



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:22 AM UTC

PDB ID : 3VTH / pdb_00003vth
Title : Crystal structure of full-length HypF in the phosphate- and nucleotide-bound form
Authors : Shomura, Y.; Higuchi, Y.
Deposited on : 2012-05-30
Resolution : 2.00 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

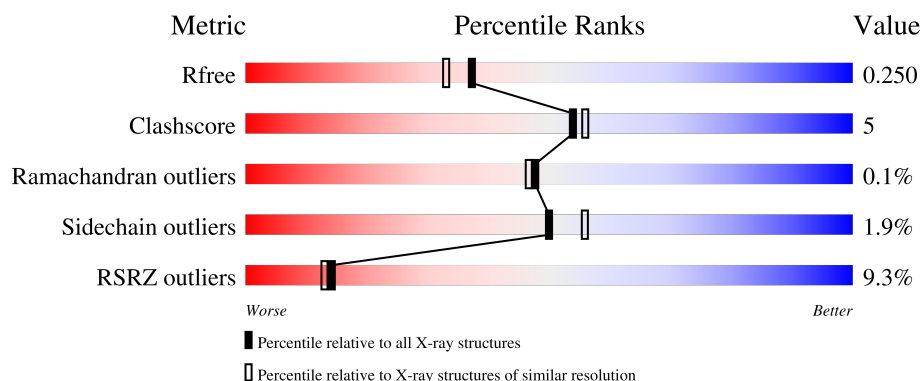
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	761	3% 90% 9%
1	B	761	14% 70% 12% 17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11800 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 Hydrogenase maturation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	4	0
			6058	3870	1033	1124	31			
1	B	630	Total	C	N	O	S	0	0	0
			5059	3236	867	931	25			

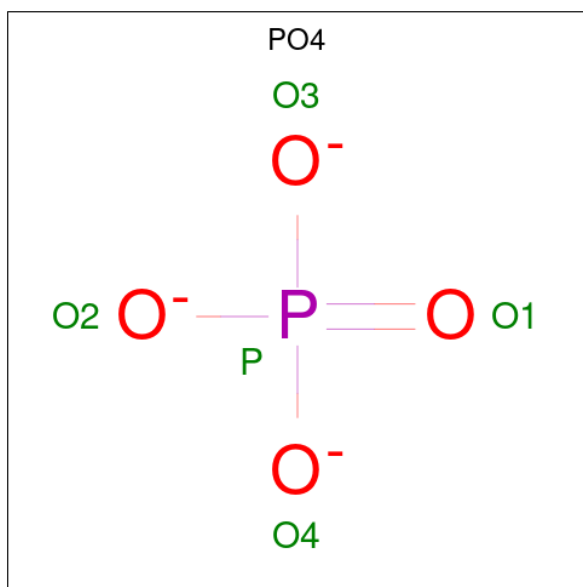
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	SER	-	expression tag	UNP Q8RDB0
A	753	ALA	-	expression tag	UNP Q8RDB0
A	754	TRP	-	expression tag	UNP Q8RDB0
A	755	SER	-	expression tag	UNP Q8RDB0
A	756	HIS	-	expression tag	UNP Q8RDB0
A	757	PRO	-	expression tag	UNP Q8RDB0
A	758	GLN	-	expression tag	UNP Q8RDB0
A	759	PHE	-	expression tag	UNP Q8RDB0
A	760	GLU	-	expression tag	UNP Q8RDB0
A	761	LYS	-	expression tag	UNP Q8RDB0
B	752	SER	-	expression tag	UNP Q8RDB0
B	753	ALA	-	expression tag	UNP Q8RDB0
B	754	TRP	-	expression tag	UNP Q8RDB0
B	755	SER	-	expression tag	UNP Q8RDB0
B	756	HIS	-	expression tag	UNP Q8RDB0
B	757	PRO	-	expression tag	UNP Q8RDB0
B	758	GLN	-	expression tag	UNP Q8RDB0
B	759	PHE	-	expression tag	UNP Q8RDB0
B	760	GLU	-	expression tag	UNP Q8RDB0
B	761	LYS	-	expression tag	UNP Q8RDB0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

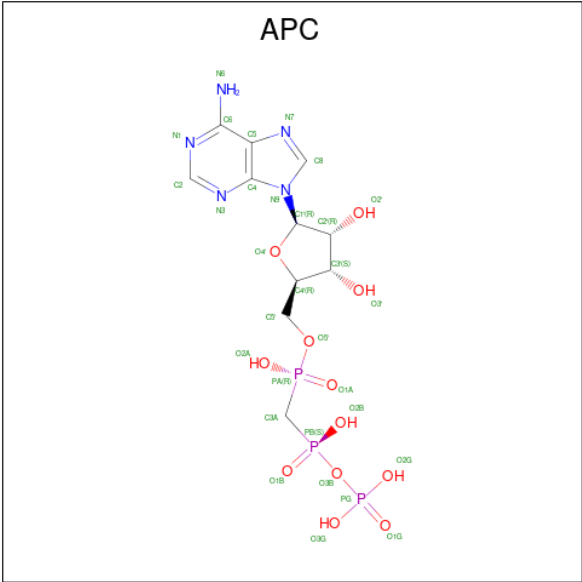
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

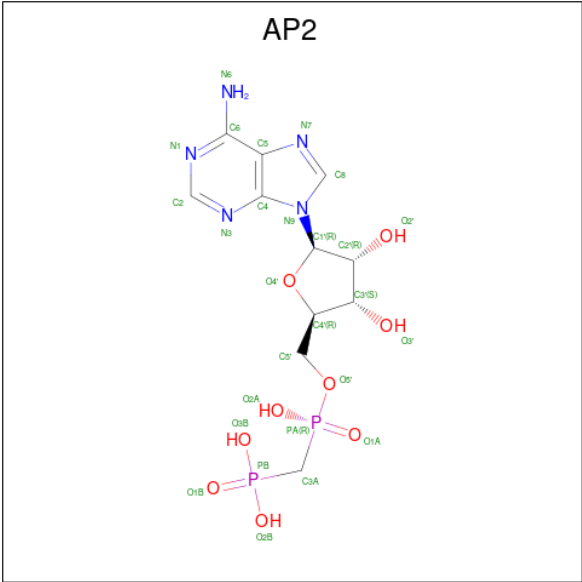


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: AP2) (formula: C₁₁H₁₇N₅O₉P₂).

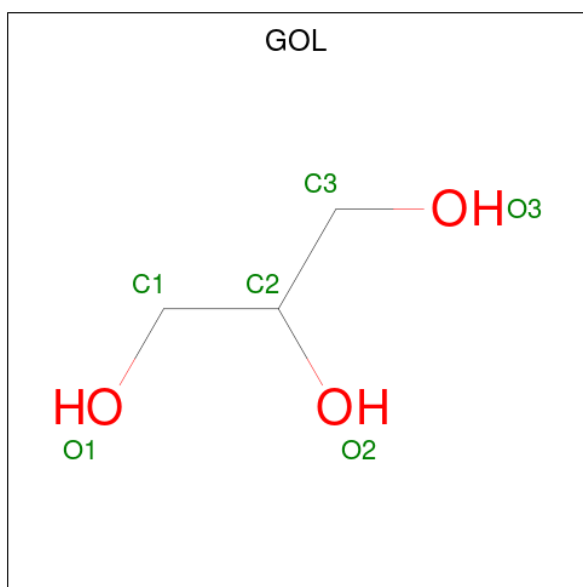


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
6	B	1	Total	C	N	O	P	0	0
			27	11	5	9	2		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		
7	B	1	Total	Fe	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

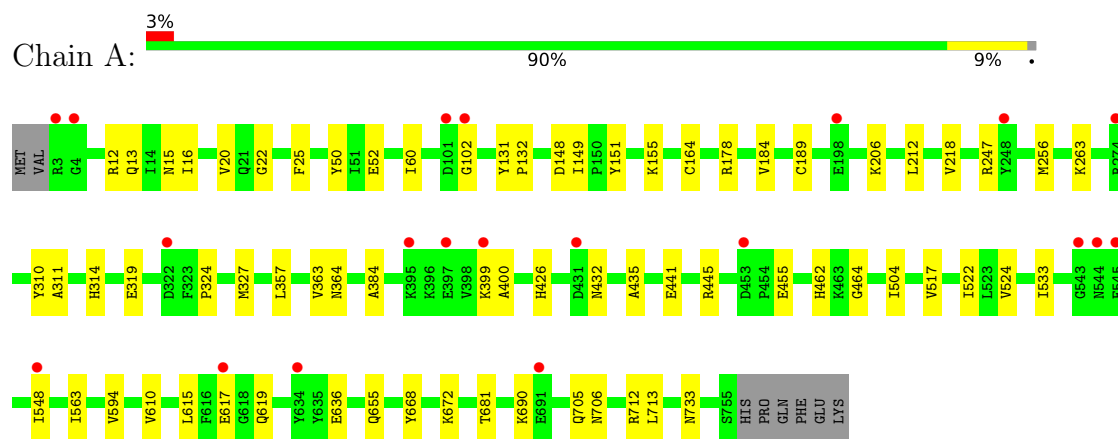
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	400	Total	O	0	0
			400	400		
9	B	107	Total	O	0	0
			107	107		

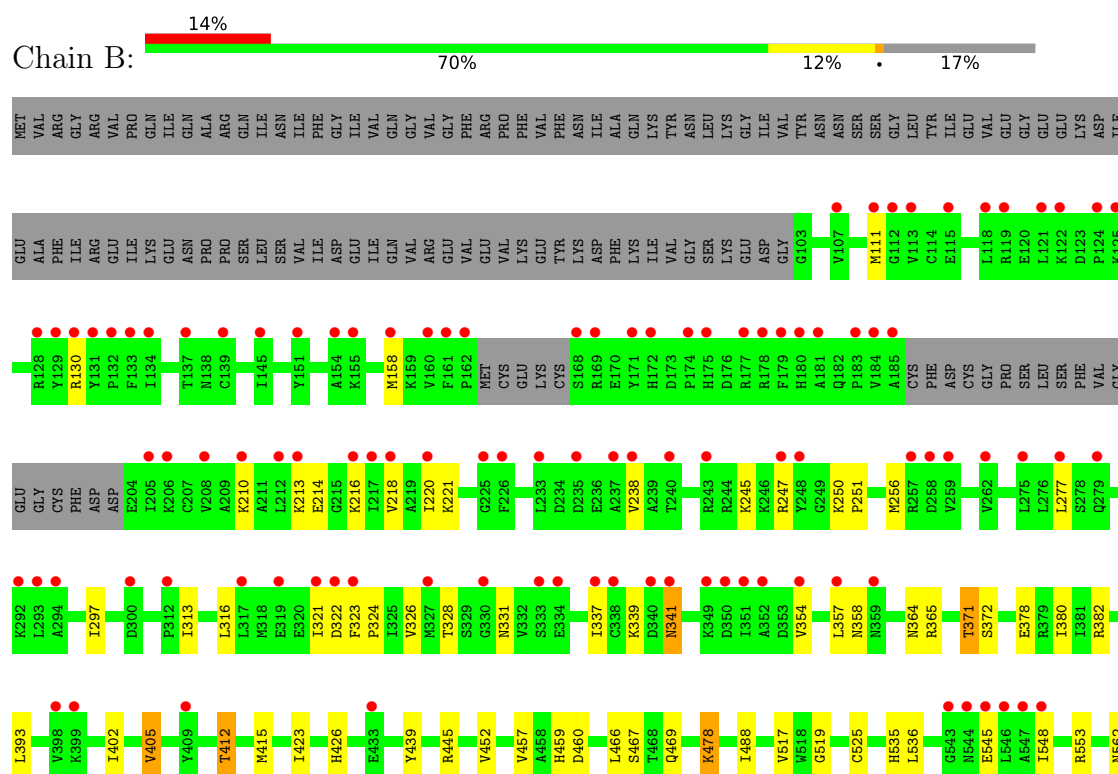
3 Residue-property plots

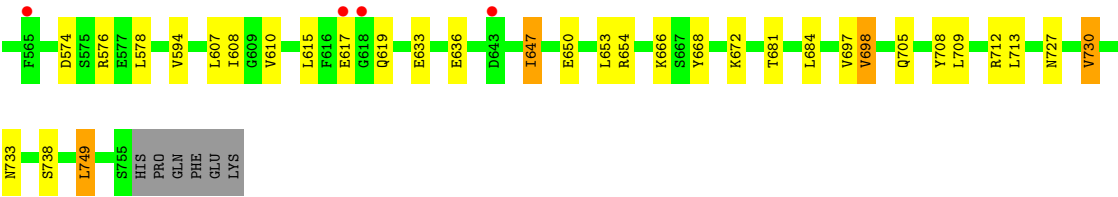
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hydrogenase maturation factor



• Molecule 1: Hydrogenase maturation factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	232.98Å 232.98Å 65.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.00) 96.9 (20.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.238 0.222 , 0.250	Depositor DCC
R_{free} test set	6728 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, ZN, FE, AP2, PO4, APC

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	0.66	1/6192 (0.0%)	0.82	2/8341 (0.0%)
1	B	0.54	0/5161	0.81	3/6952 (0.0%)
All	All	0.61	1/11353 (0.0%)	0.81	5/15293 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	610	VAL	C-O	-5.35	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	N-CA-C	5.60	123.37	115.30
1	B	111	MET	N-CA-C	5.26	117.38	109.23
1	A	563	ILE	N-CA-C	5.19	115.81	110.36
1	B	617	GLU	N-CA-C	5.17	117.33	111.02
1	B	525	CYS	N-CA-C	5.04	116.85	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6058	0	6064	47	0
1	B	5059	0	5084	64	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	0	0
3	B	10	0	0	0	0
4	A	31	0	14	3	0
4	B	31	0	14	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	14	1	0
6	B	27	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	12	0	16	0	0
8	B	6	0	8	0	0
9	A	400	0	0	7	0
9	B	107	0	0	2	0
All	All	11800	0	11228	111	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 5.

All (111) 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:A:13:GLN:HE21	1:A:15:ASN:HD21	1.20	0.88
1:B:405:VAL:HG22	1:B:439:TYR:OH	1.77	0.84
1:A:636:GLU:H	1:A:655:GLN:HE22	1.28	0.79
1:B:321:ILE:HG13	1:B:322:ASP:H	1.49	0.76
1:A:615:LEU:H	1:A:619:GLN:NE2	1.84	0.76
1:B:321:ILE:HD11	1:B:323:PHE:CZ	2.22	0.74
1:B:615:LEU:H	1:B:619:GLN:HE22	1.35	0.74
1:B:245:LYS:HE3	1:B:331:ASN:O	1.87	0.73
1:B:615:LEU:H	1:B:619:GLN:NE2	1.87	0.71
1:A:615:LEU:H	1:A:619:GLN:HE22	1.40	0.69
1:B:247:ARG:HE	1:B:250:LYS:HB2	1.59	0.67
1:A:247:ARG:HE	4:A:804:APC:H3A2	1.61	0.66
1:B:247:ARG:NH2	1:B:251:PRO:O	2.30	0.65
1:B:371:THR:HG23	1:B:380:ILE:HA	1.79	0.64
1:A:311:ALA:H	1:A:314:HIS:HD2	1.46	0.63
1:B:321:ILE:HG13	1:B:322:ASP:N	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLU:N	1:A:655:GLN:HE22	1.98	0.61
1:B:221:LYS:HD3	1:B:358:ASN:CB	2.30	0.61
1:A:462:HIS:HD2	1:A:464:GLY:H	1.46	0.61
1:A:247:ARG:HH21	4:A:804:APC:H3A1	1.67	0.60
1:B:221:LYS:HD3	1:B:358:ASN:HB2	1.84	0.59
1:B:371:THR:HG21	1:B:378:GLU:OE2	2.01	0.59
1:B:727:ASN:HB3	1:B:730:VAL:O	2.03	0.58
1:A:247:ARG:HE	4:A:804:APC:C3A	2.16	0.58
1:B:402:ILE:HD11	1:B:749:LEU:HD13	1.85	0.58
1:B:341:ASN:HD21	1:B:357:LEU:HD13	1.69	0.57
1:A:705:GLN:NE2	1:A:733:ASN:HD22	2.02	0.57
1:A:311:ALA:H	1:A:314:HIS:CD2	2.22	0.57
1:B:371:THR:HG22	1:B:372:SER:H	1.68	0.57
1:B:256:MET:HG2	1:B:324:PRO:HB3	1.86	0.56
1:A:314:HIS:CE1	9:A:1300:HOH:O	2.59	0.56
1:A:712:ARG:HD2	9:A:1023:HOH:O	2.06	0.55
1:B:705:GLN:NE2	1:B:733:ASN:HD22	2.05	0.55
1:B:339:LYS:HB3	1:B:365:ARG:HB3	1.88	0.55
1:B:412:THR:HG22	1:B:738:SER:OG	2.08	0.54
1:A:256:MET:HG2	1:A:324:PRO:HB3	1.90	0.54
1:B:364:ASN:HB3	1:B:445:ARG:NH1	2.23	0.54
1:A:310:TYR:H	1:A:314:HIS:HD2	1.54	0.54
1:B:562:ASN:HD22	1:B:654:ARG:HD3	1.73	0.54
1:B:220:ILE:HD11	1:B:313:ILE:HD12	1.89	0.54
1:A:22:GLY:HA2	1:A:151:TYR:CE1	2.42	0.53
1:A:426:HIS:HD2	9:A:902:HOH:O	1.91	0.53
1:B:405:VAL:HG13	1:B:467:SER:HB2	1.90	0.53
1:B:545:GLU:O	1:B:548:ILE:HG13	2.09	0.53
1:A:178:ARG:HD3	1:A:184:VAL:HG23	1.91	0.52
1:B:214:GLU:HG3	1:B:216:LYS:HG3	1.90	0.52
1:A:504:ILE:HG12	1:A:522:ILE:HD12	1.91	0.51
1:B:574:ASP:OD1	1:B:576:ARG:HG2	2.11	0.51
1:B:245:LYS:HZ2	1:B:328:THR:HG22	1.75	0.51
1:B:459:HIS:HD2	1:B:460:ASP:O	1.92	0.51
1:A:681:THR:HG21	1:A:713:LEU:HD21	1.92	0.51
1:B:328:THR:HG23	4:B:804:APC:O1A	2.11	0.51
1:A:712:ARG:HD3	9:A:1118:HOH:O	2.11	0.51
1:A:400:ALA:HB1	1:A:455:GLU:OE1	2.11	0.51
1:A:462:HIS:CD2	1:A:464:GLY:H	2.27	0.50
1:B:158:MET:HE2	1:B:158:MET:HA	1.92	0.50
1:A:50:TYR:CE1	1:A:52:GLU:HG3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:HIS:HD2	1:B:536:LEU:O	1.96	0.49
1:A:212:LEU:HD21	1:A:218:VAL:HG22	1.94	0.49
1:B:331:ASN:HD22	1:B:337:ILE:HA	1.77	0.49
1:A:148:ASP:HB3	1:A:155:LYS:HD3	1.94	0.48
1:B:633:GLU:OE2	1:B:668:TYR:OH	2.31	0.48
1:B:412:THR:HG21	1:B:423:ILE:HD11	1.96	0.48
1:B:668:TYR:CZ	1:B:672:LYS:HD2	2.48	0.48
1:A:524:VAL:HG23	1:A:533:ILE:HG13	1.95	0.48
1:B:382:ARG:HD3	9:B:930:HOH:O	2.11	0.48
1:B:382:ARG:HD2	1:B:426:HIS:CG	2.48	0.47
1:B:364:ASN:HB3	1:B:445:ARG:HH11	1.78	0.47
1:A:363:VAL:O	1:A:445:ARG:NH1	2.48	0.47
1:A:310:TYR:H	1:A:314:HIS:CD2	2.32	0.46
1:B:517:VAL:HB	1:B:594:VAL:HG12	1.97	0.46
1:B:238:VAL:HG11	1:B:297:ILE:HD11	1.96	0.46
1:A:364:ASN:HD22	1:A:445:ARG:HH11	1.63	0.46
1:B:218:VAL:HG12	1:B:354:VAL:HG23	1.97	0.45
1:B:647:ILE:CD1	1:B:684:LEU:HD11	2.46	0.45
1:B:210:LYS:HA	1:B:213:LYS:HG2	1.97	0.45
1:A:314:HIS:HE1	9:A:1300:HOH:O	1.97	0.45
1:A:426:HIS:HE1	9:A:940:HOH:O	1.99	0.45
1:B:607:LEU:HD12	1:B:653:LEU:HD22	1.99	0.45
1:A:164:CYS:HB3	1:A:189:CYS:HB3	1.98	0.44
1:A:149:ILE:C	1:A:149:ILE:HD12	2.42	0.44
1:A:462:HIS:HD2	1:A:464:GLY:N	2.13	0.44
1:B:466:LEU:HD23	1:B:469:GLN:NE2	2.32	0.44
1:B:488:ILE:HG23	1:B:698:VAL:HG22	1.99	0.44
1:B:412:THR:CG2	1:B:738:SER:OG	2.66	0.43
1:B:457:VAL:CG1	1:B:478:LYS:HD3	2.47	0.43
1:A:50:TYR:HE1	1:A:52:GLU:HG3	1.82	0.43
1:B:578:LEU:C	1:B:578:LEU:HD13	2.43	0.43
1:B:247:ARG:NH1	4:B:804:APC:O1A	2.52	0.43
1:B:415:MET:HE3	1:B:452:VAL:HG21	1.99	0.43
1:A:432:ASN:ND2	1:A:435:ALA:H	2.16	0.43
1:A:517:VAL:HB	1:A:594:VAL:HG12	2.00	0.43
1:B:337:ILE:O	1:B:365:ARG:HD3	2.20	0.42
1:B:221:LYS:HD3	1:B:358:ASN:HB3	2.02	0.42
1:B:650:GLU:HG2	9:B:951:HOH:O	2.19	0.42
1:B:708:TYR:CZ	1:B:712:ARG:HD3	2.55	0.42
1:A:706:ASN:HB2	6:A:806:AP2:N1	2.34	0.42
1:B:681:THR:HG21	1:B:713:LEU:HD21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:HA	1:A:132:PRO:HD3	1.82	0.41
1:B:130:ARG:HG3	1:B:316:LEU:HD22	2.02	0.41
1:A:548:ILE:HG23	1:A:617:GLU:OE1	2.21	0.41
1:A:206:LYS:HE3	1:A:206:LYS:HB2	1.79	0.41
1:B:562:ASN:ND2	1:B:654:ARG:HD3	2.34	0.41
1:B:382:ARG:HD2	1:B:426:HIS:CE1	2.56	0.41
1:A:327:MET:HE3	9:A:908:HOH:O	2.20	0.41
1:A:668:TYR:CE2	1:A:672:LYS:HD2	2.56	0.41
1:B:245:LYS:CE	1:B:331:ASN:O	2.63	0.41
1:B:608:ILE:HG13	1:B:610:VAL:HG23	2.03	0.41
1:B:608:ILE:O	1:B:666:LYS:HE3	2.21	0.41
1:A:16:ILE:HG22	1:A:20:VAL:HG11	2.03	0.40
1:A:12:ARG:HG3	1:A:60:ILE:HG21	2.02	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	755/761 (99%)	729 (97%)	25 (3%)	1 (0%)	48	46
1	B	624/761 (82%)	598 (96%)	25 (4%)	1 (0%)	43	42
All	All	1379/1522 (91%)	1327 (96%)	50 (4%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ALA
1	B	519	GLY

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	657/661 (99%)	650 (99%)	7 (1%)	65	73
1	B	545/661 (82%)	529 (97%)	16 (3%)	37	40
All	All	1202/1322 (91%)	1179 (98%)	23 (2%)	50	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	263	LYS
1	A	319	GLU
1	A	357	LEU
1	A	399	LYS
1	A	441	GLU
1	A	690	LYS
1	B	277	LEU
1	B	326	VAL
1	B	341	ASN
1	B	371	THR
1	B	393	LEU
1	B	405	VAL
1	B	412	THR
1	B	478	LYS
1	B	553	ARG
1	B	636	GLU
1	B	647	ILE
1	B	697	VAL
1	B	698	VAL
1	B	709	LEU
1	B	730	VAL
1	B	749	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	ASN
1	A	44	ASN
1	A	70	ASN
1	A	314	HIS
1	A	364	ASN
1	A	411	ASN
1	A	426	HIS
1	A	432	ASN
1	A	437	ASN
1	A	462	HIS
1	A	562	ASN
1	A	619	GLN
1	A	655	GLN
1	A	705	GLN
1	A	727	ASN
1	B	135	ASN
1	B	180	HIS
1	B	331	ASN
1	B	341	ASN
1	B	364	ASN
1	B	459	HIS
1	B	516	ASN
1	B	535	HIS
1	B	562	ASN
1	B	619	GLN
1	B	675	ASN
1	B	705	GLN
1	B	727	ASN
1	B	746	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	APC	A	804	5	29,33,33	1.56	6 (20%)	44,52,52	1.85	11 (25%)
3	PO4	A	810	-	4,4,4	0.88	0	6,6,6	0.51	0
4	APC	B	804	5	29,33,33	1.61	7 (24%)	44,52,52	1.89	13 (29%)
3	PO4	A	809	-	4,4,4	0.88	0	6,6,6	0.67	0
8	GOL	A	813	-	5,5,5	0.34	0	5,5,5	0.22	0
6	AP2	B	806	7	26,29,29	1.59	4 (15%)	40,45,45	2.06	13 (32%)
3	PO4	A	808	-	4,4,4	1.03	0	6,6,6	0.46	0
8	GOL	A	812	-	5,5,5	0.34	0	5,5,5	0.60	0
8	GOL	B	801	-	5,5,5	0.42	0	5,5,5	0.59	0
3	PO4	A	803	-	4,4,4	0.99	0	6,6,6	0.54	0
3	PO4	A	811	-	4,4,4	0.87	0	6,6,6	0.57	0
6	AP2	A	806	7	26,29,29	1.58	6 (23%)	40,45,45	2.11	15 (37%)
3	PO4	B	808	-	4,4,4	1.06	0	6,6,6	0.57	0
3	PO4	B	803	-	4,4,4	0.82	0	6,6,6	0.51	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	APC	A	804	5	-	4/19/38/38	0/3/3/3
4	APC	B	804	5	-	4/19/38/38	0/3/3/3
8	GOL	A	813	-	-	0/4/4/4	-
6	AP2	B	806	7	-	1/16/32/32	0/3/3/3
8	GOL	B	801	-	-	0/4/4/4	-
8	GOL	A	812	-	-	2/4/4/4	-
6	AP2	A	806	7	-	0/16/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	806	AP2	C5-C4	5.18	1.48	1.39
4	B	804	APC	C5-C4	4.92	1.47	1.39
6	A	806	AP2	C5-C4	4.91	1.47	1.39
4	A	804	APC	C5-C4	4.71	1.47	1.39
4	B	804	APC	PB-O3B	3.52	1.62	1.58
4	A	804	APC	PA-O2A	-3.02	1.49	1.56
6	B	806	AP2	C5-C6	2.98	1.49	1.41
6	A	806	AP2	C5-C6	2.85	1.48	1.41
4	B	804	APC	C5-C6	2.74	1.48	1.41
4	A	804	APC	C5-C6	2.66	1.48	1.41
4	A	804	APC	PB-O3B	2.63	1.61	1.58
6	A	806	AP2	C8-N7	2.50	1.36	1.31
6	B	806	AP2	C8-N7	2.40	1.36	1.31
4	A	804	APC	C4-N9	-2.36	1.32	1.37
4	A	804	APC	C8-N7	2.30	1.36	1.31
4	B	804	APC	C8-N7	2.24	1.36	1.31
4	B	804	APC	PA-O2A	-2.24	1.50	1.56
4	B	804	APC	C5-N7	-2.19	1.35	1.39
6	A	806	AP2	C5-N7	-2.14	1.35	1.39
6	A	806	AP2	PB-O2B	-2.12	1.50	1.55
4	B	804	APC	PB-O2B	-2.12	1.51	1.56
6	B	806	AP2	PA-O2A	-2.10	1.51	1.56
6	A	806	AP2	PA-O2A	-2.05	1.51	1.56

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	AP2	C5-C4-N3	-5.46	119.20	126.72
6	A	806	AP2	C5-C4-N3	-5.30	119.42	126.72
4	B	804	APC	C5-C4-N3	-5.29	119.43	126.72
4	B	804	APC	N3-C4-N9	4.64	135.06	127.17
4	A	804	APC	C5-C4-N3	-4.38	120.69	126.72
6	B	806	AP2	N3-C4-N9	4.22	134.34	127.17
6	A	806	AP2	O1B-PB-C3A	-4.16	102.30	111.37
4	A	804	APC	C4-N9-C8	4.11	110.06	105.74
6	A	806	AP2	N3-C4-N9	4.05	134.06	127.17
4	A	804	APC	N3-C4-N9	4.04	134.04	127.17
6	B	806	AP2	C2-N3-C4	3.75	120.98	111.83
6	A	806	AP2	N3-C2-N1	-3.73	122.94	128.58
6	B	806	AP2	C4-C5-N7	-3.65	106.40	110.58
6	A	806	AP2	C2-N3-C4	3.62	120.66	111.83
6	B	806	AP2	N3-C2-N1	-3.61	123.11	128.58
4	B	804	APC	C2-N3-C4	3.59	120.60	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	APC	N3-C2-N1	-3.47	123.32	128.58
4	B	804	APC	C4-N9-C8	3.46	109.37	105.74
6	B	806	AP2	O1B-PB-C3A	-3.40	103.95	111.37
4	A	804	APC	N3-C2-N1	-3.27	123.64	128.58
6	A	806	AP2	C4-C5-N7	-3.18	106.94	110.58
4	B	804	APC	C4-C5-N7	-3.17	106.95	110.58
6	A	806	AP2	O1A-PA-C3A	-3.17	100.71	109.05
4	A	804	APC	C2-N3-C4	3.08	119.36	111.83
6	A	806	AP2	O2A-PA-O1A	2.94	119.52	109.95
6	B	806	AP2	O1A-PA-C3A	-2.92	101.36	109.05
4	A	804	APC	N9-C8-N7	-2.89	109.84	113.94
4	A	804	APC	C2'-C1'-N9	-2.77	106.41	113.30
4	A	804	APC	C4-C5-N7	-2.75	107.43	110.58
4	B	804	APC	C5-N7-C8	2.60	107.54	103.45
6	B	806	AP2	O2A-PA-O1A	2.58	118.34	109.95
4	A	804	APC	C5-N7-C8	2.52	107.40	103.45
6	A	806	AP2	C2'-C1'-N9	-2.50	107.09	113.30
6	B	806	AP2	C4-N9-C8	2.49	108.35	105.74
6	B	806	AP2	C5-N7-C8	2.48	107.34	103.45
6	B	806	AP2	C6-C5-N7	2.47	136.86	132.09
6	B	806	AP2	O4'-C1'-N9	2.46	112.81	108.09
6	A	806	AP2	O3B-PB-O2B	2.44	114.92	107.96
6	A	806	AP2	O4'-C1'-N9	2.44	112.78	108.09
6	A	806	AP2	C2-N1-C6	2.37	122.63	118.73
4	B	804	APC	O2B-PB-O1B	2.37	117.66	109.95
4	A	804	APC	C6-C5-N7	2.36	136.63	132.09
4	B	804	APC	N9-C8-N7	-2.34	110.62	113.94
6	A	806	AP2	C5-N7-C8	2.33	107.11	103.45
6	A	806	AP2	O2A-PA-C3A	2.29	116.21	106.73
4	B	804	APC	C6-C5-N7	2.24	136.42	132.09
4	A	804	APC	C2-N1-C6	2.24	122.41	118.73
4	B	804	APC	PB-O3B-PG	-2.14	124.77	132.45
4	B	804	APC	O2A-PA-O1A	2.10	116.77	109.95
6	B	806	AP2	C2-N1-C6	2.08	122.15	118.73
6	A	806	AP2	C6-C5-N7	2.07	136.08	132.09
4	B	804	APC	C2-N1-C6	2.01	122.04	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	APC	PA-C3A-PB-O2B

Continued on next page...

Continued from previous page...

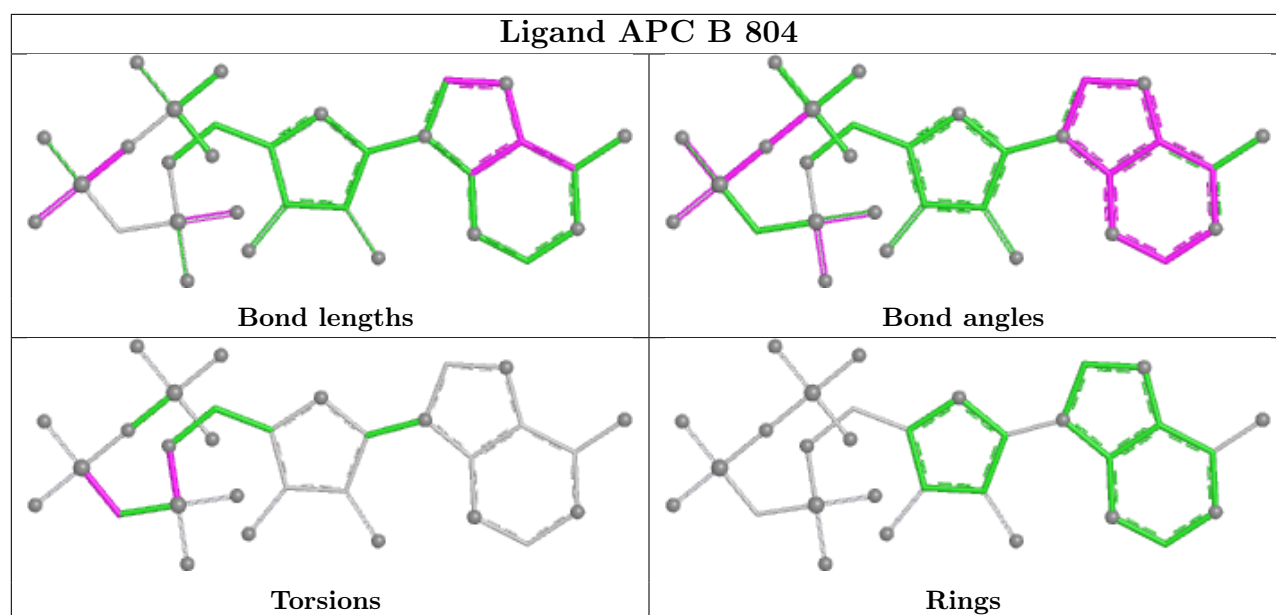
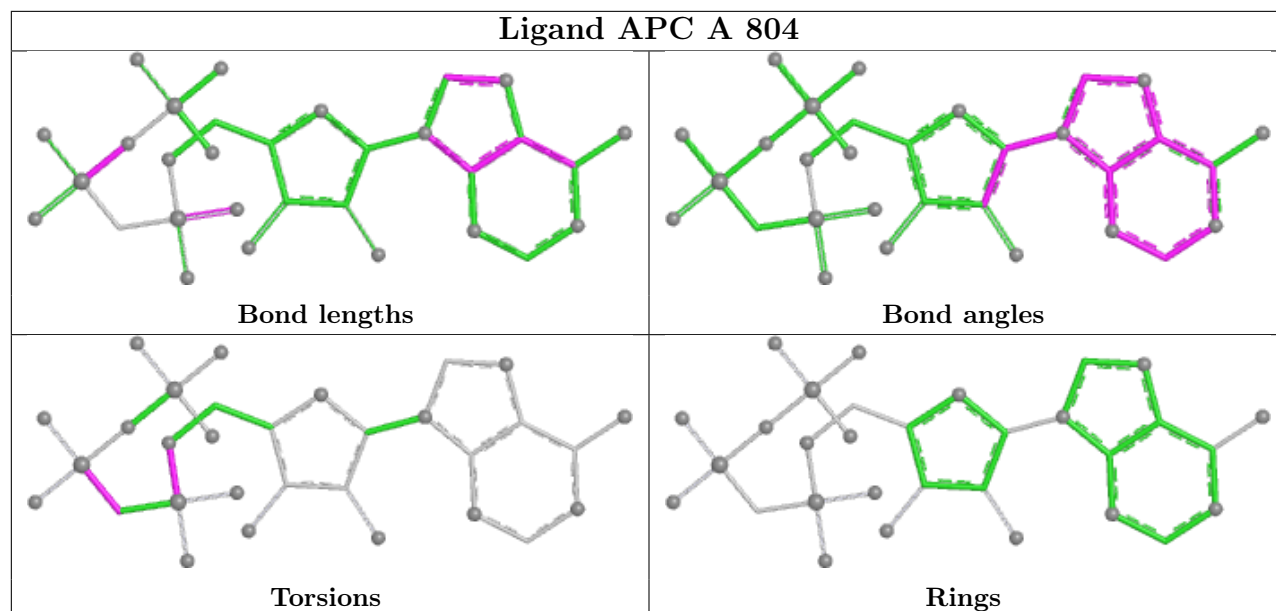
Mol	Chain	Res	Type	Atoms
4	A	804	APC	PA-C3A-PB-O3B
4	B	804	APC	PA-C3A-PB-O1B
4	B	804	APC	PA-C3A-PB-O2B
4	B	804	APC	PA-C3A-PB-O3B
4	B	804	APC	C5'-O5'-PA-O2A
8	A	812	GOL	C1-C2-C3-O3
8	A	812	GOL	O2-C2-C3-O3
6	B	806	AP2	C5'-O5'-PA-C3A
4	A	804	APC	PA-C3A-PB-O1B
4	A	804	APC	C5'-O5'-PA-O1A

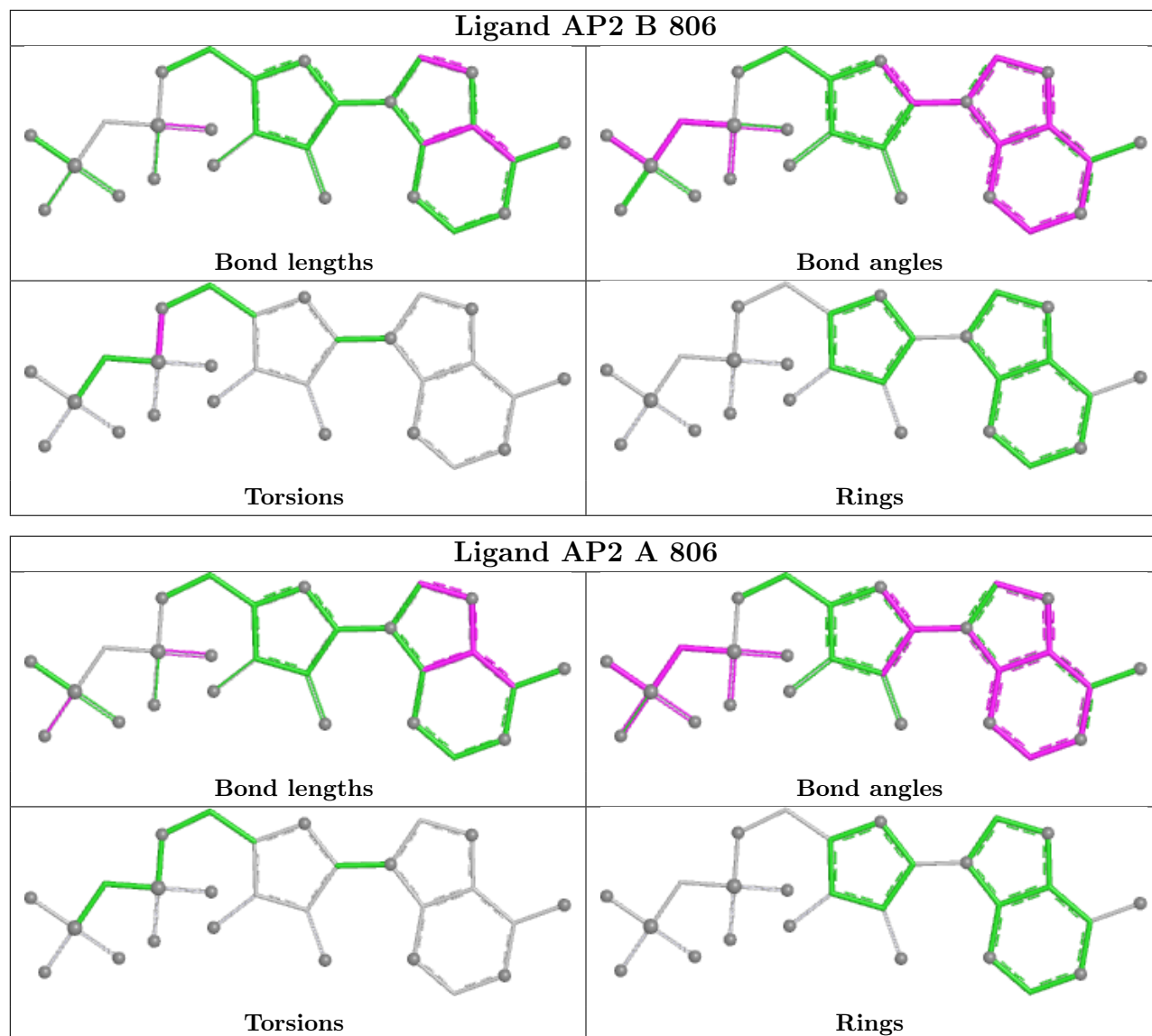
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	APC	3	0
4	B	804	APC	2	0
6	A	806	AP2	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	753/761 (98%)	-0.02	20 (2%) 56 55	18, 33, 49, 70	4 (0%)
1	B	630/761 (82%)	0.87	108 (17%) 4 4	27, 56, 118, 149	0
All	All	1383/1522 (90%)	0.38	128 (9%) 14 13	18, 39, 105, 149	4 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	6.4
1	B	168	SER	4.8
1	B	184	VAL	4.5
1	B	134	ILE	4.4
1	B	248	TYR	4.4
1	A	543	GLY	4.1
1	B	115	GLU	4.0
1	B	238	VAL	3.9
1	B	547	ALA	3.9
1	B	399	LYS	3.9
1	B	162	PRO	3.9
1	B	546	LEU	3.6
1	B	217	ILE	3.6
1	B	277	LEU	3.5
1	B	169	ARG	3.5
1	B	220	ILE	3.5
1	B	179	PHE	3.4
1	B	293	LEU	3.4
1	B	350	ASP	3.4
1	B	237	ALA	3.4
1	B	323	PHE	3.4
1	A	322	ASP	3.4
1	B	178	ARG	3.4
1	B	122	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	548	ILE	3.4
1	B	247	ARG	3.3
1	B	154	ALA	3.2
1	B	174	PRO	3.2
1	B	543	GLY	3.2
1	B	125	LYS	3.2
1	B	171	TYR	3.1
1	A	544	ASN	3.1
1	A	4	GLY	3.0
1	B	128	ARG	3.0
1	B	155	LYS	3.0
1	B	118	LEU	3.0
1	B	327	MET	2.9
1	B	107	VAL	2.9
1	B	145	ILE	2.9
1	B	161	PHE	2.9
1	B	113	VAL	2.9
1	B	240	THR	2.9
1	B	548	ILE	2.8
1	B	565	PHE	2.8
1	B	354	VAL	2.8
1	B	181	ALA	2.8
1	B	160	VAL	2.8
1	B	259	VAL	2.8
1	B	205	ILE	2.8
1	B	177	ARG	2.7
1	B	333	SER	2.7
1	A	397	GLU	2.7
1	B	545	GLU	2.7
1	B	111	MET	2.7
1	B	317	LEU	2.7
1	A	453	ASP	2.7
1	A	399	LYS	2.7
1	A	102	GLY	2.7
1	B	330	GLY	2.7
1	B	119	ARG	2.7
1	B	617	GLU	2.7
1	B	340	ASP	2.7
1	B	294	ALA	2.6
1	B	341	ASN	2.6
1	B	349	LYS	2.6
1	B	337	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	691	GLU	2.6
1	B	124	PRO	2.6
1	A	431	ASP	2.6
1	B	210	LYS	2.6
1	A	545	GLU	2.5
1	B	351	ILE	2.5
1	B	398	VAL	2.5
1	B	292	LYS	2.5
1	B	130	ARG	2.5
1	B	258	ASP	2.5
1	B	352	ALA	2.5
1	B	226	PHE	2.5
1	B	180	HIS	2.5
1	B	151	TYR	2.5
1	B	409	TYR	2.5
1	B	121	LEU	2.5
1	B	175	HIS	2.5
1	B	208	VAL	2.4
1	B	137	THR	2.4
1	B	279	GLN	2.4
1	B	218	VAL	2.4
1	B	338	CYS	2.4
1	B	158	MET	2.4
1	B	183	PRO	2.4
1	A	274	ARG	2.4
1	B	216	LYS	2.4
1	B	544	ASN	2.4
1	B	319	GLU	2.4
1	B	235	ASP	2.4
1	B	300	ASP	2.4
1	B	212	LEU	2.4
1	B	359	ASN	2.4
1	A	248	TYR	2.3
1	B	334	GLU	2.3
1	B	172	HIS	2.3
1	B	225	GLY	2.3
1	B	321	ILE	2.3
1	B	129	TYR	2.3
1	B	132	PRO	2.2
1	B	643	ASP	2.2
1	B	233	LEU	2.2
1	B	275	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	257	ARG	2.2
1	B	213	LYS	2.2
1	B	618	GLY	2.2
1	A	198	GLU	2.2
1	B	433	GLU	2.2
1	B	357	LEU	2.2
1	A	634	TYR	2.2
1	B	112	GLY	2.2
1	A	617	GLU	2.1
1	B	243	ARG	2.1
1	B	131	TYR	2.1
1	A	101	ASP	2.1
1	B	322	ASP	2.1
1	B	262	VAL	2.1
1	B	139	CYS	2.1
1	B	133	PHE	2.1
1	A	395	LYS	2.1
1	A	3	ARG	2.1
1	B	206	LYS	2.0
1	B	312	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	B	805	1/1	0.61	0.20	86,86,86,86	0
3	PO4	A	809	5/5	0.67	0.14	70,71,72,72	0
3	PO4	A	811	5/5	0.74	0.13	83,83,84,84	0

Continued on next page...

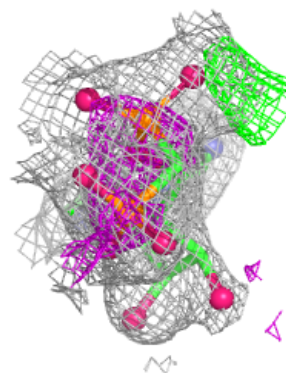
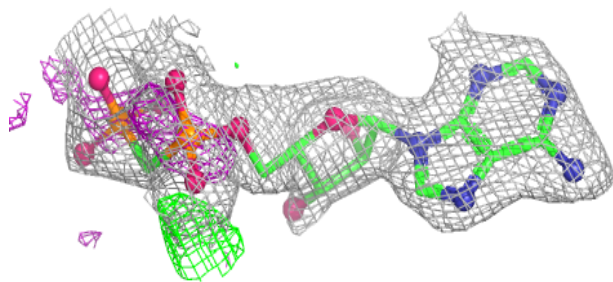
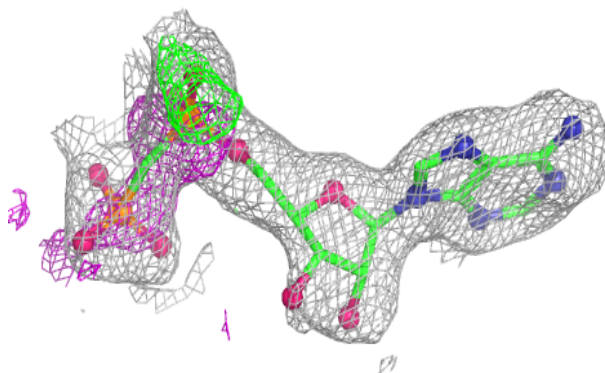
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	803	5/5	0.80	0.12	60,60,60,61	0
3	PO4	A	810	5/5	0.80	0.17	58,58,60,61	0
5	MG	A	805	1/1	0.86	0.11	45,45,45,45	0
6	AP2	B	806	27/27	0.87	0.12	45,53,56,57	0
3	PO4	A	808	5/5	0.88	0.12	51,51,54,54	0
8	GOL	A	812	6/6	0.89	0.09	37,39,43,47	0
4	APC	B	804	31/31	0.90	0.10	55,59,72,74	0
3	PO4	B	808	5/5	0.92	0.09	58,58,59,59	0
8	GOL	B	801	6/6	0.92	0.08	27,30,31,31	0
6	AP2	A	806	27/27	0.93	0.09	29,37,39,40	0
8	GOL	A	813	6/6	0.95	0.07	30,32,33,34	0
4	APC	A	804	31/31	0.97	0.06	28,32,35,37	0
3	PO4	A	803	5/5	0.98	0.05	23,24,26,27	0
2	ZN	B	802	1/1	0.98	0.05	97,97,97,97	0
7	FE	B	807	1/1	1.00	0.03	37,37,37,37	0
2	ZN	A	801	1/1	1.00	0.01	27,27,27,27	0
2	ZN	A	802	1/1	1.00	0.03	35,35,35,35	0
7	FE	A	807	1/1	1.00	0.03	27,27,27,27	0

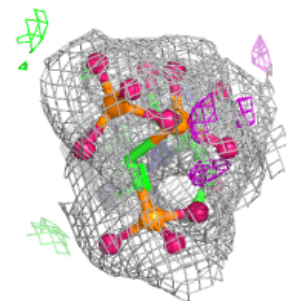
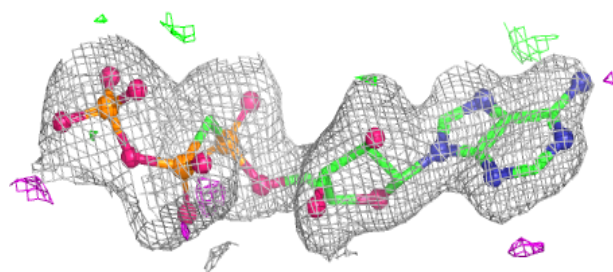
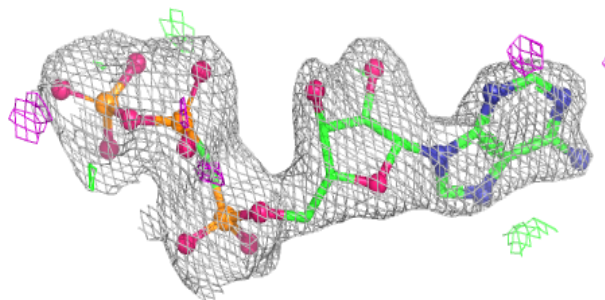
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AP2 B 806:

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

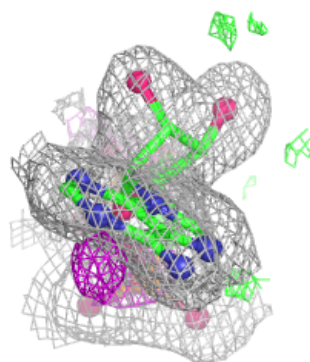
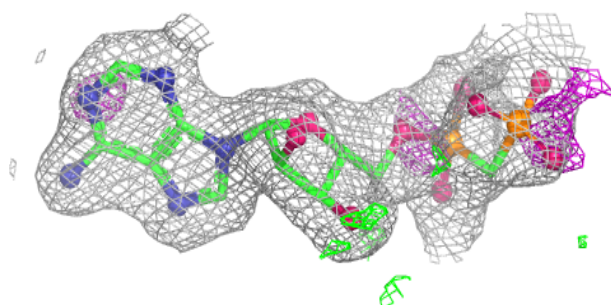
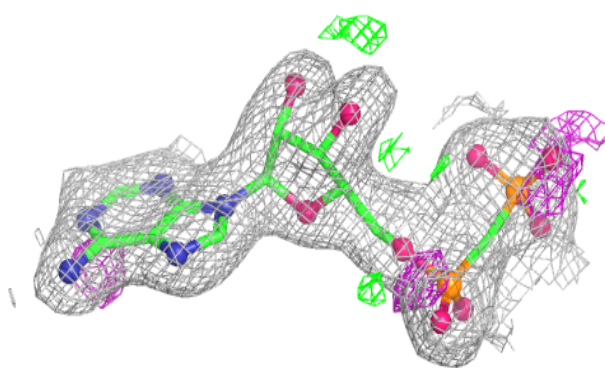
**Electron density around APC B 804:**

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

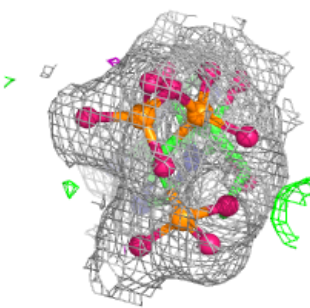
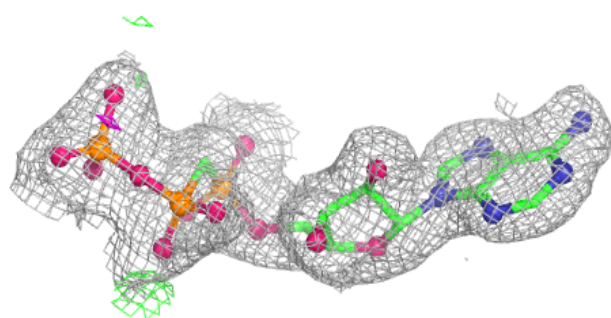
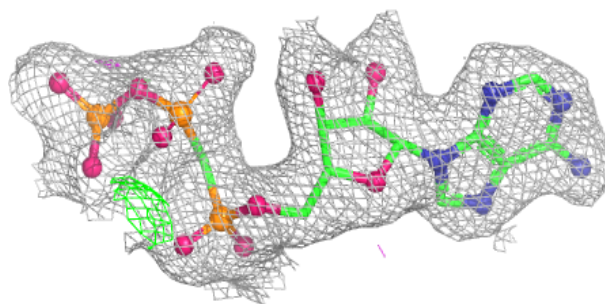


Electron density around AP2 A 806:

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

**Electron density around APC A 804:**

$2mF_o-DF_c$ (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.