



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2025 – 05:15 PM JST

PDB ID : 9KQH / pdb_00009kqh
Title : Crystal structure of Finegoldia magna DinG in complex with ssDNA and ADPNP
Authors : Cheng, K.; Gao, T.
Deposited on : 2024-11-25
Resolution : 2.26 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

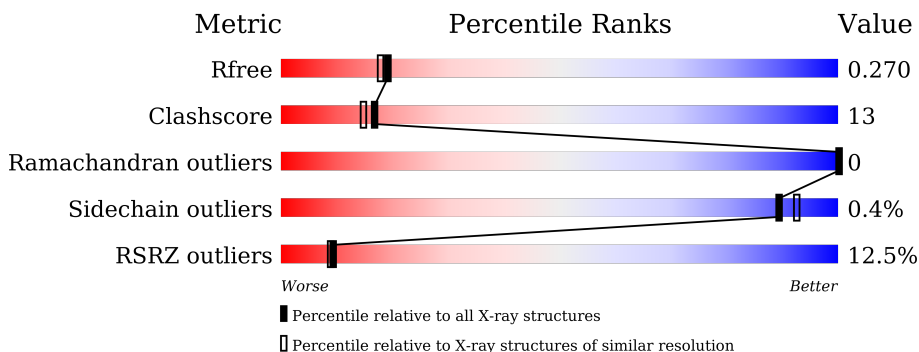
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	748	<div> <div>12%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
2	B	12	<div> <div>17%</div> <div>83%</div> <div>17%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6437 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 DNA 5'-3' helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	738	6057	3901	975	1151	30	0	0	0

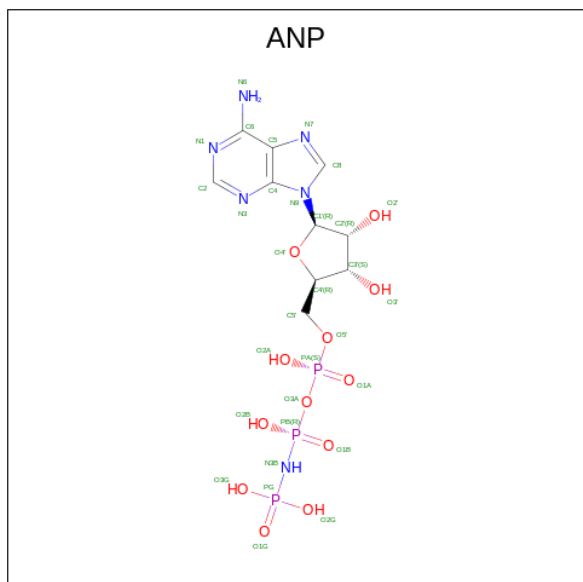
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ALA	ASP	engineered mutation	UNP B0S2X2

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

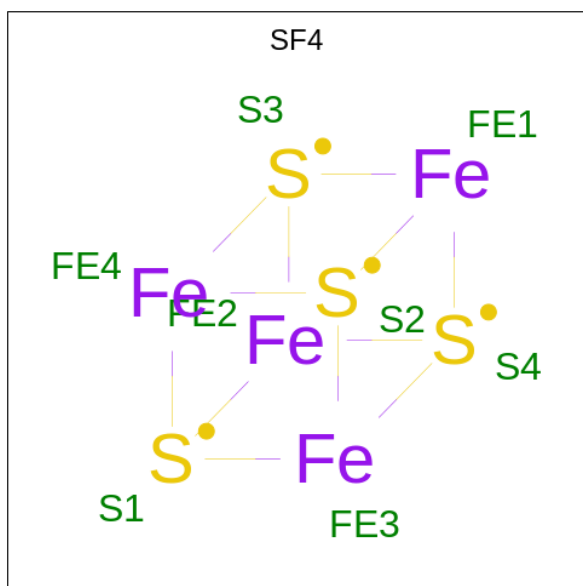
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	12	220	110	22	77	11	0	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	10	Total	O	0	0
			10	10		

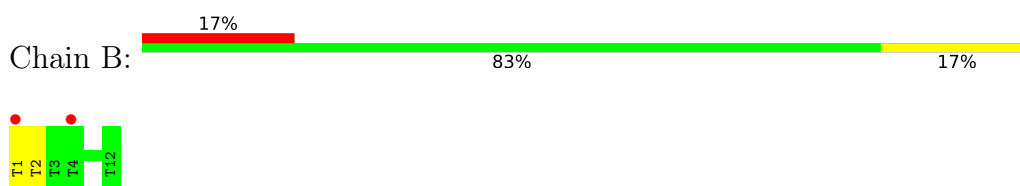
3 Residue-property plots [i](#)

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: DNA 5'-3' helicase



• Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.86Å 123.53Å 84.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.51 – 2.26 31.51 – 2.26	Depositor EDS
% Data completeness (in resolution range)	94.3 (31.51-2.26) 94.3 (31.51-2.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.240 , 0.271 0.239 , 0.270	Depositor DCC
R_{free} test set	2229 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6437	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.80	0/6175	1.07	5/8315 (0.1%)
2	B	0.55	0/241	1.05	0/372
All	All	0.79	0/6416	1.07	5/8687 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	295	GLU	N-CA-C	-6.76	104.85	113.23
1	A	93	THR	N-CA-C	-5.58	106.46	113.72
1	A	370	TYR	N-CA-C	-5.54	105.21	112.41
1	A	281	VAL	N-CA-CB	5.30	118.04	112.21
1	A	738	PRO	N-CA-CB	-5.17	96.92	102.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	25	ARG	Sidechain
1	A	364	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	554	ARG	Sidechain
1	A	590	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	719	ARG	Sidechain
1	A	73	ARG	Sidechain
1	A	94	ARG	Sidechain

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	6057	0	6061	155	1
2	B	220	0	130	2	0
3	A	31	0	13	4	0
4	A	8	0	0	0	0
5	A	111	0	0	8	0
5	B	10	0	0	0	0
All	All	6437	0	6204	158	1

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 13.

All (158) 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:126:ASP:OD1	1:A:147:ASN:OD1	1.60	1.18
1:A:17:GLU:OE1	1:A:105:LYS:NZ	1.78	1.14
1:A:111:VAL:HG11	1:A:131:LEU:HD21	1.50	0.91
1:A:214:MET:HE3	1:A:535:LEU:HD21	1.53	0.90
1:A:105:LYS:HZ2	1:A:105:LYS:HB3	1.44	0.82
1:A:278:LYS:HB2	1:A:335:LEU:HD22	1.63	0.80
1:A:126:ASP:CG	1:A:147:ASN:OD1	2.24	0.80
1:A:214:MET:HE3	1:A:535:LEU:CD2	2.12	0.80
1:A:530:PHE:CE1	1:A:547:LEU:HD11	2.18	0.78
1:A:516:ASN:ND2	5:A:904:HOH:O	2.16	0.78
1:A:527:SER:OG	5:A:901:HOH:O	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:HG23	1:A:143:PHE:HE1	1.47	0.77
1:A:105:LYS:NZ	1:A:105:LYS:HB3	2.00	0.76
1:A:363:LYS:HD2	1:A:363:LYS:H	1.50	0.76
1:A:126:ASP:OD1	1:A:147:ASN:CG	2.30	0.75
1:A:343:ASN:OD1	5:A:902:HOH:O	2.03	0.74
1:A:276:ILE:HB	1:A:281:VAL:HG13	1.68	0.74
1:A:21:ASP:OD1	1:A:299:GLY:N	2.21	0.74
1:A:604:PRO:HG3	1:A:673:SER:HB3	1.69	0.73
1:A:592:ILE:O	1:A:599:LYS:HE2	1.90	0.71
1:A:592:ILE:HG22	1:A:599:LYS:HD3	1.72	0.71
1:A:520:ASN:HA	1:A:523:LYS:HD2	1.72	0.70
1:A:566:VAL:HG21	1:A:747:TRP:HA	1.73	0.70
1:A:567:ASN:HD21	1:A:726:GLU:HG2	1.56	0.70
1:A:281:VAL:HA	1:A:324:LYS:HE2	1.73	0.69
1:A:360:VAL:HG22	1:A:360:VAL:O	1.93	0.69
1:A:111:VAL:HG11	1:A:131:LEU:CD2	2.22	0.69
1:A:132:THR:HG23	1:A:143:PHE:CE1	2.27	0.69
1:A:682:GLU:OE2	5:A:903:HOH:O	2.10	0.68
1:A:453:CYS:O	1:A:457:MET:HG3	1.93	0.68
1:A:464:GLU:HA	1:A:464:GLU:OE1	1.93	0.67
1:A:207:THR:O	1:A:526:LYS:HE2	1.95	0.66
1:A:674:VAL:HG23	1:A:676:LEU:HG	1.78	0.66
1:A:592:ILE:CG2	1:A:599:LYS:HD3	2.27	0.65
1:A:634:GLU:O	1:A:637:SER:OG	2.15	0.65
1:A:310:ASP:OD1	1:A:314:ASN:ND2	2.31	0.64
1:A:276:ILE:HB	1:A:281:VAL:CG1	2.28	0.63
1:A:573:THR:OG1	1:A:731:ASP:OD2	2.17	0.63
1:A:278:LYS:CB	1:A:335:LEU:HD22	2.28	0.63
1:A:219:THR:HG23	3:A:801:ANP:HNB1	1.64	0.62
1:A:703:VAL:HG11	1:A:738:PRO:HG2	1.81	0.62
1:A:571:ILE:HD11	1:A:585:ILE:HG12	1.82	0.62
1:A:3:LYS:HD3	1:A:66:VAL:HG22	1.82	0.61
1:A:21:ASP:OD1	1:A:298:LYS:HA	2.00	0.61
1:A:552:ASN:O	1:A:553:ILE:HD13	2.00	0.61
1:A:206:ALA:HA	1:A:211:VAL:HG22	1.82	0.61
1:A:335:LEU:HD12	1:A:338:GLU:OE2	2.01	0.61
1:A:132:THR:CG2	1:A:143:PHE:HE1	2.14	0.60
1:A:369:PRO:HG2	1:A:524:LYS:HB3	1.86	0.58
1:A:34:LYS:NZ	5:A:910:HOH:O	2.35	0.58
1:A:563:ASN:HB3	1:A:724:THR:HG22	1.85	0.58
1:A:278:LYS:HG3	1:A:335:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LYS:O	1:A:748:LYS:HD3	2.04	0.57
1:A:105:LYS:NZ	1:A:105:LYS:CB	2.62	0.56
1:A:111:VAL:CG1	1:A:131:LEU:HD21	2.29	0.56
1:A:360:VAL:O	1:A:360:VAL:CG2	2.54	0.56
1:A:134:TYR:HE1	1:A:136:THR:HG22	1.70	0.56
1:A:329:LYS:HD3	1:A:330:TYR:CE1	2.40	0.56
1:A:406:GLU:HG3	1:A:472:LYS:HD2	1.87	0.55
1:A:205:SER:O	1:A:209:GLN:HG3	2.07	0.54
1:A:412:LYS:HD3	1:A:460:PHE:HB2	1.90	0.54
1:A:714:GLY:HA3	1:A:747:TRP:CH2	2.43	0.54
1:A:574:ARG:HH12	1:A:732:ASP:CG	2.15	0.53
1:A:299:GLY:HA3	1:A:303:ARG:NH1	2.24	0.53
1:A:551:TYR:CE2	1:A:553:ILE:HD11	2.43	0.53
1:A:276:ILE:CB	1:A:281:VAL:HG13	2.38	0.53
1:A:454:LYS:HD2	1:A:481:ASN:OD1	2.09	0.53
1:A:21:ASP:CG	1:A:298:LYS:HA	2.33	0.53
1:A:73:ARG:HH11	1:A:73:ARG:HB3	1.72	0.53
1:A:84:THR:HG21	1:A:118:TYR:HE2	1.74	0.52
1:A:278:LYS:CG	1:A:335:LEU:HD22	2.40	0.52
1:A:413:GLU:OE2	1:A:467:LYS:HE2	2.09	0.52
1:A:495:VAL:HG22	1:A:496:THR:N	2.25	0.51
1:A:450:CYS:HB3	1:A:480:ILE:HG23	1.92	0.51
1:A:661:LEU:HD22	1:A:661:LEU:N	2.26	0.51
1:A:265:GLN:HG2	1:A:266:LYS:HD2	1.93	0.50
1:A:451:VAL:O	1:A:455:GLU:HG2	2.11	0.50
1:A:244:PHE:HE1	1:A:373:MET:HG2	1.77	0.50
1:A:457:MET:HE3	1:A:473:VAL:CG1	2.41	0.50
2:B:1:DT:H2"	2:B:2:DT:C5	2.47	0.50
1:A:732:ASP:O	1:A:735:ASP:OD1	2.29	0.50
1:A:101:TYR:O	1:A:108:TRP:NE1	2.45	0.50
1:A:643:SER:HB2	1:A:645:ILE:HG12	1.94	0.49
1:A:84:THR:HG21	1:A:118:TYR:CE2	2.47	0.49
1:A:307:CYS:SG	1:A:326:TYR:HB3	2.52	0.49
1:A:454:LYS:HG3	1:A:477:TYR:CE1	2.46	0.49
1:A:618:PHE:CZ	1:A:620:ILE:HD11	2.48	0.49
1:A:517:ILE:HG13	5:A:975:HOH:O	2.13	0.49
1:A:563:ASN:CB	1:A:724:THR:HG22	2.42	0.48
1:A:630:MET:HA	1:A:633:LEU:HD12	1.96	0.48
1:A:130:GLN:O	1:A:131:LEU:HD23	2.14	0.48
1:A:720:THR:OG1	1:A:722:THR:HG22	2.13	0.48
1:A:214:MET:HE3	1:A:535:LEU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:CG2	1:A:281:VAL:HG13	2.43	0.48
1:A:72:GLY:HA3	1:A:114:TYR:HE1	1.77	0.48
1:A:278:LYS:HB2	1:A:335:LEU:CD2	2.38	0.48
1:A:83:LYS:HD2	1:A:126:ASP:OD2	2.14	0.47
1:A:412:LYS:O	1:A:415:LYS:HG2	2.15	0.47
1:A:571:ILE:HG12	1:A:730:ILE:HG22	1.96	0.47
1:A:57:LEU:HD11	1:A:77:ILE:HD11	1.96	0.47
1:A:569:ILE:HG22	1:A:571:ILE:HG23	1.95	0.47
3:A:801:ANP:O1B	3:A:801:ANP:H5'2	2.15	0.47
1:A:412:LYS:HD3	1:A:460:PHE:HA	1.98	0.46
1:A:3:LYS:HE2	1:A:172:THR:HG21	1.96	0.46
1:A:573:THR:HG21	1:A:672:ILE:O	2.15	0.46
1:A:636:LEU:HD21	1:A:655:PHE:CD1	2.50	0.46
1:A:171:ILE:O	1:A:175:ILE:HG12	2.16	0.46
1:A:616:CYS:HB3	1:A:618:PHE:CE1	2.51	0.46
1:A:34:LYS:HB3	1:A:488:ASP:OD1	2.16	0.45
1:A:300:HIS:HD2	1:A:333:CYS:H	1.64	0.45
1:A:571:ILE:HG21	1:A:584:LYS:HD2	1.96	0.45
1:A:634:GLU:HA	1:A:637:SER:OG	2.16	0.45
1:A:174:HIS:CE1	1:A:271:LYS:HG3	2.51	0.45
1:A:244:PHE:CE1	1:A:373:MET:HG2	2.51	0.45
1:A:687:LYS:HG3	1:A:697:GLY:C	2.41	0.45
1:A:7:LEU:HD11	1:A:164:TYR:CE1	2.52	0.45
1:A:435:PRO:HA	1:A:500:SER:HB2	1.99	0.45
2:B:1:DT:H2''	2:B:2:DT:C6	2.52	0.45
1:A:246:LEU:HA	1:A:350:CYS:O	2.17	0.45
1:A:393:TYR:CE1	1:A:482:LYS:HE2	2.52	0.44
1:A:229:PHE:N	1:A:230:PRO:HD2	2.32	0.44
1:A:373:MET:HE3	1:A:373:MET:HB2	1.85	0.44
1:A:394:SER:HA	1:A:507:TYR:O	2.17	0.43
1:A:461:LEU:HA	1:A:470:TYR:HE1	1.82	0.43
1:A:574:ARG:NH1	1:A:732:ASP:OD2	2.47	0.43
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.71	0.43
1:A:132:THR:CG2	1:A:143:PHE:CE1	2.97	0.43
1:A:246:LEU:HD12	1:A:377:VAL:HG22	2.00	0.43
1:A:448:ASP:O	1:A:452:ARG:HG2	2.18	0.43
1:A:18:ARG:HA	1:A:106:TYR:OH	2.19	0.43
1:A:658:GLY:O	1:A:659:VAL:C	2.62	0.42
1:A:296:PHE:CD1	1:A:296:PHE:N	2.88	0.42
1:A:189:TYR:HH	3:A:801:ANP:HO2'	1.63	0.42
1:A:126:ASP:OD2	1:A:147:ASN:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:VAL:C	5:A:906:HOH:O	2.62	0.42
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.84	0.42
1:A:189:TYR:OH	3:A:801:ANP:O2'	2.34	0.42
1:A:672:ILE:HD13	1:A:730:ILE:HD12	2.01	0.42
1:A:105:LYS:HZ2	1:A:105:LYS:CB	2.20	0.42
1:A:253:LYS:HE2	1:A:274:GLU:HG3	2.02	0.41
1:A:495:VAL:CG2	1:A:496:THR:N	2.83	0.41
1:A:85:LEU:HD12	1:A:128:ASP:O	2.20	0.41
1:A:95:ASP:HB2	1:A:98:GLU:HG3	2.02	0.41
1:A:159:SER:O	1:A:163:LYS:HG3	2.20	0.41
1:A:187:PHE:CE2	1:A:189:TYR:HB2	2.55	0.41
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.85	0.41
1:A:695:LYS:HE2	5:A:993:HOH:O	2.20	0.41
1:A:623:GLN:NE2	1:A:655:PHE:HD2	2.18	0.41
1:A:108:TRP:HA	1:A:111:VAL:HG22	2.03	0.41
1:A:299:GLY:O	1:A:300:HIS:C	2.64	0.41
1:A:636:LEU:HD21	1:A:655:PHE:CE1	2.56	0.41
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.89	0.41
1:A:716:ARG:HA	1:A:716:ARG:HD3	1.76	0.41
1:A:214:MET:CE	1:A:535:LEU:HG	2.51	0.41
1:A:213:LEU:HD11	1:A:553:ILE:HG12	2.03	0.41
1:A:544:VAL:HG23	1:A:545:LEU:HG	2.04	0.40
1:A:621:LEU:O	1:A:647:ALA:HA	2.21	0.40
1:A:681:VAL:O	1:A:685:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLN:NE2	1:A:691:ASP:O[2_655]	2.19	0.01

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	734/748 (98%)	708 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	681/691 (99%)	678 (100%)	3 (0%)	89	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	745	ASN
1	A	746	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	110	GLN
1	A	209	GLN
1	A	257	ASN
1	A	265	GLN
1	A	300	HIS
1	A	382	ASN
1	A	419	ASN
1	A	528	ASN
1	A	623	GLN
1	A	638	GLN
1	A	644	ASN
1	A	667	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 ⓘ

2 ligands are modelled in this entry.

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	SF4	A	802	1	0,12,12	-	-	-		
3	ANP	A	801	-	29,33,33	1.19	5 (17%)	31,52,52	1.19	5 (16%)

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	SF4	A	802	1	-	-	0/6/5/5
3	ANP	A	801	-	-	2/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	PG-O1G	2.90	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	PB-O1B	2.85	1.50	1.46
3	A	801	ANP	PB-O2B	-2.27	1.50	1.56
3	A	801	ANP	PG-O2G	-2.18	1.50	1.56
3	A	801	ANP	PG-O3G	-2.15	1.51	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	O2B-PB-O1B	4.08	118.48	109.92
3	A	801	ANP	C5-C6-N6	2.30	123.85	120.35
3	A	801	ANP	O2G-PG-O1G	-2.20	107.92	113.45
3	A	801	ANP	O3A-PB-N3B	-2.18	100.55	106.59
3	A	801	ANP	O3G-PG-O1G	-2.07	108.24	113.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ANP	PB-N3B-PG-O1G
3	A	801	ANP	O4'-C4'-C5'-O5'

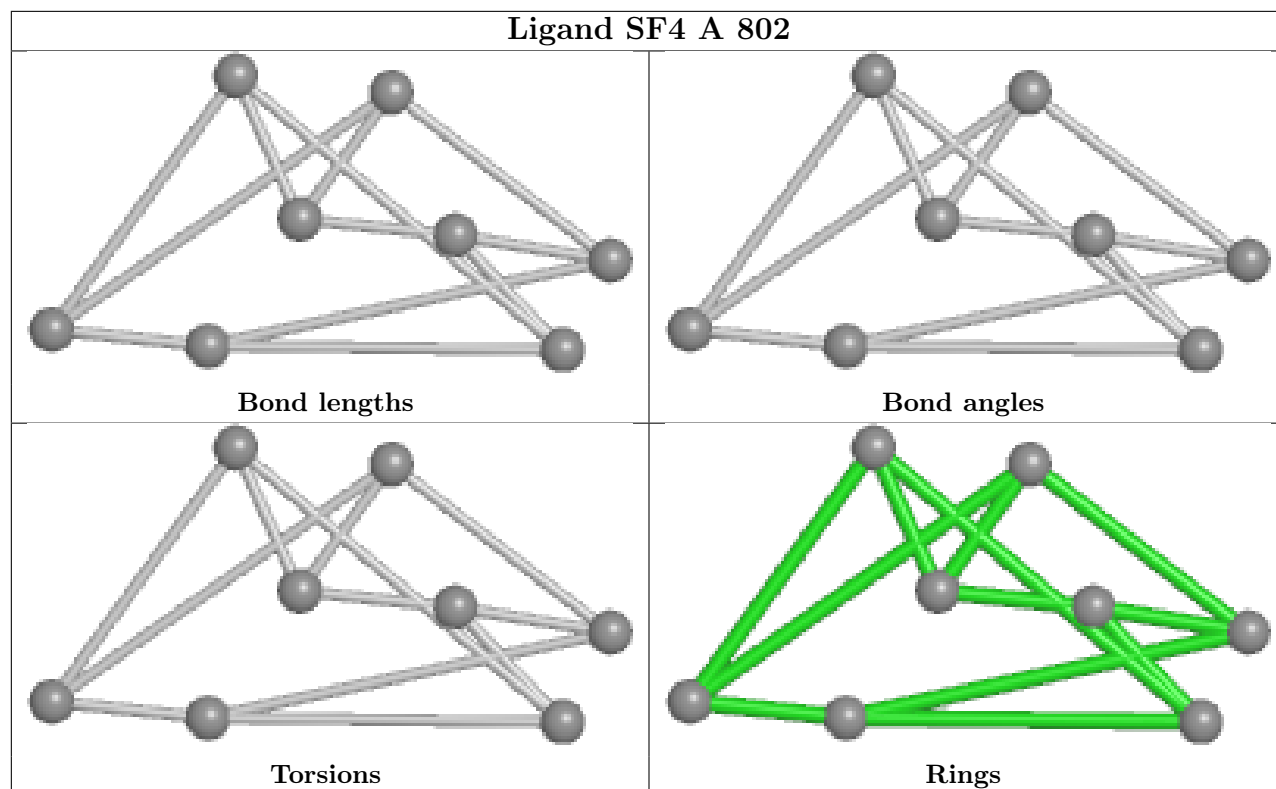
There are no ring outliers.

1 monomer is involved in 4 short contacts:

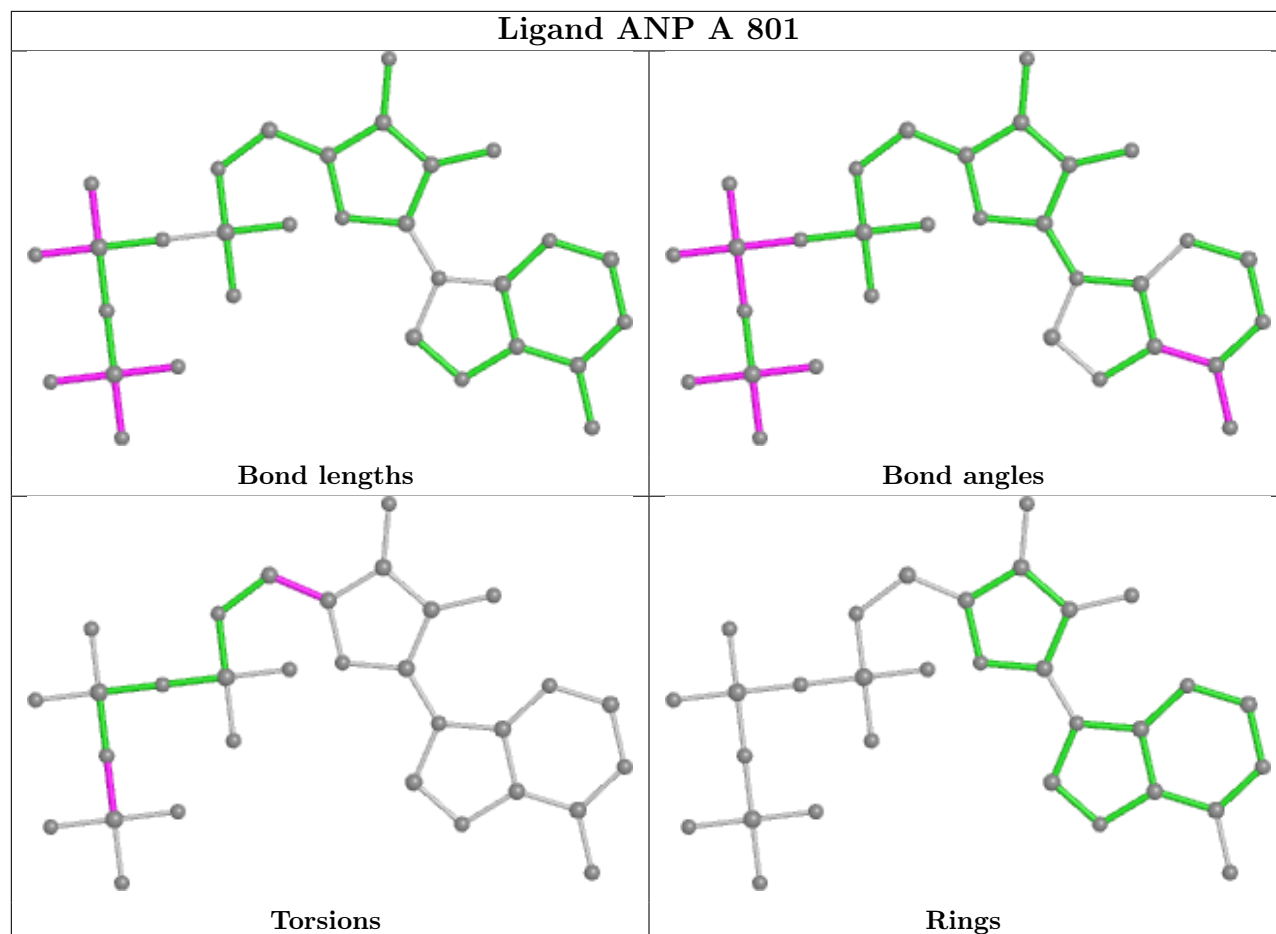
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ANP	4	0

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 SF4 A 802



Ligand ANP A 801



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	738/748 (98%)	1.00	92 (12%) 9 9	21, 46, 76, 92	0
2	B	12/12 (100%)	0.71	2 (16%) 5 5	35, 59, 83, 85	0
All	All	750/760 (98%)	1.00	94 (12%) 9 9	21, 46, 76, 92	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	664	ASP	5.2
1	A	409	ASP	4.9
1	A	294	CYS	4.2
1	A	26	PHE	4.0
1	A	143	PHE	4.0
1	A	49	ILE	3.8
1	A	458	THR	3.8
1	A	672	ILE	3.7
1	A	722	THR	3.6
1	A	23	ASP	3.5
1	A	282	CYS	3.5
1	A	462	VAL	3.4
1	A	407	LEU	3.4
1	A	412	LYS	3.3
1	A	468	PRO	3.3
1	A	477	TYR	3.3
1	A	480	ILE	3.2
1	A	645	ILE	3.2
1	A	329	LYS	3.1
1	A	621	LEU	3.1
1	A	96	LEU	3.1
1	A	168	THR	3.0
1	A	283	ILE	3.0
1	A	636	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	644	ASN	3.0
1	A	408	VAL	3.0
1	A	136	THR	2.9
1	A	520	ASN	2.9
1	A	169	GLU	2.8
1	A	358	PRO	2.8
1	A	284	ASN	2.8
1	A	720	THR	2.8
1	A	403	CYS	2.7
1	A	615	ILE	2.7
1	A	659	VAL	2.7
1	A	469	TYR	2.7
1	A	94	ARG	2.6
1	A	46	GLU	2.6
1	A	723	ASP	2.6
1	A	101	TYR	2.6
1	A	648	PHE	2.6
1	A	626	THR	2.6
1	A	633	LEU	2.6
1	A	673	SER	2.5
1	A	50	GLY	2.5
1	A	42	MET	2.5
1	A	597	GLY	2.5
1	A	295	GLU	2.4
1	A	657	GLU	2.4
1	A	616	CYS	2.4
1	A	24	ASP	2.4
1	A	502	ASN	2.4
1	A	639	PHE	2.4
1	A	496	THR	2.4
1	A	22	ILE	2.4
1	A	459	LYS	2.3
1	A	661	LEU	2.3
1	A	138	THR	2.3
1	A	620	ILE	2.3
1	A	35	GLU	2.3
1	A	473	VAL	2.3
1	A	333	CYS	2.3
1	A	126	ASP	2.3
1	A	660	ASP	2.3
1	A	28	ASN	2.2
1	A	652	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	100	GLU	2.2
1	A	27	ARG	2.2
1	A	51	PHE	2.2
1	A	280	LYS	2.2
1	A	625	ARG	2.2
1	A	476	VAL	2.2
1	A	4	GLU	2.2
1	A	33	ALA	2.2
1	A	81	ASN	2.1
1	A	552	ASN	2.1
1	A	745	ASN	2.1
2	B	1	DT	2.1
1	A	123	ASP	2.1
1	A	492	ASP	2.1
1	A	662	SER	2.1
1	A	147	ASN	2.1
1	A	503	ASP	2.1
1	A	281	VAL	2.1
1	A	330	TYR	2.1
1	A	478	PHE	2.1
2	B	4	DT	2.1
1	A	466	ASP	2.0
1	A	2	LYS	2.0
1	A	628	THR	2.0
1	A	606	TYR	2.0
1	A	433	GLY	2.0
1	A	607	SER	2.0
1	A	221	ILE	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,

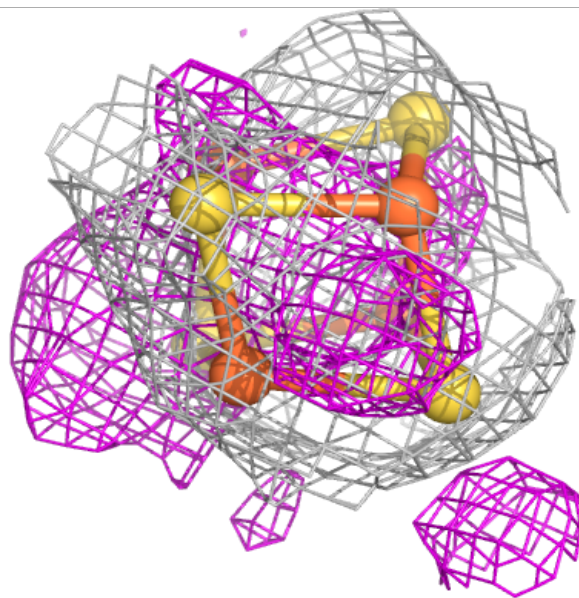
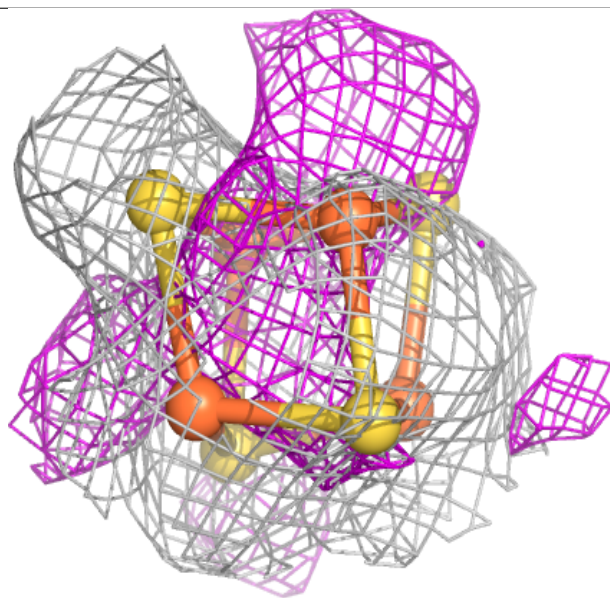
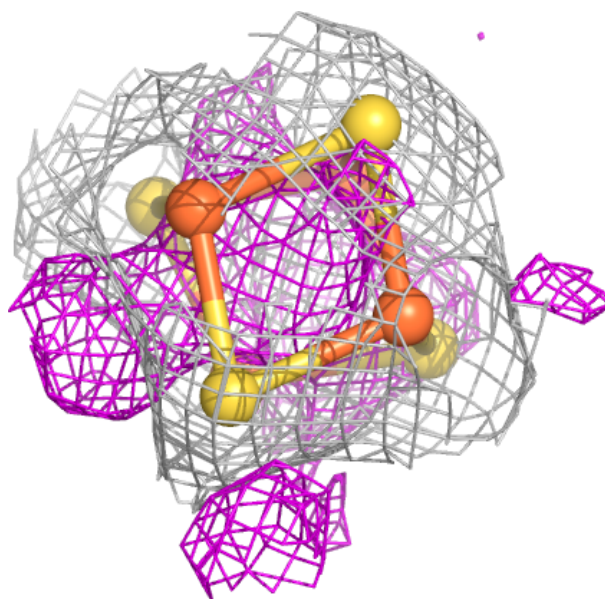
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SF4	A	802	8/8	0.63	0.14	103,139,185,191	0
3	ANP	A	801	31/31	0.82	0.15	51,65,102,119	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.

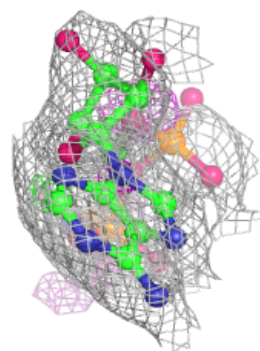
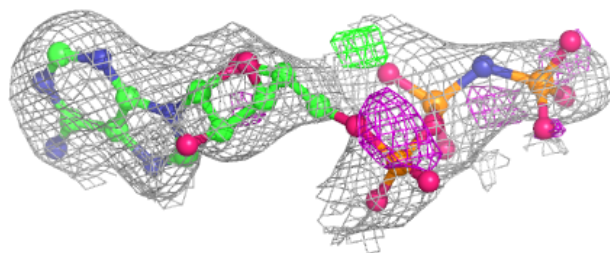
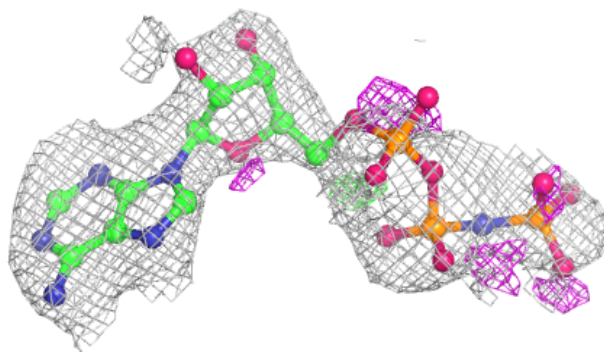
Electron density around SF4 A 802:

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 801:

$2mF_o-DF_c$ (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.