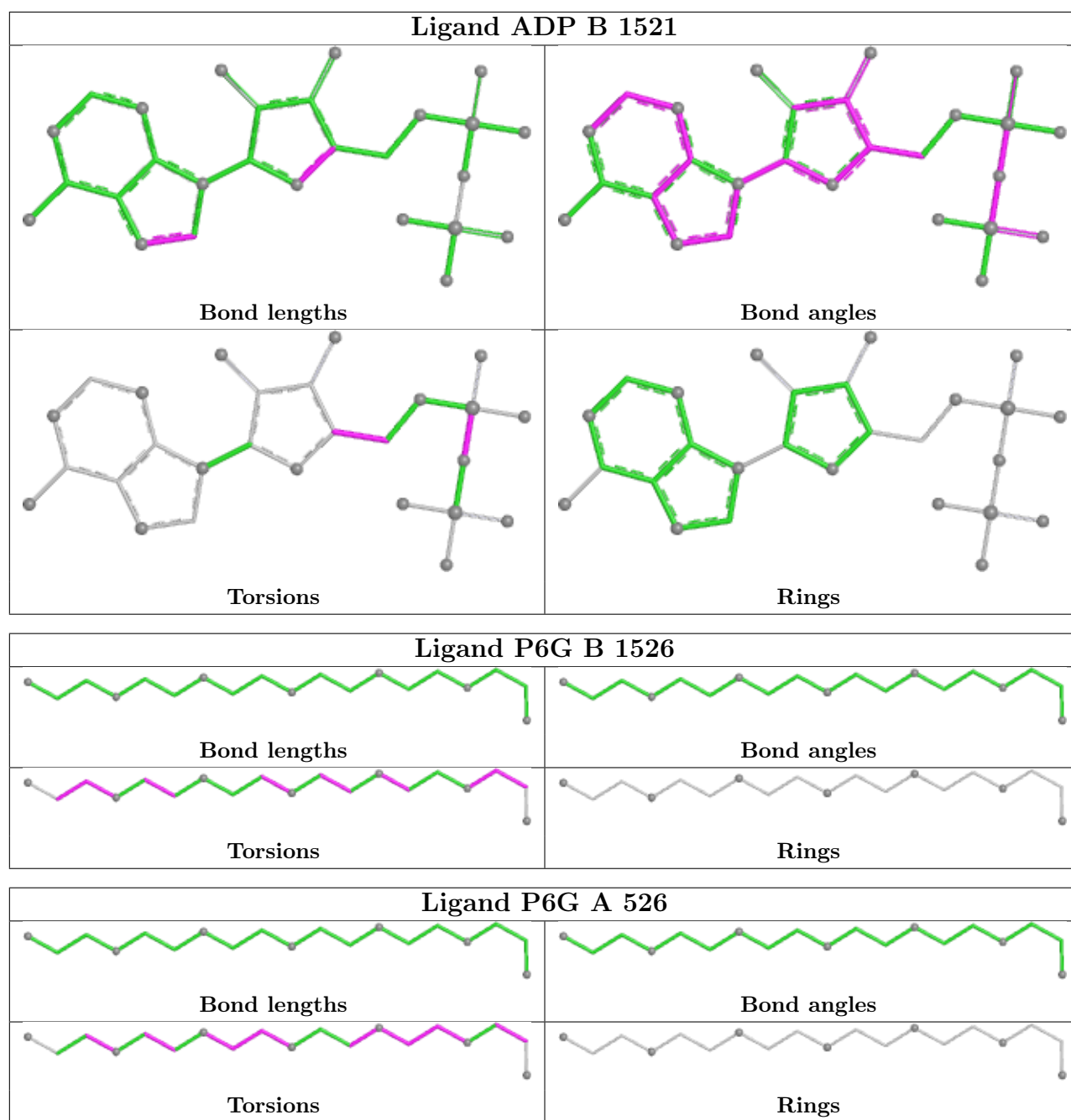
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 P2S A 520







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	507/518 (97%)	0.19	16 (3%) 50 53	7, 23, 53, 84	0
1	B	503/518 (97%)	0.44	34 (6%) 23 25	9, 28, 63, 93	0
All	All	1010/1036 (97%)	0.32	50 (4%) 34 36	7, 26, 60, 93	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	514	LEU	4.9
1	B	514	LEU	4.5
1	B	513	TRP	4.0
1	A	223	SER	3.8
1	B	510	PHE	3.8
1	A	511	ALA	3.6
1	B	275	ALA	3.6
1	B	172	ALA	3.4
1	B	163	LYS	3.3
1	B	512	VAL	3.1
1	A	513	TRP	3.1
1	A	226	TYR	3.1
1	A	221	THR	3.1
1	B	277	ILE	3.0
1	A	510	PHE	3.0
1	B	393	ILE	3.0
1	B	170	ALA	2.9
1	A	311	SER	2.8
1	A	167	ILE	2.8
1	A	275	ALA	2.7
1	B	214	THR	2.7
1	B	511	ALA	2.7
1	A	209	LEU	2.7
1	B	372	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLU	2.6
1	B	394	GLY	2.6
1	B	397	THR	2.6
1	B	398	ALA	2.5
1	B	283	GLY	2.5
1	A	512	VAL	2.5
1	B	164	SER	2.5
1	B	271	SER	2.4
1	B	370	LEU	2.4
1	B	509	PRO	2.4
1	A	220	LYS	2.4
1	B	269	THR	2.4
1	B	218	PHE	2.3
1	B	165	GLY	2.3
1	B	221	THR	2.3
1	B	216	LEU	2.3
1	A	224	GLY	2.3
1	A	266	ALA	2.2
1	B	270	PRO	2.2
1	B	395	CYS	2.2
1	B	371	ALA	2.1
1	B	290	SER	2.1
1	B	284	LYS	2.1
1	B	286	LEU	2.1
1	A	515	GLU	2.1
1	B	293	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

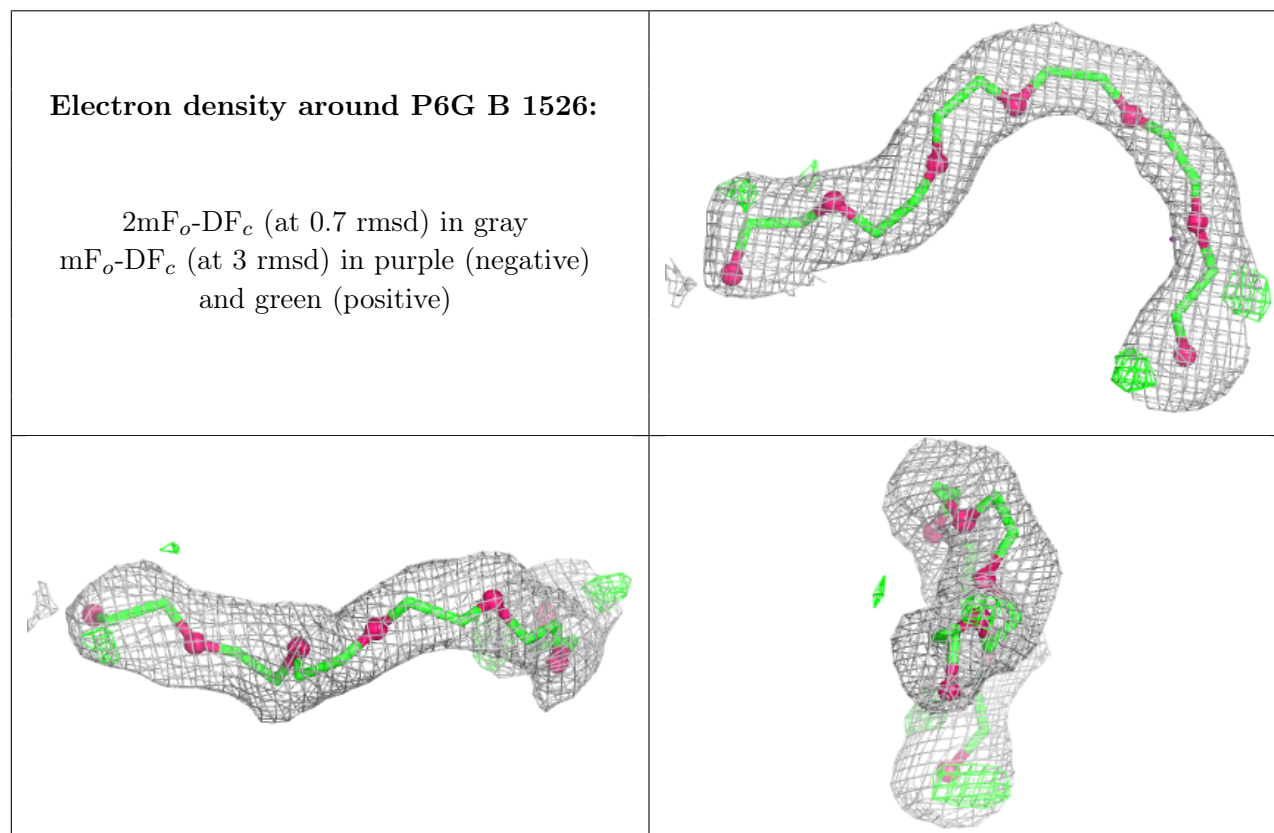
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

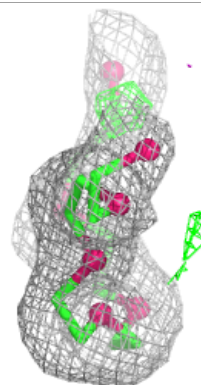
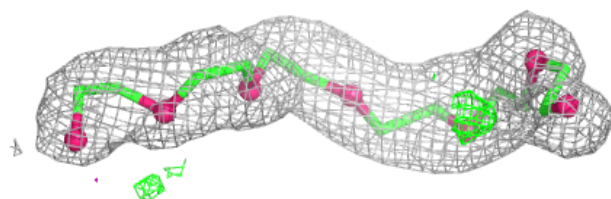
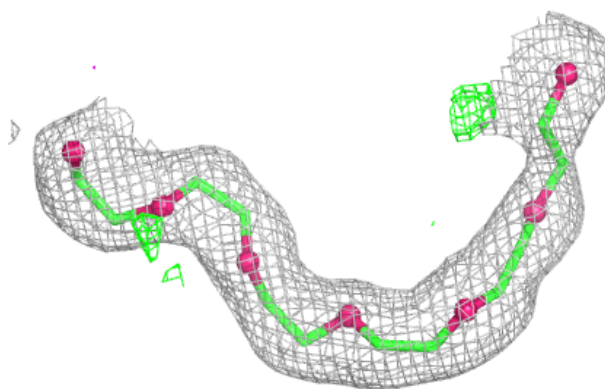
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	P6G	B	1526	19/19	0.82	0.13	29,34,48,49	0
2	MG	B	1523	1/1	0.86	0.06	11,11,11,11	0
2	MG	B	1522	1/1	0.88	0.08	21,21,21,21	0
2	MG	B	1524	1/1	0.90	0.05	15,15,15,15	0
2	MG	A	522	1/1	0.91	0.05	18,18,18,18	0
2	MG	A	524	1/1	0.91	0.04	14,14,14,14	0
5	P6G	A	526	19/19	0.92	0.10	27,34,45,45	0
2	MG	A	523	1/1	0.92	0.06	15,15,15,15	0
2	MG	B	1525	1/1	0.95	0.06	31,31,31,31	0
3	P2S	B	1520	21/21	0.96	0.07	12,18,26,28	0
4	ADP	B	1521	27/27	0.97	0.06	7,11,16,18	0
3	P2S	A	520	21/21	0.97	0.07	9,16,24,26	0
4	ADP	A	521	27/27	0.97	0.05	3,11,15,18	0
2	MG	A	525	1/1	0.98	0.06	14,14,14,14	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.



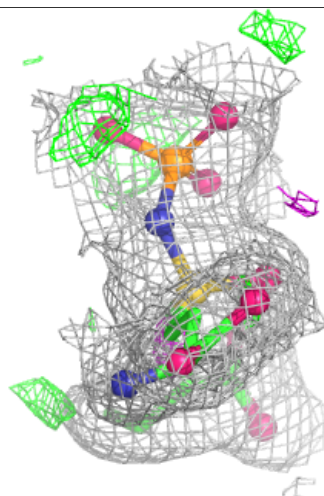
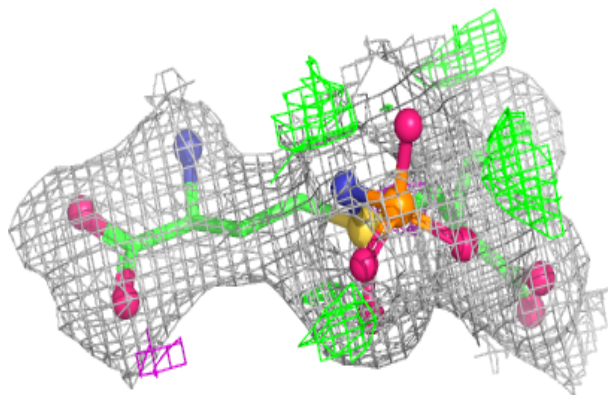
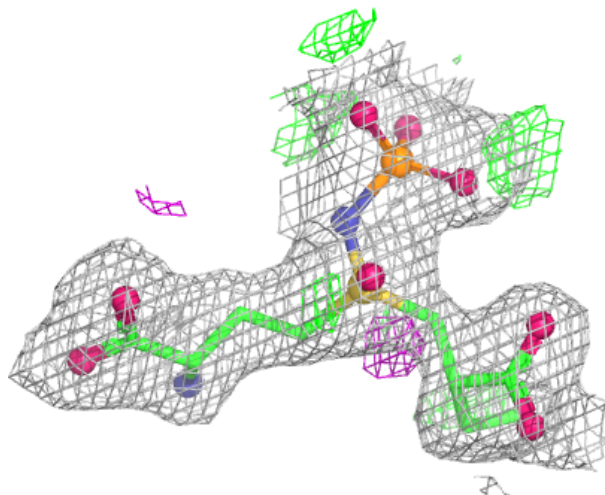
Electron density around P6G A 526:

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



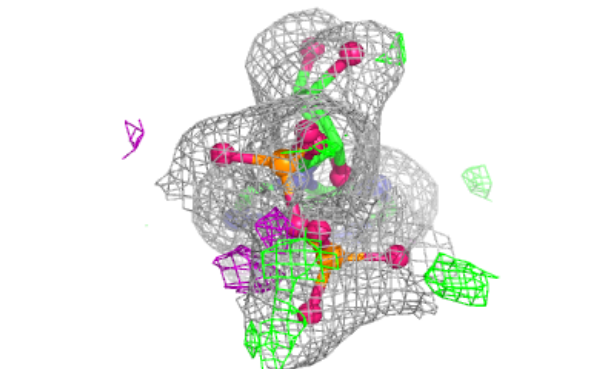
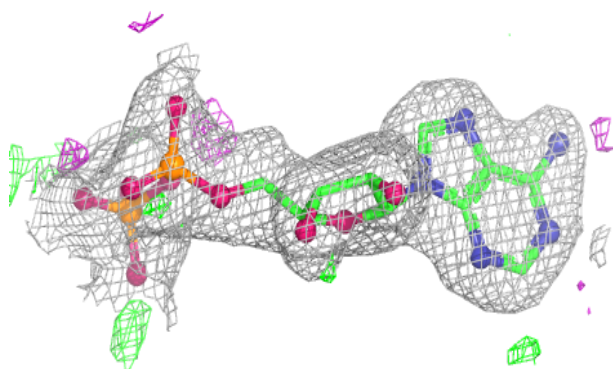
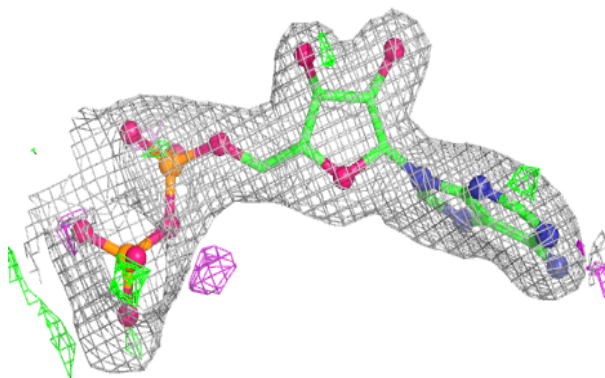
Electron density around P2S B 1520:

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

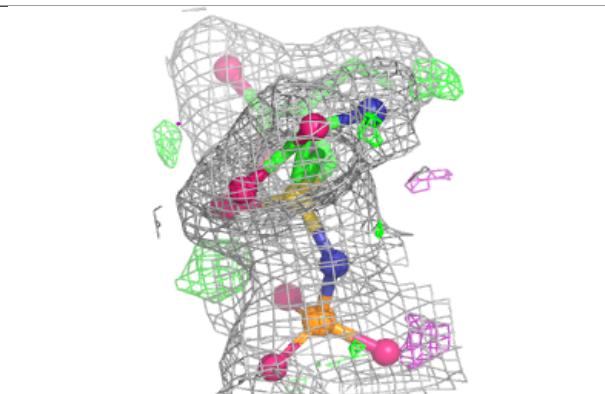
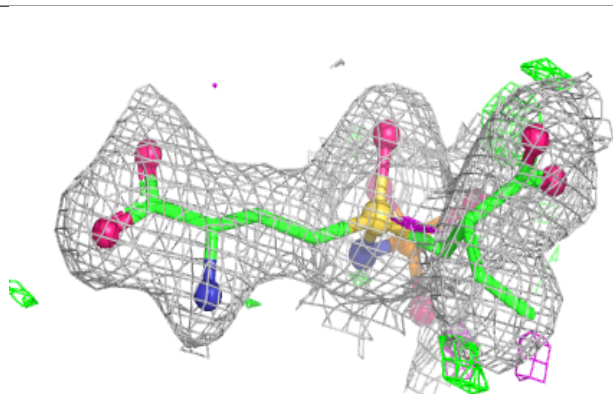
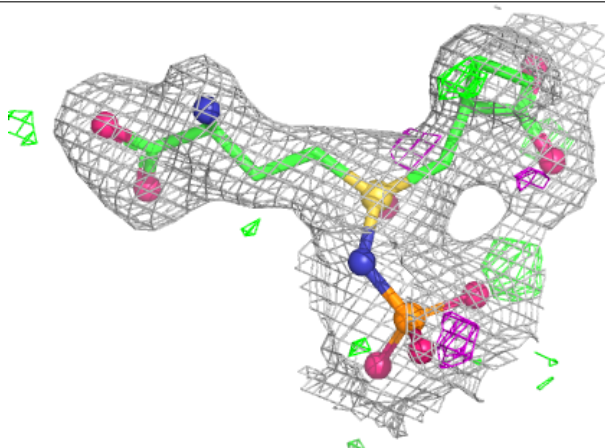


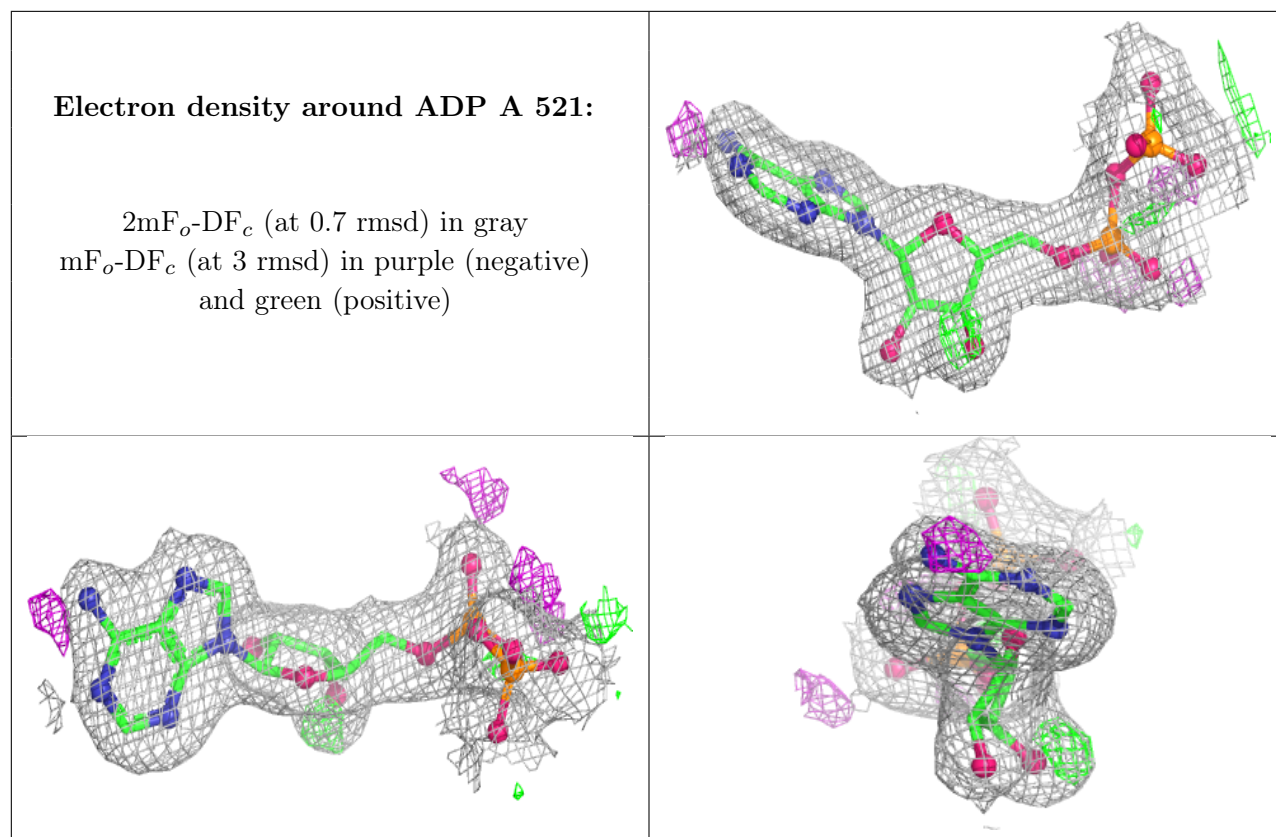
Electron density around ADP B 1521:

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

**Electron density around P2S A 520:**

$2mF_o-DF_c$ (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.