



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:04 AM EDT

PDB ID : 2BIF
Title : 6-PHOSPHOFRUCTO-2-KINASE/FRUCTOSE-2,6-BISPHOSPHATASE
H256A MUTANT WITH F6P IN PHOSPHATASE ACTIVE SITE
Authors : Yuen, M.H.; Hasemann, C.A.
Deposited on : 1998-10-26
Resolution : 2.40 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 : 2.23.2
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) : 2.23.2

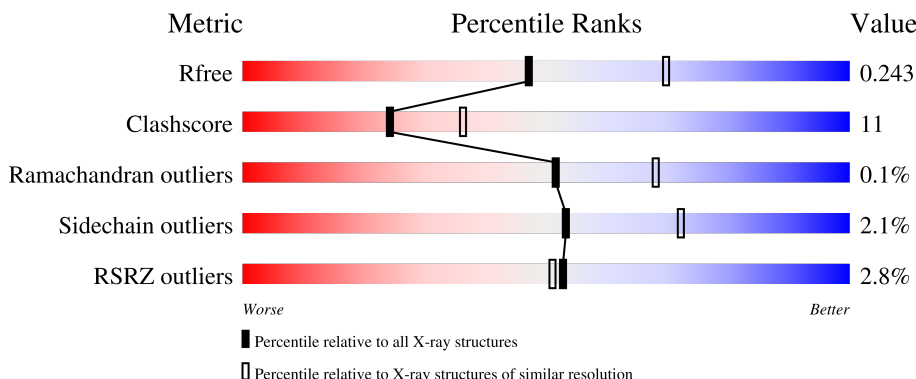
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	469	 4% 70% 20% • 8%
1	B	469	 % 70% 21% • 8%

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	PO4	B	545	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7444 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.

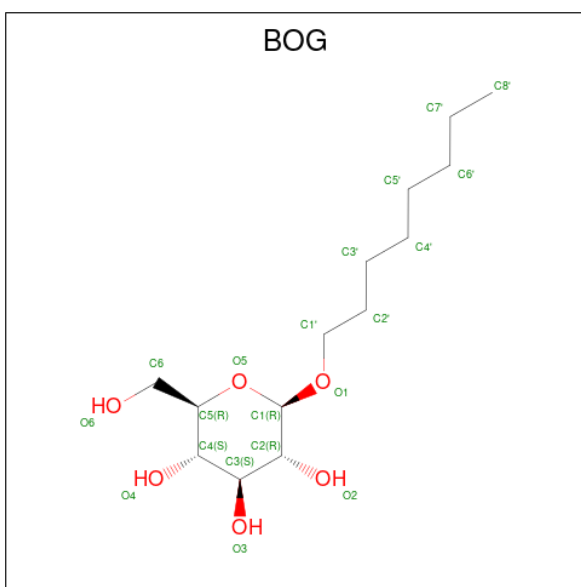
- Molecule 1 is a protein called PROTEIN (6-PHOSPHOFRUCTO-2-KINASE/FRUCTOSE-2,6-BISPHOSPHATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	1	0
			3508	2218	607	663	20			
1	B	432	Total	C	N	O	S	0	1	0
			3506	2217	604	665	20			

There are 12 discrepancies between the modelled and reference sequences:

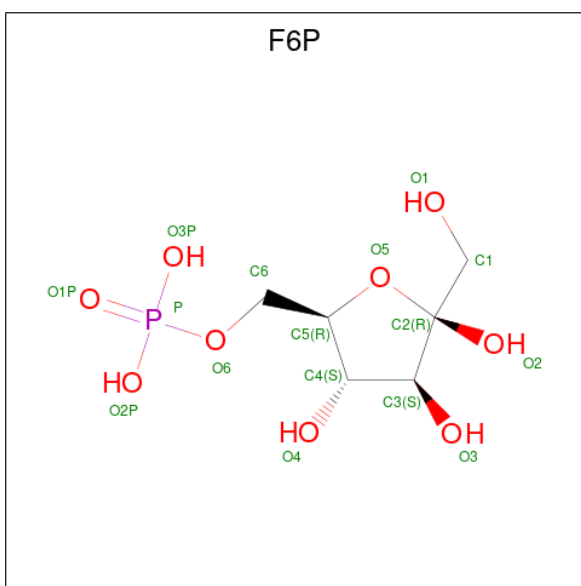
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	SEE REMARK 999	UNP P25114
B	0	MET	-	SEE REMARK 999	UNP P25114
A	15	PHE	TRP	engineered mutation	UNP P25114
B	15	PHE	TRP	engineered mutation	UNP P25114
A	64	PHE	TRP	engineered mutation	UNP P25114
B	64	PHE	TRP	engineered mutation	UNP P25114
A	256	ALA	HIS	engineered mutation	UNP P25114
B	256	ALA	HIS	engineered mutation	UNP P25114
A	299	PHE	TRP	engineered mutation	UNP P25114
B	299	PHE	TRP	engineered mutation	UNP P25114
A	320	PHE	TRP	engineered mutation	UNP P25114
B	320	PHE	TRP	engineered mutation	UNP P25114

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).

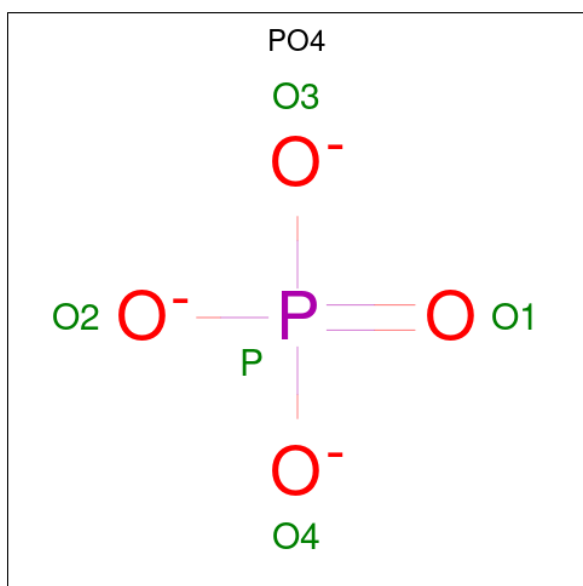


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

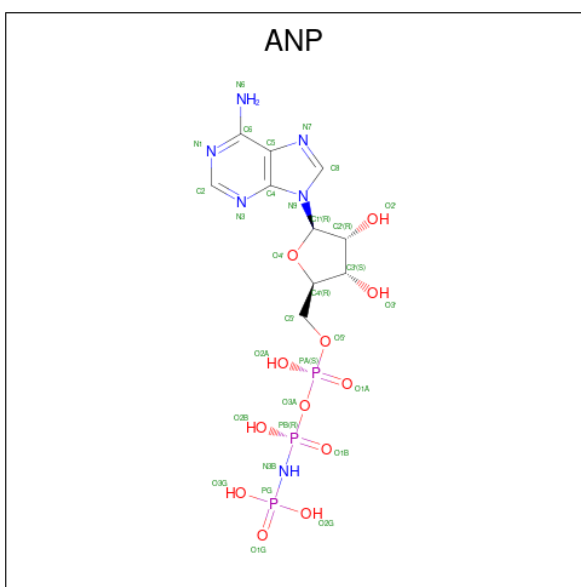
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



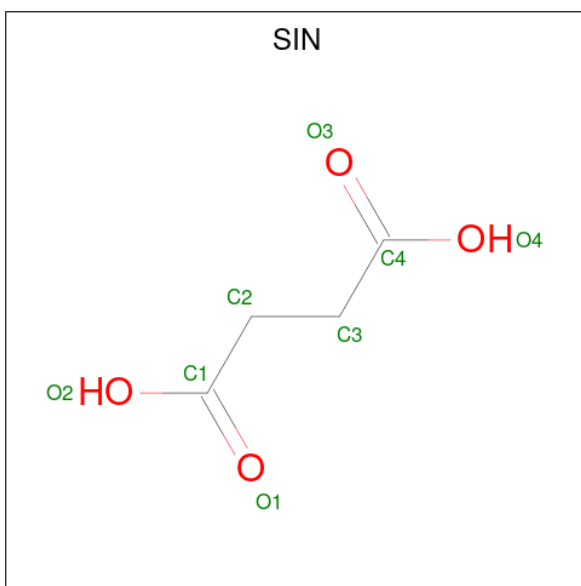
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



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

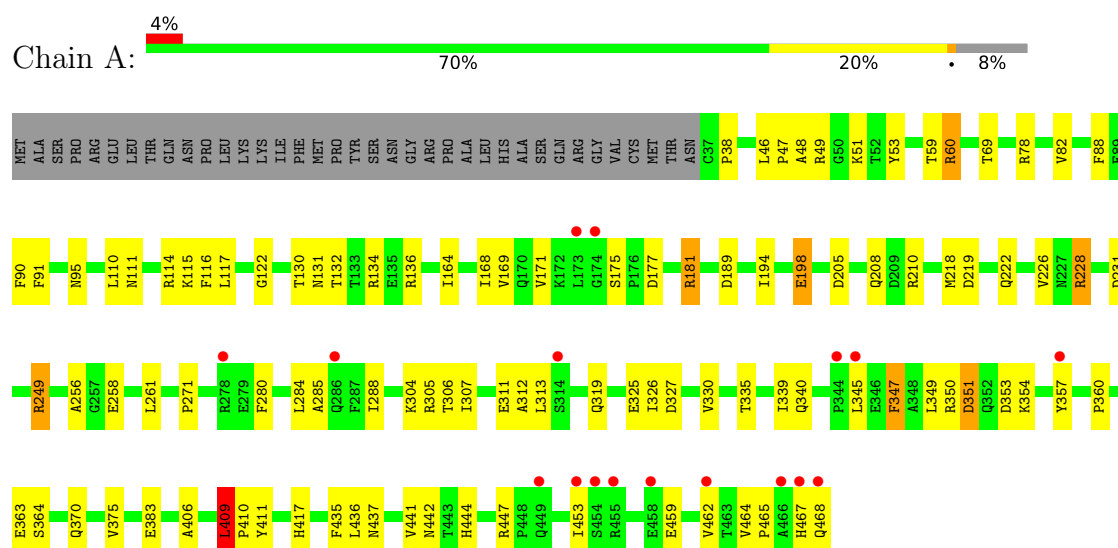
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	122	Total 122	O 122	0	0
8	B	153	Total 153	O 153	0	0

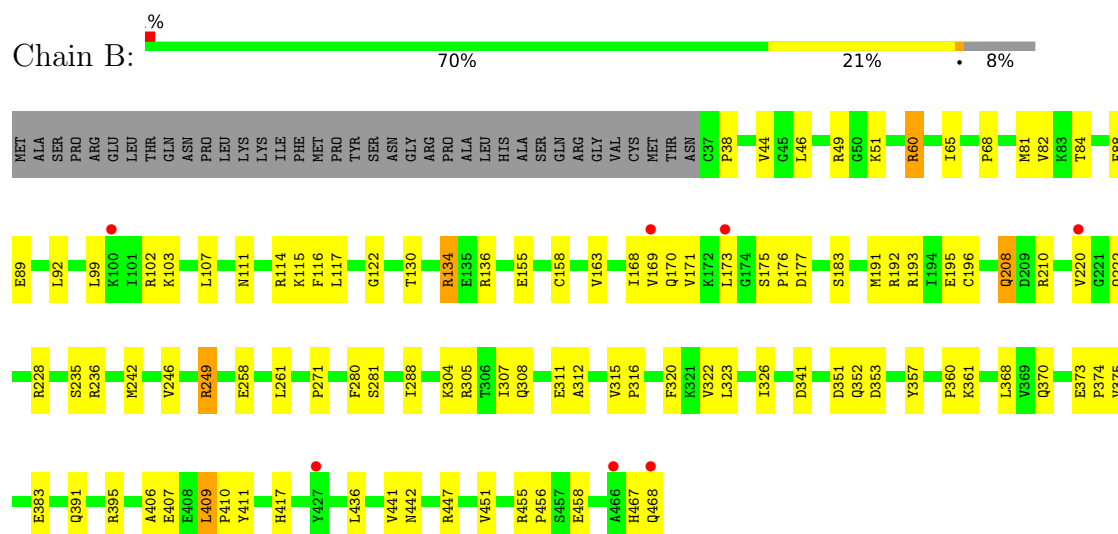
3 Residue-property plots

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: PROTEIN (6-PHOSPHOFRUCTO-2-KINASE/FRUCTOSE-2,6-BISPHOSPHATASE)



- Molecule 1: PROTEIN (6-PHOSPHOFRUCTO-2-KINASE/FRUCTOSE-2,6-BISPHOSPHATASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.74Å 73.51Å 76.70Å 116.90° 99.31° 105.20°	Depositor
Resolution (Å)	30.00 – 2.40 29.59 – 2.42	Depositor EDS
% Data completeness (in resolution range)	86.5 (30.00-2.40) 90.9 (29.59-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.70 (at 2.42Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.200 , 0.244 0.204 , 0.243	Depositor DCC
R_{free} test set	3943 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	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	0.92	EDS
Total number of atoms	7444	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: MG, SIN, F6P, PO4, BOG, ANP

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	0.58	0/3581	0.75	4/4839 (0.1%)
1	B	0.56	0/3579	0.76	3/4838 (0.1%)
All	All	0.57	0/7160	0.76	7/9677 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	B	134	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	A	409	LEU	CA-CB-CG	6.66	130.61	115.30
1	A	347	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	B	409	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	181	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	210	ARG	NE-CZ-NH1	5.20	122.90	120.30

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	3508	0	3472	81	0
1	B	3506	0	3465	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	56	4	0
2	B	20	0	28	7	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	A	31	0	13	2	0
7	A	8	0	4	0	0
7	B	8	0	4	0	0
8	A	122	0	0	10	0
8	B	153	0	0	7	0
All	All	7444	0	7064	156	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 (156) 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:220:VAL:HG11	1:B:246:VAL:HG22	1.59	0.83
1:A:375:VAL:HG13	2:B:525:BOG:H8'3	1.61	0.82
1:B:92:LEU:HD23	1:B:196:CYS:SG	2.19	0.81
1:A:375:VAL:HG13	2:B:525:BOG:C8'	2.11	0.81
1:A:370:GLN:HG2	8:A:709:HOH:O	1.81	0.80
1:A:181:ARG:HD2	8:A:637:HOH:O	1.84	0.77
1:A:134:ARG:NH2	1:A:208:GLN:HG3	2.01	0.76
1:B:171:VAL:O	1:B:175:SER:HB3	1.86	0.75
1:A:134:ARG:HH22	1:A:208:GLN:HG3	1.51	0.74
1:A:219:ASP:HB2	1:A:222:GLN:HB3	1.70	0.73
1:A:285:ALA:HA	1:A:313:LEU:HD23	1.71	0.73
1:B:220:VAL:HG11	1:B:246:VAL:CG2	2.19	0.72
1:B:370:GLN:HG2	8:B:899:HOH:O	1.88	0.72
1:B:193:ARG:HD2	8:B:905:HOH:O	1.91	0.70
1:B:351:ASP:HB3	1:B:451:VAL:HG13	1.75	0.69
1:A:90:PHE:HA	1:A:95:ASN:ND2	2.08	0.69
1:B:353:ASP:HB3	1:B:357:TYR:CD1	2.28	0.68
1:B:447:ARG:HE	1:B:451:VAL:HG21	1.60	0.65
1:B:352:GLN:HG2	1:B:451:VAL:HG12	1.79	0.65
1:A:345:LEU:CD1	1:A:453:ILE:HD11	2.26	0.65
1:B:169:VAL:O	1:B:173:LEU:HG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HA	1:A:95:ASN:HD22	1.61	0.65
1:A:285:ALA:HA	1:A:313:LEU:CD2	2.27	0.64
1:B:353:ASP:HB3	1:B:357:TYR:HD1	1.63	0.64
1:B:38:PRO:HB3	1:B:117:LEU:HD22	1.79	0.63
1:A:340:GLN:HA	1:A:340:GLN:OE1	1.98	0.63
1:A:305:ARG:HG2	8:A:638:HOH:O	1.98	0.62
1:B:65:ILE:HD12	2:B:525:BOG:HO4	1.64	0.62
1:B:280:PHE:CE1	1:B:436:LEU:HD12	2.35	0.61
1:A:110:LEU:HD11	2:A:510:BOG:H8'3	1.83	0.61
1:A:48:ALA:H	6:A:500:ANP:HNB1	1.48	0.60
1:A:78:ARG:HB2	8:A:711:HOH:O	2.01	0.60
1:B:220:VAL:HG12	1:B:220:VAL:O	2.02	0.60
1:A:467:HIS:O	1:A:468:GLN:HB2	1.99	0.60
1:A:134:ARG:HD3	8:A:704:HOH:O	2.00	0.60
1:A:319:GLN:HG2	8:A:663:HOH:O	2.00	0.59
1:A:38:PRO:HB2	1:A:117:LEU:HD13	1.83	0.59
1:A:171:VAL:O	1:A:175:SER:HB3	2.02	0.59
1:A:228:ARG:NH1	1:B:222:GLN:OE1	2.36	0.58
1:A:280:PHE:CE1	1:A:417:HIS:HA	2.39	0.57
1:A:53:TYR:CD2	6:A:500:ANP:H8	2.39	0.57
1:A:78:ARG:O	1:A:82:VAL:HG22	2.05	0.57
1:B:65:ILE:HD12	2:B:525:BOG:O4	2.05	0.56
1:A:280:PHE:CE1	1:A:436:LEU:HD12	2.40	0.56
1:B:451:VAL:HG12	1:B:451:VAL:O	2.04	0.56
1:B:183:SER:HA	8:B:947:HOH:O	2.05	0.56
1:A:205:ASP:HB3	1:A:208:GLN:HB2	1.86	0.56
1:B:456:PRO:HB2	1:B:458:GLU:OE1	2.06	0.56
1:A:256:ALA:HB2	1:A:306:THR:HG22	1.88	0.56
1:A:375:VAL:HG13	2:B:525:BOG:H8'2	1.88	0.55
1:A:164:ILE:O	1:A:168:ILE:HG13	2.06	0.55
1:A:411:TYR:CE1	1:A:447:ARG:HB2	2.41	0.55
1:A:110:LEU:CD1	2:A:510:BOG:H8'3	2.36	0.55
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.71	0.55
1:A:130:THR:HB	1:A:132:THR:HG23	1.88	0.55
1:B:451:VAL:HA	1:B:455:ARG:NH1	2.21	0.55
1:A:350:ARG:HA	1:A:357:TYR:HB2	1.89	0.55
1:A:88:PHE:HB3	1:A:189:ASP:OD1	2.06	0.54
1:A:307:ILE:O	1:A:311:GLU:HG2	2.08	0.54
1:A:285:ALA:CA	1:A:313:LEU:HD23	2.36	0.54
1:A:349:LEU:O	1:A:357:TYR:HD2	1.91	0.53
1:A:258:GLU:OE2	1:A:441:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:OE2	1:B:441:VAL:HG23	2.08	0.53
1:B:134:ARG:HH12	1:B:208:GLN:CD	2.12	0.53
1:A:46:LEU:O	1:A:49:ARG:HB2	2.09	0.53
1:B:89:GLU:HA	1:B:92:LEU:HG	1.91	0.53
1:B:341:ASP:HA	8:B:917:HOH:O	2.09	0.53
1:B:111:ASN:OD1	1:B:114:ARG:NH1	2.42	0.52
1:B:280:PHE:HE1	1:B:436:LEU:HD12	1.75	0.52
1:B:103:LYS:HG2	1:B:136:ARG:HH22	1.75	0.52
1:A:375:VAL:CG1	2:B:525:BOG:H8'3	2.37	0.51
1:A:111:ASN:ND2	1:A:115:LYS:HE3	2.25	0.51
1:B:169:VAL:O	1:B:169:VAL:HG12	2.11	0.51
1:B:305:ARG:HG2	8:B:822:HOH:O	2.11	0.51
1:A:345:LEU:HD12	1:A:453:ILE:HD11	1.92	0.51
2:A:555:BOG:H7'2	1:B:375:VAL:HG22	1.92	0.51
1:A:406:ALA:O	1:A:410:PRO:HD3	2.11	0.50
1:B:352:GLN:CG	1:B:451:VAL:HG12	2.40	0.50
1:B:249:ARG:HG2	1:B:383:GLU:HA	1.94	0.50
1:B:441:VAL:HG12	1:B:442:ASN:N	2.27	0.50
1:A:364:SER:HA	8:A:646:HOH:O	2.12	0.49
1:A:51:LYS:HE3	1:A:130:THR:HA	1.93	0.49
1:A:330:VAL:CG2	1:A:360:PRO:HD2	2.43	0.49
1:A:353:ASP:HB3	1:A:357:TYR:CD2	2.47	0.49
1:B:81:MET:HB2	8:B:933:HOH:O	2.12	0.49
1:B:220:VAL:CG1	1:B:246:VAL:HG22	2.39	0.49
1:B:175:SER:OG	1:B:177:ASP:HB2	2.13	0.48
1:B:307:ILE:O	1:B:311:GLU:HG2	2.14	0.48
1:A:325:GLU:HG3	1:A:326:ILE:N	2.29	0.48
1:A:169:VAL:HG12	1:A:169:VAL:O	2.14	0.47
1:A:116:PHE:CZ	1:A:122:GLY:HA3	2.49	0.47
1:B:60:ARG:C	1:B:60:ARG:HD3	2.35	0.47
1:A:435:PHE:CE2	1:A:437:ASN:HA	2.50	0.47
1:B:210:ARG:HG2	1:B:210:ARG:NH1	2.29	0.47
1:B:281:SER:HB3	1:B:312:ALA:HB2	1.97	0.46
1:A:60:ARG:C	1:A:60:ARG:HD3	2.36	0.46
1:B:88:PHE:CE2	1:B:192:ARG:HD2	2.51	0.46
1:B:406:ALA:O	1:B:410:PRO:HD3	2.15	0.46
1:B:373[B]:GLU:HB2	1:B:374:PRO:HD3	1.96	0.46
1:B:280:PHE:CE1	1:B:417:HIS:HA	2.50	0.46
1:A:345:LEU:O	1:A:349:LEU:HG	2.15	0.46
1:B:353:ASP:HB3	1:B:357:TYR:CE1	2.50	0.46
1:A:441:VAL:HG12	1:A:442:ASN:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:HA	1:A:136:ARG:HD3	1.97	0.46
1:A:222:GLN:OE1	1:B:228:ARG:NH1	2.48	0.46
1:B:467:HIS:O	1:B:468:GLN:CB	2.64	0.46
1:A:285:ALA:HB2	1:A:312:ALA:O	2.15	0.45
1:B:99:LEU:HD23	1:B:102:ARG:HH21	1.80	0.45
1:A:330:VAL:HG22	1:A:360:PRO:HD2	1.99	0.45
1:A:261:LEU:HG	1:A:271:PRO:HB3	1.99	0.45
2:A:555:BOG:H8'2	1:B:323:LEU:HD11	1.98	0.45
1:B:320:PHE:HB3	1:B:322:VAL:HG12	1.97	0.45
1:B:49:ARG:HG3	1:B:158:CYS:H	1.82	0.45
1:A:249:ARG:HG2	1:A:383:GLU:HA	1.99	0.44
1:B:467:HIS:O	1:B:468:GLN:HB2	2.16	0.44
1:A:231:ASP:HB2	8:A:622:HOH:O	2.18	0.44
1:B:411:TYR:CE1	1:B:447:ARG:HB2	2.52	0.44
1:A:409:LEU:C	1:A:409:LEU:HD12	2.38	0.44
1:B:261:LEU:HG	1:B:271:PRO:HB3	2.00	0.43
1:B:391:GLN:O	1:B:395:ARG:HG3	2.18	0.43
1:B:158:CYS:SG	1:B:163:VAL:HG11	2.58	0.43
1:B:315:VAL:HG13	1:B:316:PRO:HD2	2.01	0.43
1:A:327:ASP:HB3	1:A:363:GLU:HG3	2.00	0.43
1:B:38:PRO:HB2	1:B:117:LEU:HD13	2.00	0.43
1:B:373[A]:GLU:HB3	1:B:374:PRO:HD3	1.99	0.43
1:B:407:GLU:HB2	8:B:948:HOH:O	2.18	0.43
1:A:59:THR:HG23	1:A:69:THR:HG22	2.01	0.43
1:A:171:VAL:HG22	8:A:645:HOH:O	2.18	0.43
1:A:175:SER:OG	1:A:177:ASP:HB2	2.19	0.42
1:B:44:VAL:O	1:B:155:GLU:HA	2.18	0.42
1:A:47:PRO:HB2	1:A:194:ILE:HG12	2.01	0.42
1:B:360:PRO:O	1:B:361:LYS:HB2	2.20	0.42
1:A:46:LEU:HD11	1:A:198:GLU:HG3	2.01	0.42
1:A:459:GLU:O	1:A:462:VAL:HG12	2.19	0.42
1:A:444:HIS:O	1:A:465:PRO:HG3	2.20	0.42
1:B:111:ASN:HD21	1:B:115:LYS:HE3	1.85	0.42
1:B:175:SER:HA	1:B:176:PRO:HD3	1.84	0.42
1:B:46:LEU:O	1:B:49:ARG:HB2	2.20	0.41
1:B:51:LYS:HE3	1:B:130:THR:HA	2.02	0.41
1:B:373[B]:GLU:OE1	2:B:525:BOG:H61	2.20	0.41
1:A:354:LYS:HB2	8:A:628:HOH:O	2.20	0.41
1:B:168:ILE:C	1:B:170:GLN:H	2.24	0.41
1:A:226:VAL:HG21	1:B:242:MET:HE1	2.02	0.41
1:B:116:PHE:CZ	1:B:122:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:O	1:A:175:SER:CB	2.68	0.41
1:A:284:LEU:HA	1:A:436:LEU:HD13	2.03	0.41
1:A:464:VAL:HA	1:A:465:PRO:HD3	1.96	0.41
1:A:347:PHE:O	1:A:351:ASP:HB2	2.20	0.41
1:B:304:LYS:O	1:B:308:GLN:HG3	2.21	0.41
1:B:288:ILE:HD13	1:B:288:ILE:HA	1.90	0.40
1:A:288:ILE:HD13	1:A:288:ILE:HA	1.88	0.40
1:B:191:MET:O	1:B:195:GLU:HG3	2.21	0.40
1:B:326:ILE:HB	1:B:368:LEU:HD22	2.02	0.40
1:A:90:PHE:HD2	1:A:91:PHE:CE1	2.39	0.40
1:A:335:THR:O	1:A:339:ILE:HG13	2.21	0.40
1:B:82:VAL:C	1:B:84:THR:H	2.25	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	431/469 (92%)	409 (95%)	22 (5%)	0	100	100
1	B	431/469 (92%)	406 (94%)	24 (6%)	1 (0%)	47	62
All	All	862/938 (92%)	815 (94%)	46 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/418 (93%)	378 (98%)	9 (2%)	50	70
1	B	387/418 (93%)	380 (98%)	7 (2%)	59	76
All	All	774/836 (93%)	758 (98%)	16 (2%)	53	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	114	ARG
1	A	198	GLU
1	A	218	MET
1	A	228	ARG
1	A	249	ARG
1	A	304	LYS
1	A	351	ASP
1	A	409	LEU
1	B	60	ARG
1	B	107	LEU
1	B	208	GLN
1	B	235	SER
1	B	236	ARG
1	B	249	ARG
1	B	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	167	ASN
1	A	199	ASN
1	A	232	HIS
1	A	342	HIS
1	B	208	GLN

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Mol	Chain	Res	Type
1	B	302	GLN
1	B	342	HIS
1	B	467	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BOG	B	525	-	20,20,20	0.96	1 (5%)	25,25,25	0.71	0
5	PO4	B	530	-	4,4,4	0.71	0	6,6,6	0.88	0
6	ANP	A	500	4	29,33,33	2.11	12 (41%)	31,52,52	2.19	7 (22%)
2	BOG	A	555	-	20,20,20	0.76	0	25,25,25	0.71	0
5	PO4	A	515	-	4,4,4	1.42	1 (25%)	6,6,6	0.62	0
2	BOG	A	510	-	20,20,20	0.89	1 (5%)	25,25,25	0.83	0
3	F6P	A	520	-	15,16,16	0.77	0	17,25,25	1.21	2 (11%)
7	SIN	B	535	-	1,7,7	0.02	0	2,8,8	3.19	1 (50%)
5	PO4	B	545	-	4,4,4	3.29	3 (75%)	6,6,6	1.25	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	F6P	B	550	-	15,16,16	0.95	1 (6%)	17,25,25	1.12	3 (17%)
7	SIN	A	505	-	1,7,7	0.12	0	2,8,8	2.58	2 (100%)

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	BOG	B	525	-	-	6/11/31/31	0/1/1/1
6	ANP	A	500	4	-	3/14/38/38	0/3/3/3
2	BOG	A	555	-	-	5/11/31/31	0/1/1/1
2	BOG	A	510	-	-	7/11/31/31	0/1/1/1
3	F6P	A	520	-	-	8/9/28/28	0/1/1/1
7	SIN	B	535	-	-	0/1/5/5	-
3	F6P	B	550	-	-	3/9/28/28	0/1/1/1
7	SIN	A	505	-	-	0/1/5/5	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	ANP	PG-O3G	-4.41	1.44	1.56
6	A	500	ANP	C6-N6	4.14	1.49	1.34
5	B	545	PO4	P-O3	-4.01	1.42	1.54
5	B	545	PO4	P-O4	-3.68	1.43	1.54
5	B	545	PO4	P-O2	-3.64	1.43	1.54
6	A	500	ANP	C3'-C4'	3.34	1.61	1.53
2	A	510	BOG	O1-C1	3.26	1.45	1.40
6	A	500	ANP	PG-O2G	-3.13	1.48	1.56
6	A	500	ANP	C4-N3	2.89	1.39	1.35
6	A	500	ANP	PG-O1G	2.86	1.50	1.46
6	A	500	ANP	PB-O1B	2.79	1.50	1.46
6	A	500	ANP	PB-O3A	2.79	1.62	1.59
6	A	500	ANP	PB-O2B	-2.58	1.49	1.56
2	B	525	BOG	O1-C1	2.56	1.44	1.40
6	A	500	ANP	C5'-C4'	2.47	1.59	1.51
5	A	515	PO4	P-O4	-2.13	1.48	1.54
6	A	500	ANP	C2'-C1'	2.08	1.56	1.53
3	B	550	F6P	P-O2P	-2.06	1.46	1.54
6	A	500	ANP	O2'-C2'	2.03	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	500	ANP	O1B-PB-N3B	-5.95	103.01	111.77
6	A	500	ANP	O4'-C1'-C2'	5.20	114.52	106.93
6	A	500	ANP	O2B-PB-O1B	4.53	119.42	109.92
6	A	500	ANP	C3'-C2'-C1'	-4.31	94.48	100.98
7	B	535	SIN	C2-C3-C4	-4.05	105.87	112.67
6	A	500	ANP	O3G-PG-O2G	2.92	115.42	107.64
7	A	505	SIN	C3-C2-C1	-2.92	107.77	112.67
3	A	520	F6P	O6-P-O1P	-2.55	99.32	106.47
5	B	545	PO4	O3-P-O1	2.48	119.97	110.89
6	A	500	ANP	O2'-C2'-C1'	2.43	119.83	110.85
3	B	550	F6P	O2-C2-O5	-2.29	105.08	109.50
3	B	550	F6P	O6-P-O1P	-2.28	100.07	106.47
3	B	550	F6P	O3P-P-O1P	2.24	119.45	110.68
7	A	505	SIN	C2-C3-C4	-2.18	109.01	112.67
6	A	500	ANP	C4-C5-N7	2.09	111.58	109.40
3	A	520	F6P	O4-C4-C5	2.08	117.06	111.05

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	510	BOG	C2-C1-O1-C1'
2	A	510	BOG	O5-C1-O1-C1'
2	A	510	BOG	C2'-C1'-O1-C1
2	A	555	BOG	C2-C1-O1-C1'
2	A	555	BOG	O5-C1-O1-C1'
3	A	520	F6P	O1-C1-C2-O2
3	A	520	F6P	C6-O6-P-O1P
3	A	520	F6P	C6-O6-P-O2P
3	A	520	F6P	C6-O6-P-O3P
3	B	550	F6P	O1-C1-C2-O2
3	B	550	F6P	O1-C1-C2-C3
3	B	550	F6P	O1-C1-C2-O5
6	A	500	ANP	PB-N3B-PG-O1G
6	A	500	ANP	C5'-O5'-PA-O1A
6	A	500	ANP	C5'-O5'-PA-O3A
2	A	510	BOG	O5-C5-C6-O6
2	B	525	BOG	C4-C5-C6-O6
2	A	555	BOG	O5-C5-C6-O6
2	A	510	BOG	C4-C5-C6-O6
2	A	555	BOG	C4-C5-C6-O6

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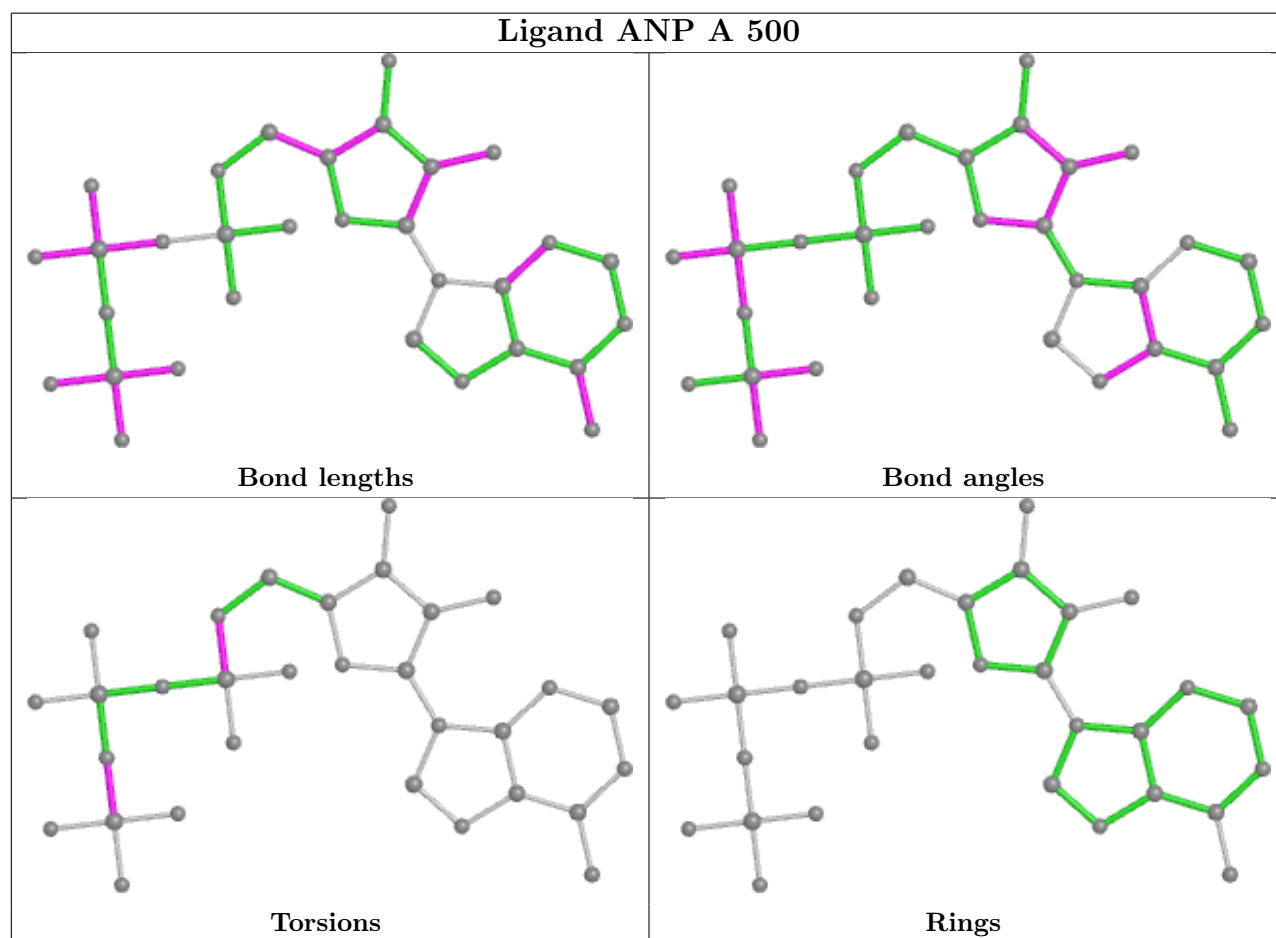
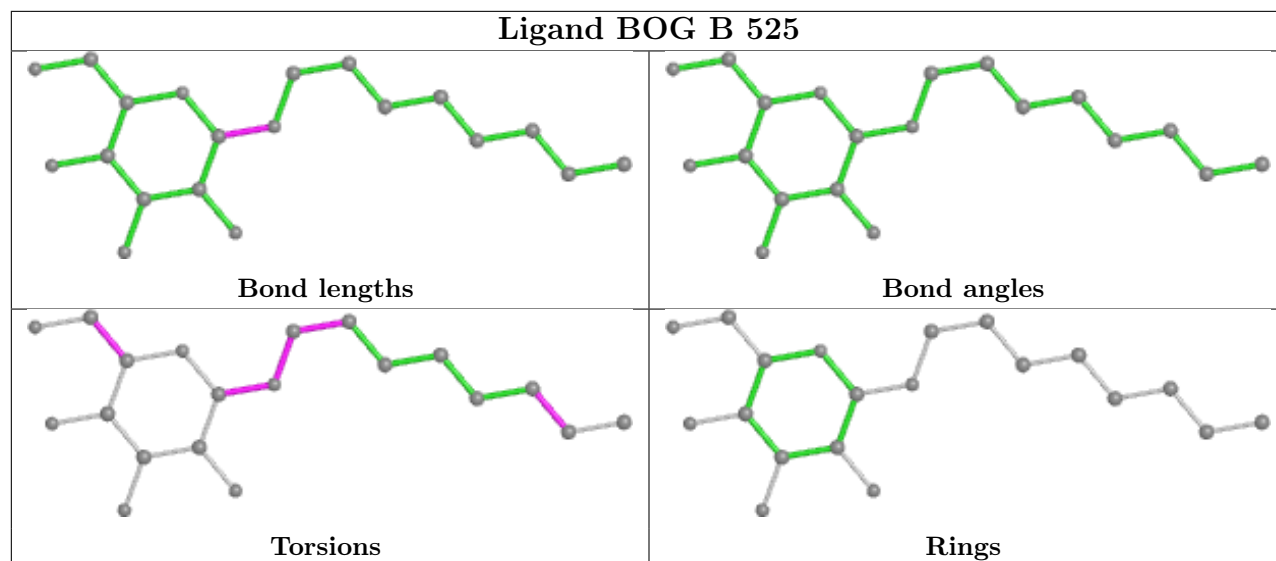
Mol	Chain	Res	Type	Atoms
2	B	525	BOG	O5-C5-C6-O6
3	A	520	F6P	O1-C1-C2-O5
2	B	525	BOG	O1-C1'-C2'-C3'
3	A	520	F6P	O1-C1-C2-C3
2	A	510	BOG	O1-C1'-C2'-C3'
2	A	555	BOG	O1-C1'-C2'-C3'
2	B	525	BOG	C2-C1-O1-C1'
3	A	520	F6P	C4-C5-C6-O6
2	B	525	BOG	C5'-C6'-C7'-C8'
2	A	510	BOG	C2'-C3'-C4'-C5'
3	A	520	F6P	O5-C5-C6-O6
2	B	525	BOG	C2'-C1'-O1-C1

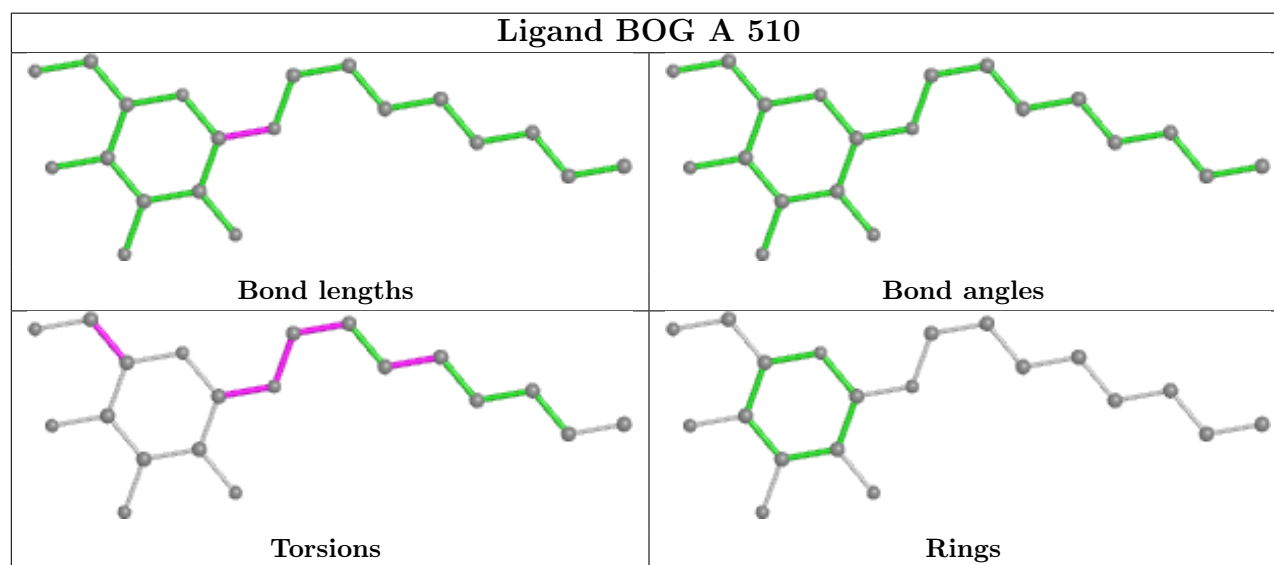
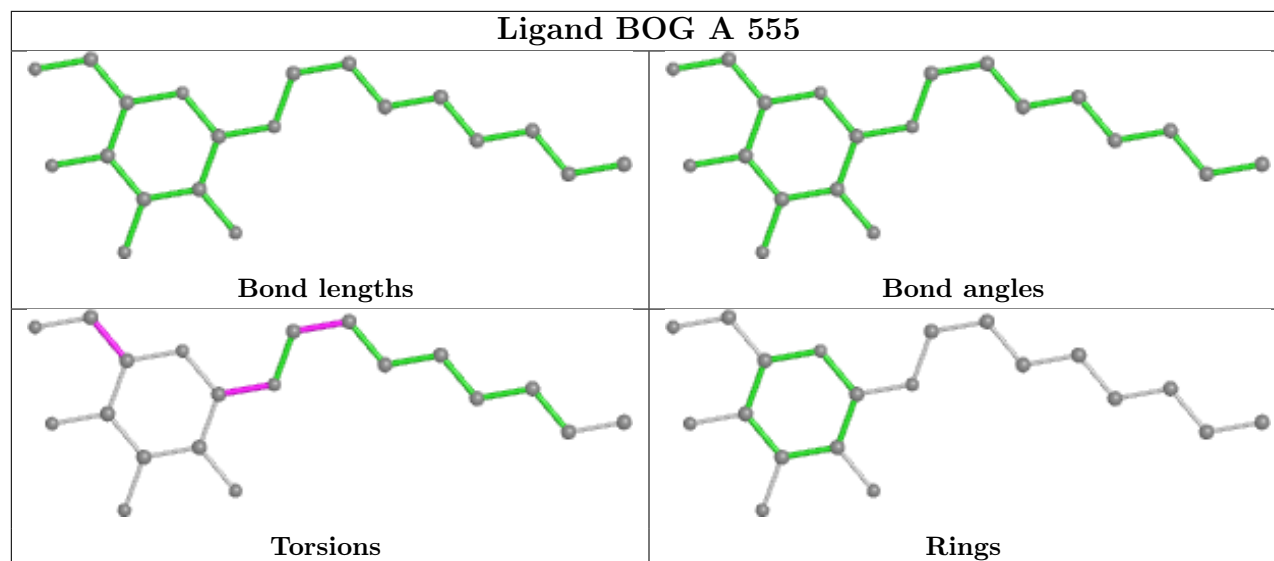
There are no ring outliers.

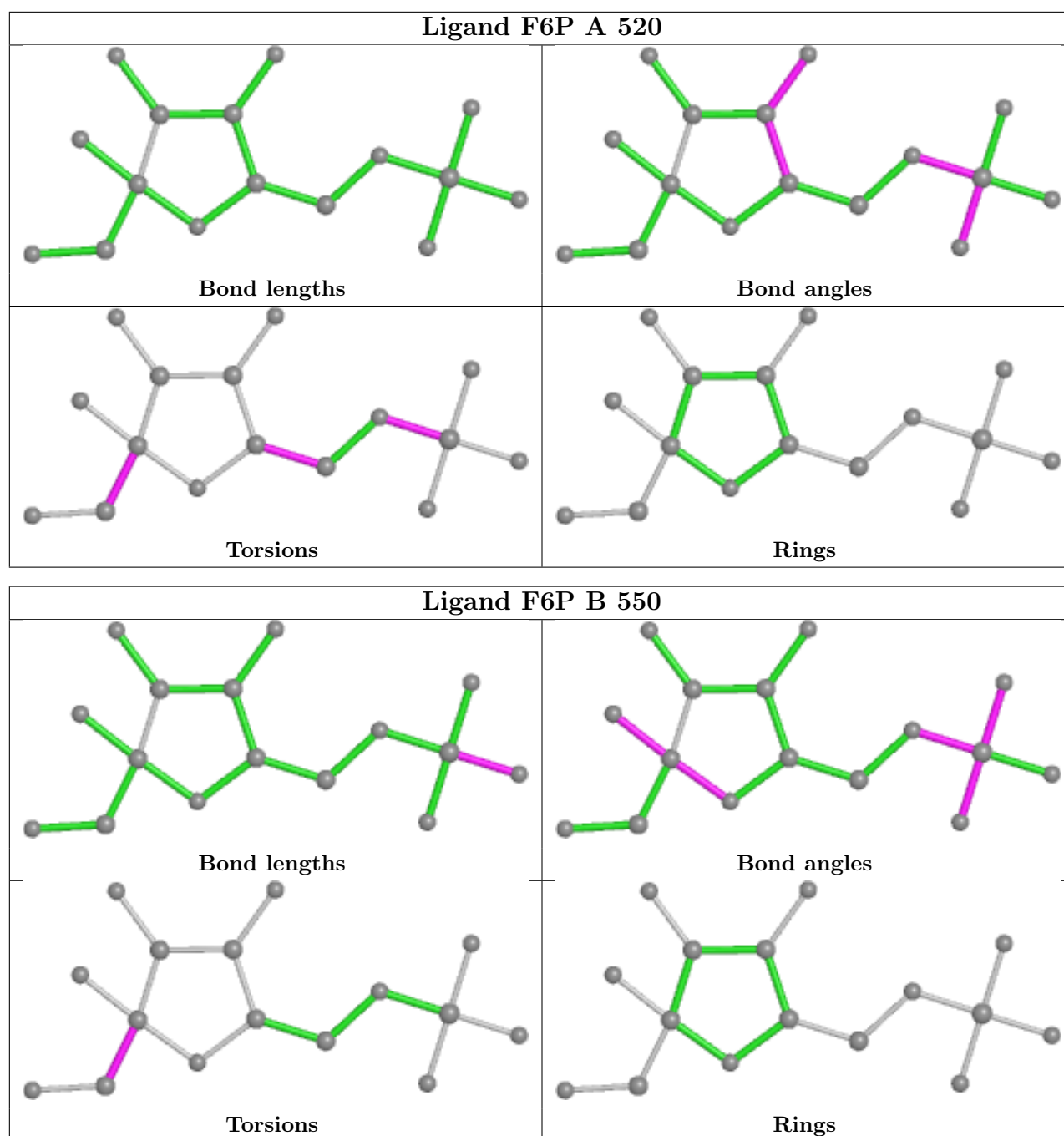
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	525	BOG	7	0
6	A	500	ANP	2	0
2	A	555	BOG	2	0
2	A	510	BOG	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.







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	432/469 (92%)	-0.09	17 (3%) 39 38	6, 35, 70, 85	0
1	B	432/469 (92%)	-0.41	7 (1%) 72 70	8, 29, 57, 75	0
All	All	864/938 (92%)	-0.25	24 (2%) 53 51	6, 32, 65, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	TYR	7.5
1	A	468	GLN	6.5
1	A	466	ALA	6.5
1	A	453	ILE	5.1
1	B	173	LEU	3.7
1	A	173	LEU	3.7
1	B	427	TYR	3.6
1	B	169	VAL	3.5
1	A	314	SER	3.2
1	A	455	ARG	3.0
1	B	220	VAL	2.8
1	A	345	LEU	2.8
1	A	462	VAL	2.6
1	A	449	GLN	2.6
1	A	344	PRO	2.5
1	A	458	GLU	2.5
1	B	468	GLN	2.4
1	A	454	SER	2.3
1	B	100	LYS	2.2
1	A	286	GLN	2.2
1	A	467	HIS	2.2
1	A	174	GLY	2.2
1	A	278	ARG	2.1
1	B	466	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

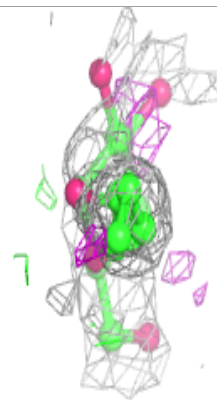
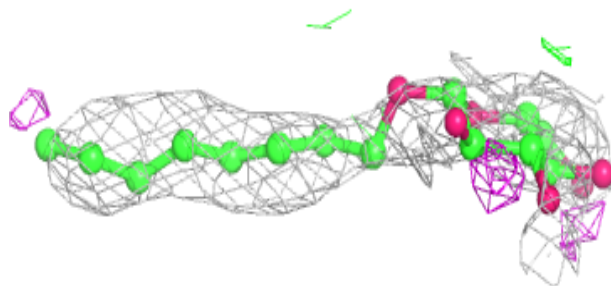
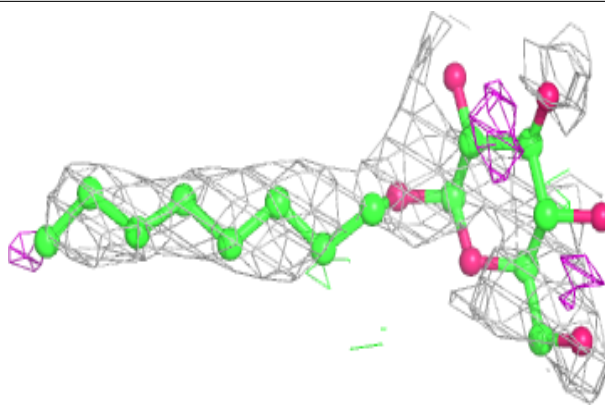
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BOG	B	525	20/20	0.61	0.38	47,84,92,96	0
2	BOG	A	555	20/20	0.75	0.23	37,63,66,67	0
4	MG	A	501	1/1	0.79	0.18	39,39,39,39	0
2	BOG	A	510	20/20	0.91	0.18	28,37,65,69	0
5	PO4	B	530	5/5	0.92	0.21	65,66,68,68	0
7	SIN	A	505	8/8	0.93	0.13	21,25,27,32	0
3	F6P	A	520	16/16	0.94	0.21	36,41,46,51	0
6	ANP	A	500	31/31	0.95	0.12	19,41,45,46	3
5	PO4	A	515	5/5	0.95	0.16	44,48,49,53	0
7	SIN	B	535	8/8	0.96	0.14	29,34,35,38	0
5	PO4	B	545	5/5	0.98	0.14	24,25,35,36	0
3	F6P	B	550	16/16	0.98	0.15	15,24,33,34	0

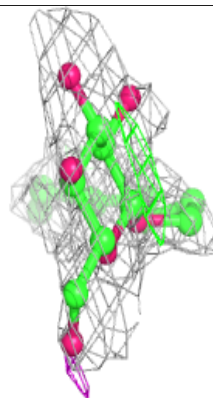
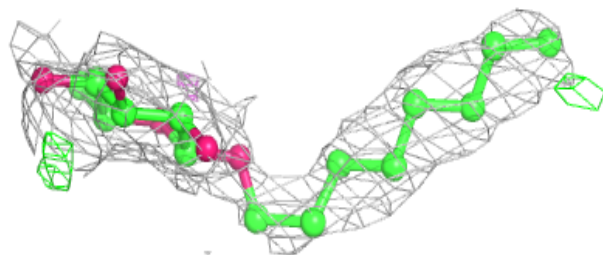
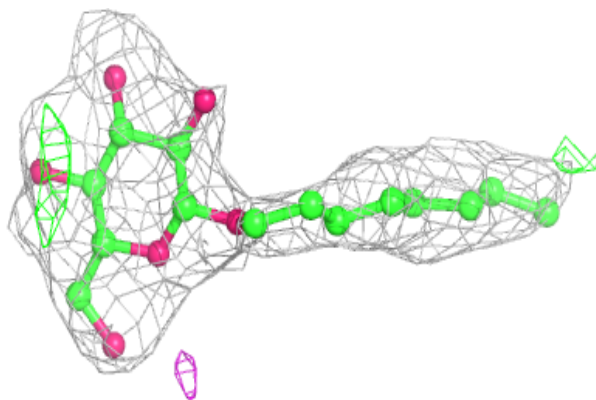
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG B 525:

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

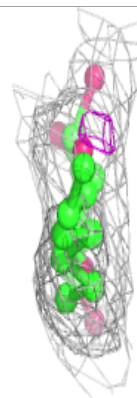
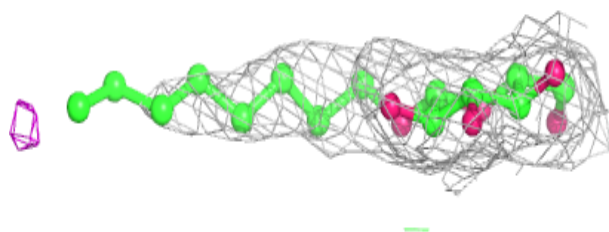
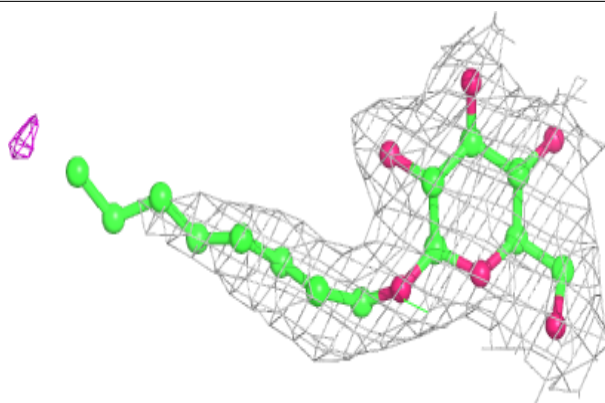
**Electron density around BOG A 555:**

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

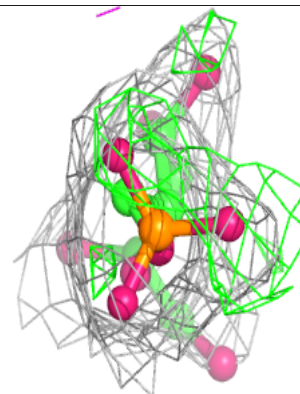
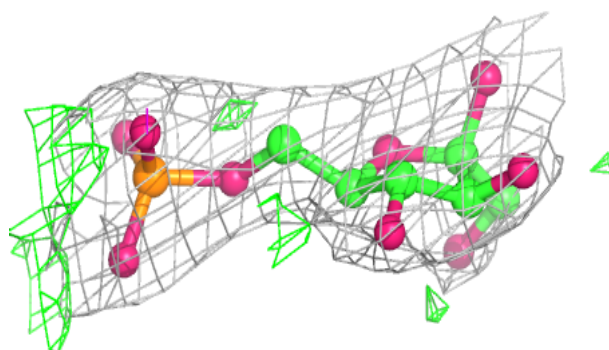
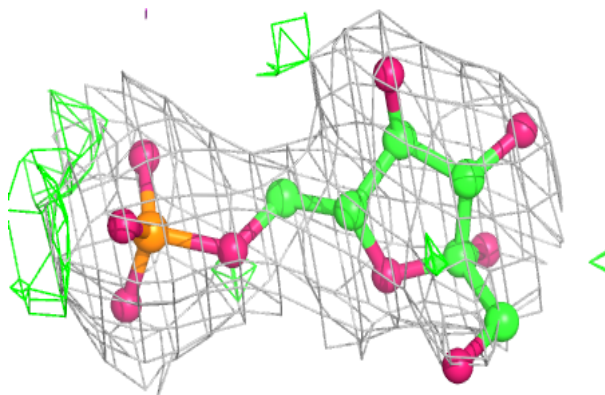


Electron density around BOG A 510:

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

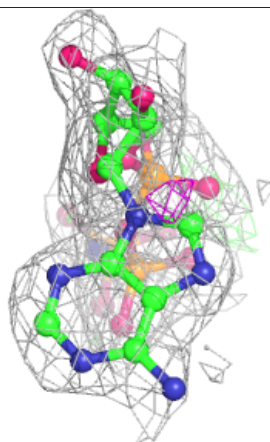
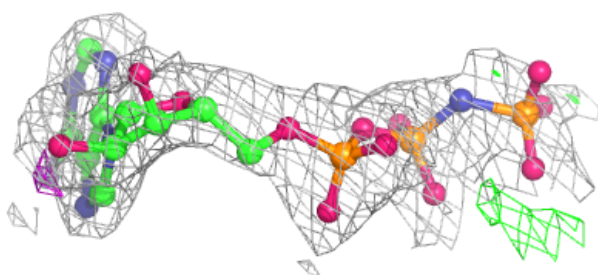
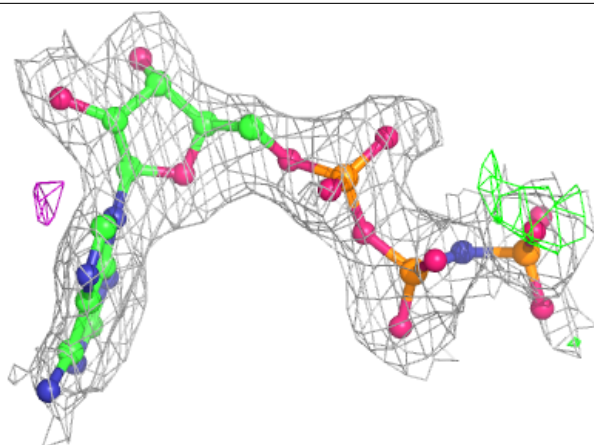
**Electron density around F6P A 520:**

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

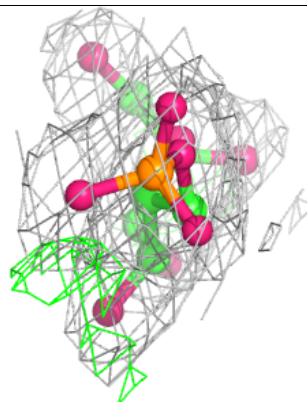
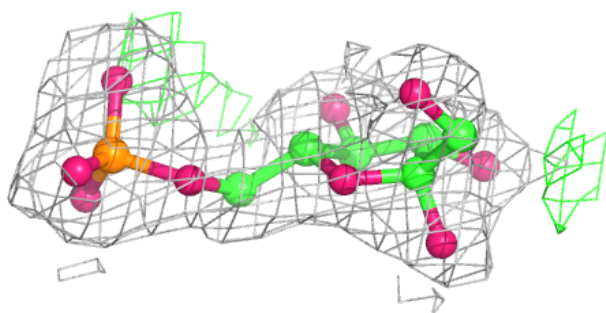
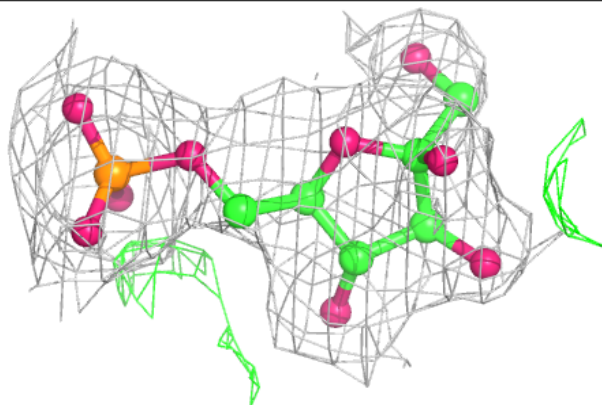


Electron density around ANP A 500:

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

**Electron density around F6P B 550:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.