wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 05:41 pm GMT

PDB ID	:	8B37
Title	:	Crystal structure of Pyrobaculum aerophilum potassium-independent proton pumping membrane integral pyrophosphatase in complex with imidodiphosphate and magnesium, and with bound sulphate
Authors	:	Strauss, J.; Wilkinson, C.; Vidilaseris, K.; Ribeiro, O.; Liu, J.; Hillier, J.; Malinen, A.; Gehl, B.; Jeuken, L.C.; Pearson, A.R.; Goldman, A.
Deposited on	:	2022-09-16
Resolution	:	3.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

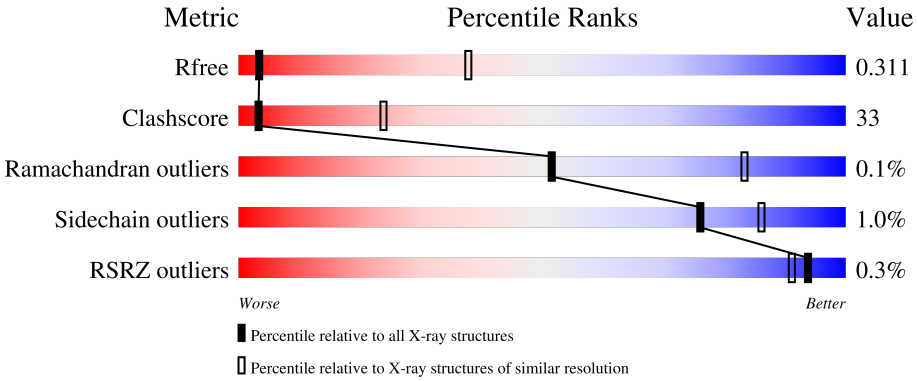
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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 <=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	729	50% 43% • 7%
1	B	729	52% 41% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15678 atoms, of which 5949 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 K(+)-insensitive pyrophosphate-energized proton pump.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	676	Total	C	H	N	O	S	0	0	0
			7808	3159	2981	769	882	17			
1	B	681	Total	C	H	N	O	S	0	0	0
			7830	3182	2968	774	889	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8ZWI8
A	-6	HIS	-	expression tag	UNP Q8ZWI8
A	-5	HIS	-	expression tag	UNP Q8ZWI8
A	-4	HIS	-	expression tag	UNP Q8ZWI8
A	-3	HIS	-	expression tag	UNP Q8ZWI8
A	-2	HIS	-	expression tag	UNP Q8ZWI8
A	-1	HIS	-	expression tag	UNP Q8ZWI8
A	0	GLY	-	expression tag	UNP Q8ZWI8
A	1	GLY	-	expression tag	UNP Q8ZWI8
B	-7	MET	-	initiating methionine	UNP Q8ZWI8
B	-6	HIS	-	expression tag	UNP Q8ZWI8
B	-5	HIS	-	expression tag	UNP Q8ZWI8
B	-4	HIS	-	expression tag	UNP Q8ZWI8
B	-3	HIS	-	expression tag	UNP Q8ZWI8
B	-2	HIS	-	expression tag	UNP Q8ZWI8
B	-1	HIS	-	expression tag	UNP Q8ZWI8
B	0	GLY	-	expression tag	UNP Q8ZWI8
B	1	GLY	-	expression tag	UNP Q8ZWI8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

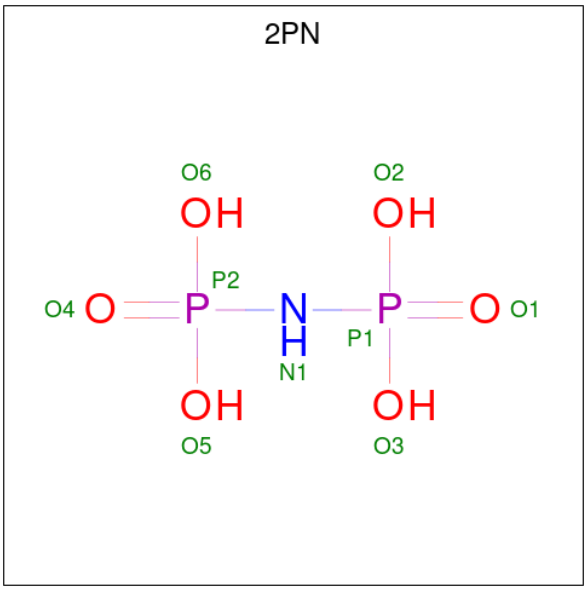
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Mg	0	0
			5	5		

Continued on next page...

Continued from previous page...

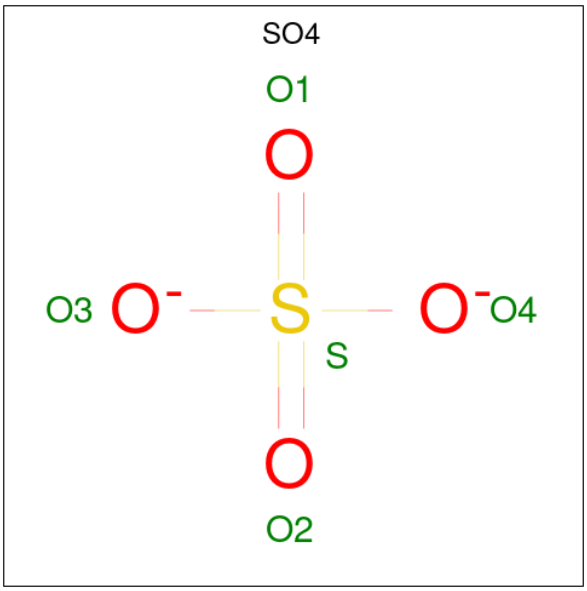
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Mg 5 5	0	0

- Molecule 3 is IMIDODIPHOSPHORIC ACID (three-letter code: 2PN) (formula: $H_5NO_6P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O P 9 1 6 2	0	0
3	B	1	Total N O P 9 1 6 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

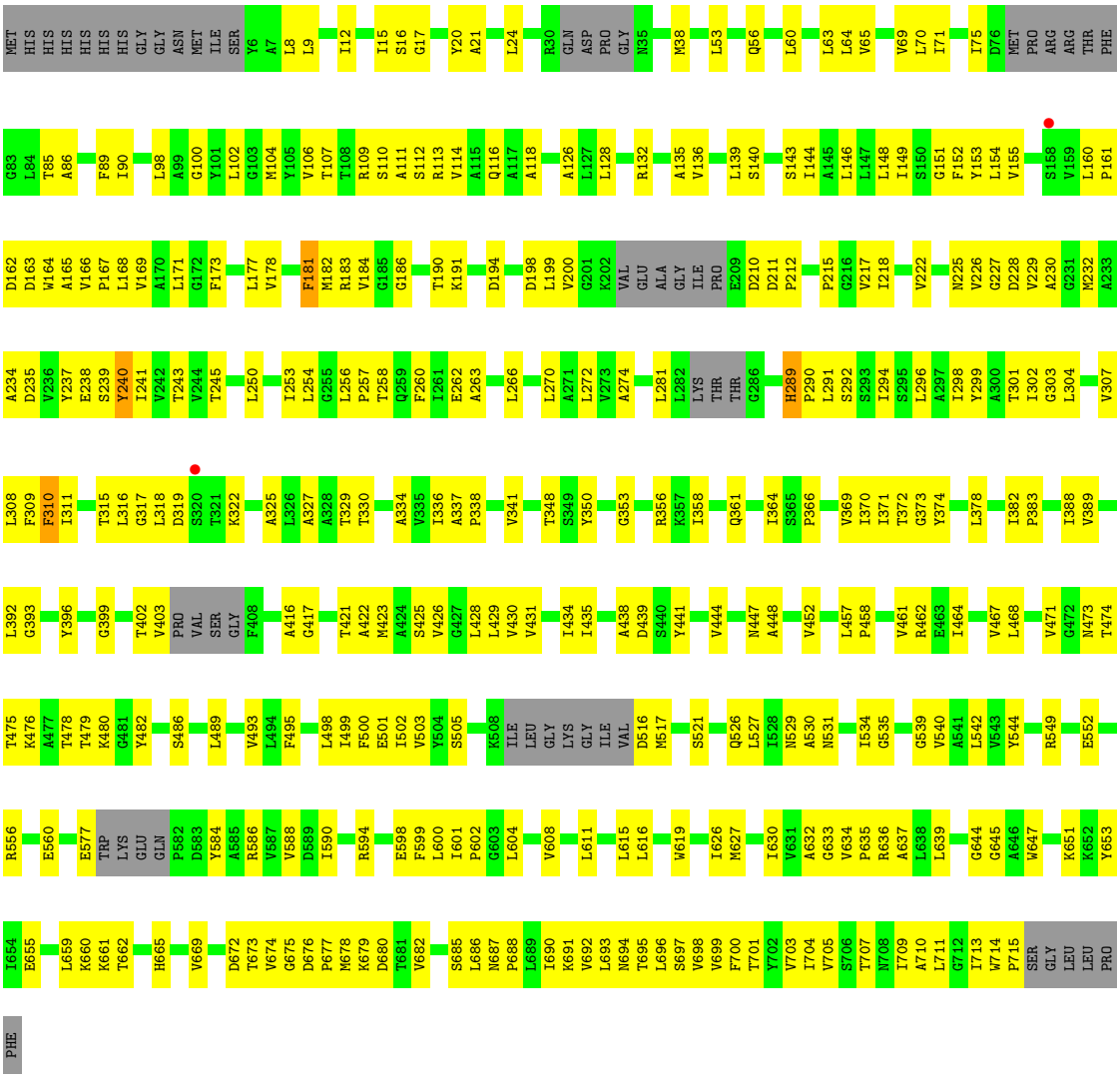
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	3	Total O 3 3	0	0

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.

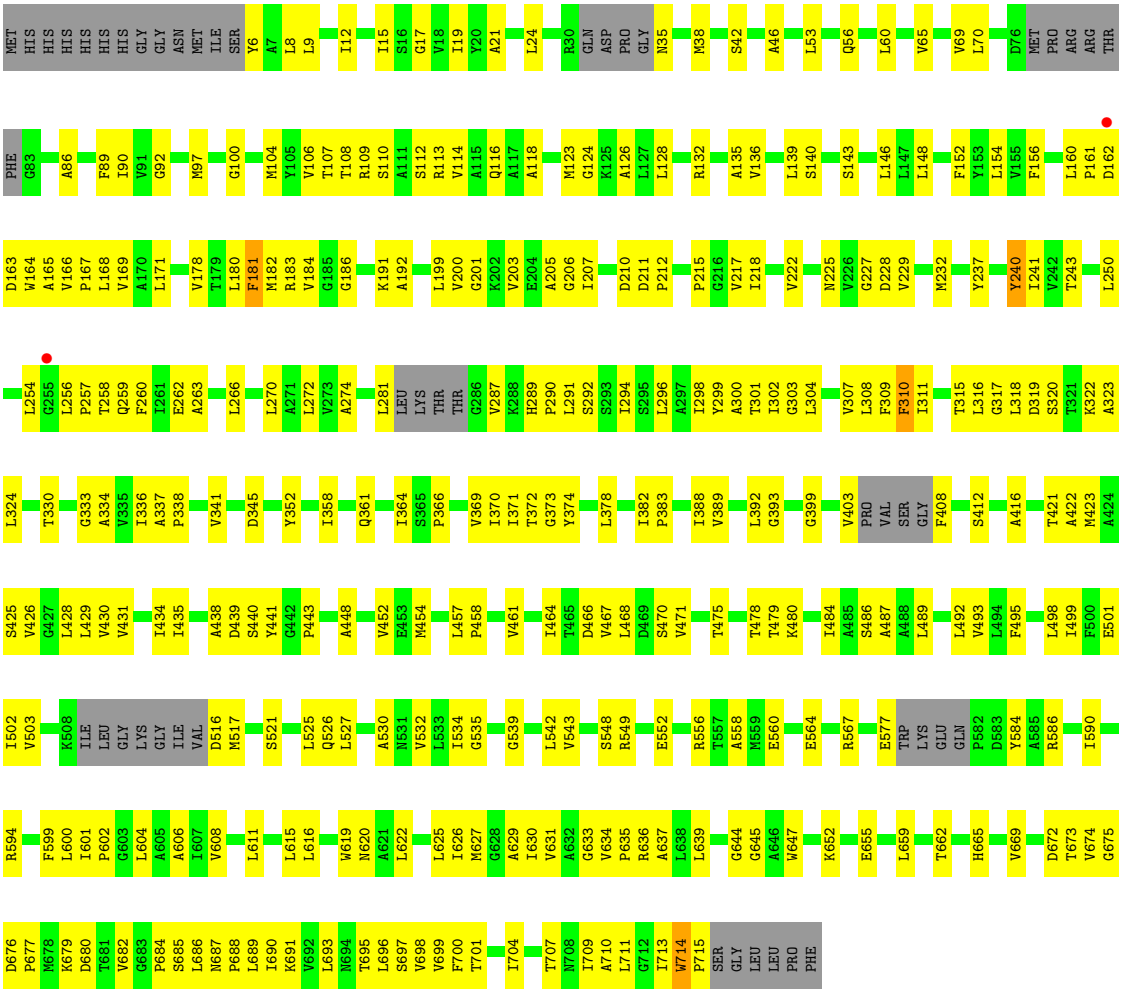
• Molecule 1: K(+)-insensitive pyrophosphate-energized proton pump

Chain A:



• Molecule 1: K(+)-insensitive pyrophosphate-energized proton pump

Chain B:


MET HIS HIS HIS HIS HIS GLY GLY ASN MET ILE SER Y6 A7 L8 L9 I12 I15 S16 G17 V18 I19 Y20 A21 L24 R30 GLN ASP PRO GLY N35 M38 S42 A46 L53 Q56 L60 V65 V69 L70 D76 MET PRO ARG ARG THR
PHE G83 A86 F89 I90 V91 G92 M97 G100 M104 Y105 V106 T107 T108 R109 S110 A111 S112 R113 V114 A115 Q116 A117 A118 M123 G124 K125 A126 L127 L128 R132 A135 V136 L139 S140 S143 L146 L147 L148 F152 Y153 L154 V155 F156 L160 P161 D162
D163 W164 A165 V166 P167 L168 V169 A170 L171 V178 T179 L180 F181 M182 R183 V184 G185 G186 K191 A192 L199 V200 G201 K202 V203 E204 A205 G206 I207 D210 D211 P212 P215 G216 V217 I218 V222 N225 V226 G227 D228 V229 M232 Y237 Y240 I241 V242 T243 L250
L254 G255 L256 P257 T258 Q259 F260 I261 E262 A263 L266 L270 A271 L272 V273 A274 L281 LEU LYS THR THR G286 V287 K288 H289 P290 L291 S292 S293 I294 S296 L296 A297 I298 Y299 A300 T301 I302 G303 L304 V307 L308 F309 F310 I311 T315 L316 G317 L318 D319 S320 T321 K322 A323
L324 T330 G333 A334 V335 I336 A337 P338 V341 D345 Y352 I358 Q361 I364 S365 P366 V369 I370 I371 T372 G373 Y374 L378 I382 P383 I388 V389 L392 G393 G399 V403 PRO VAL SER GLY F408 S412 A416 T421 A422 M423 A424
S425 V426 G427 L428 L429 V430 V431 I434 I435 A438 D439 S440 Y441 G442 P443 A448 V452 E453 M454 L457 P458 V461 I464 T465 D466 V467 L468 D469 S470 V471 T475 T478 T479 K480 I484 A485 S486 A487 A488 L489 L492 V493 L494 F495 L498 I499 P500 E501
I502 V503 K508 ILE LEU GLY LYS GLY ILE VAL D516 M517 S521 L525 Q526 L527 A530 N531 V532 L533 I534 G535 G539 L542 V543 S548 R549 E552 R556 T557 A558 M559 E560 E564 R567 E577 TRP LYS GLU GLN P582 D583 Y584 A585 R586 I590
R594 F599 L600 I601 P602 G603 L604 A605 A606 I607 V608 L611 L615 L616 W619 N620 A621 L622 L625 I626 M627 G628 A629 I630 V631 A632 G633 V634 P635 R636 A637 L638 L639 G644 G645 A646 W647 K652 E655 L659 T662 H665 V669 D672 T673 V674 G675
D676 P677 K678 K679 D680 T681 V682 G683 P684 S685 L686 N687 P688 L689 I690 K691 V692 L693 N694 T695 L696 S697 V698 V699 F700 T701 I704 T707 N708 I709 A710 L711 G712 I713 W714 P715 SER GLY LEU LEU PRO PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.19Å 88.02Å 116.75Å 90.00° 106.95° 90.00°	Depositor
Resolution (Å)	19.97 – 3.84 19.97 – 3.84	Depositor EDS
% Data completeness (in resolution range)	65.3 (19.97-3.84) 65.3 (19.97-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.289 , 0.311 0.289 , 0.311	Depositor DCC
R_{free} test set	667 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	112.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15678	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 2PN, SO4

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	0.26	1/4903 (0.0%)	0.40	0/6699
1	B	0.26	1/4940 (0.0%)	0.39	0/6752
All	All	0.26	2/9843 (0.0%)	0.39	0/13451

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLU	CD-OE2	6.88	1.33	1.25
1	B	577	GLU	CD-OE2	6.84	1.33	1.25

There are no bond angle outliers.

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	4827	2981	4935	330	0
1	B	4862	2968	4975	326	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	9	0	1	0	0
3	B	9	0	0	0	0
4	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	3	0	0	0	0
All	All	9729	5949	9911	645	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 33.

The worst 5 of 645 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:118:ALA:HB2	1:A:126:ALA:HB2	1.38	1.05
1:B:466:ASP:HB3	1:B:652:LYS:HE3	1.43	0.99
1:A:630:ILE:HG22	1:A:690:ILE:HG23	1.45	0.98
1:B:118:ALA:HB2	1:B:126:ALA:HB2	1.47	0.96
1:B:403:VAL:HG13	1:B:416:ALA:HB1	1.47	0.96

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	660/729 (90%)	645 (98%)	15 (2%)	0	100	100
1	B	667/729 (92%)	651 (98%)	15 (2%)	1 (0%)	51	83
All	All	1327/1458 (91%)	1296 (98%)	30 (2%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	475/554 (86%)	469 (99%)	6 (1%)	69 82
1	B	479/554 (86%)	475 (99%)	4 (1%)	81 89
All	All	954/1108 (86%)	944 (99%)	10 (1%)	76 86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	TYR
1	B	309	PHE
1	B	310	PHE
1	A	289	HIS
1	A	309	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	2PN	A	806	2	8,8,8	2.60	6 (75%)	8,13,13	1.58	2 (25%)
4	SO4	B	807	-	4,4,4	0.15	0	6,6,6	0.08	0
3	2PN	B	806	2	8,8,8	2.67	6 (75%)	8,13,13	1.42	1 (12%)

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
3	2PN	A	806	2	-	1/2/6/6	-
3	2PN	B	806	2	-	1/2/6/6	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	806	2PN	P2-O4	3.52	1.51	1.46
3	A	806	2PN	P2-O4	3.42	1.51	1.46
3	A	806	2PN	P1-O1	3.32	1.51	1.46
3	B	806	2PN	P1-O1	3.28	1.51	1.46
3	B	806	2PN	P2-N1	3.06	1.71	1.63

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	2PN	O4-P2-N1	-2.08	108.70	111.77
3	A	806	2PN	O6-P2-O4	-2.06	108.28	113.45
3	B	806	2PN	O6-P2-O4	-2.05	108.29	113.45

There are no chirality outliers.

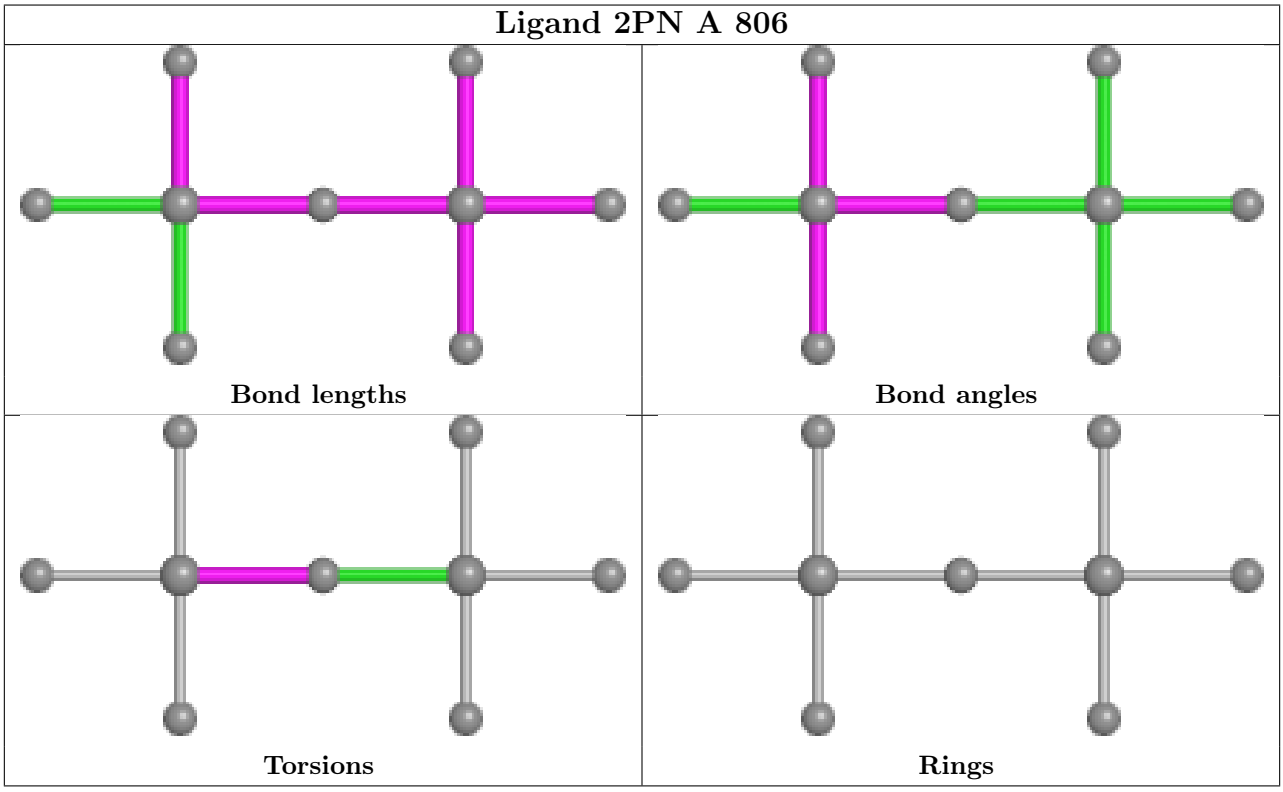
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	2PN	P1-N1-P2-O4
3	B	806	2PN	P1-N1-P2-O4

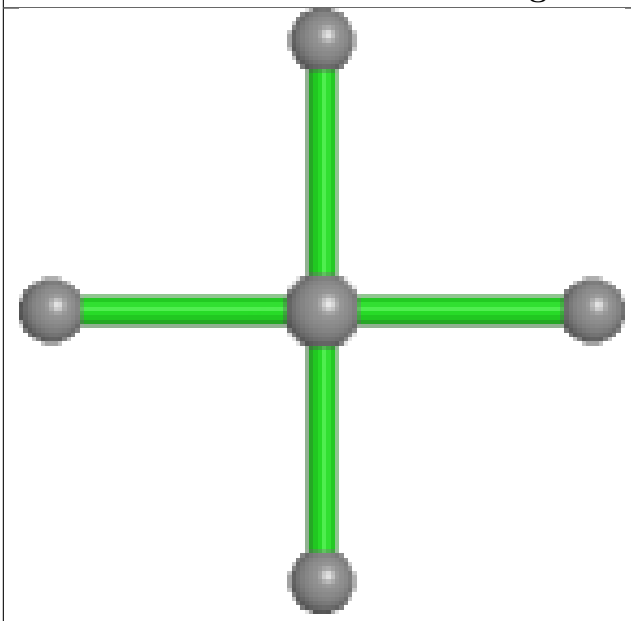
There are no ring outliers.

No monomer is involved in short contacts.

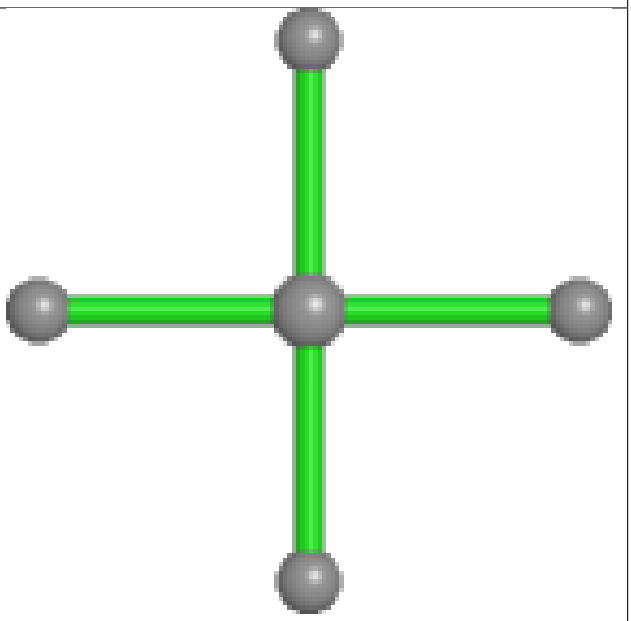
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



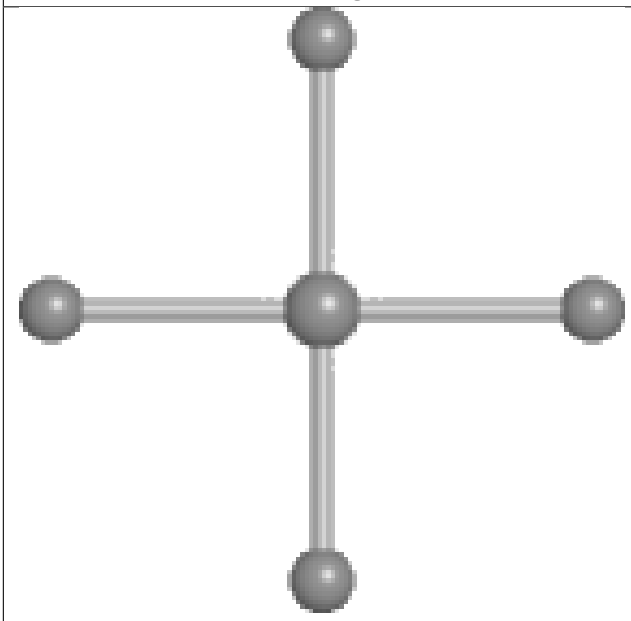
Ligand SO4 B 807



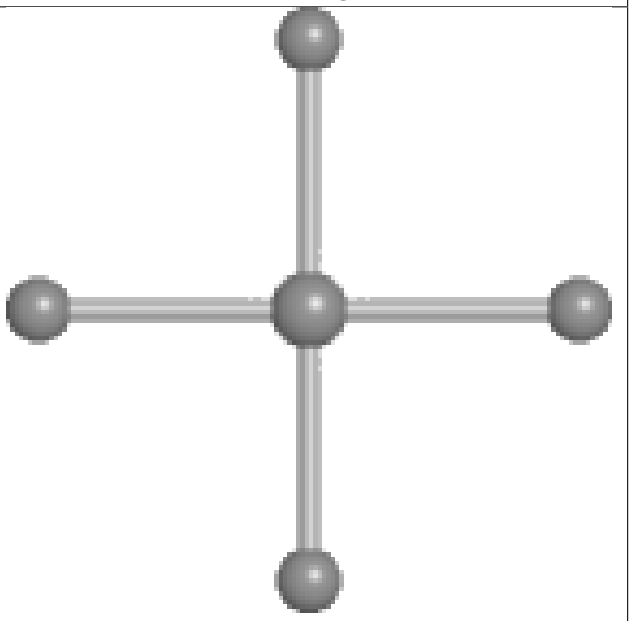
Bond lengths



Bond angles

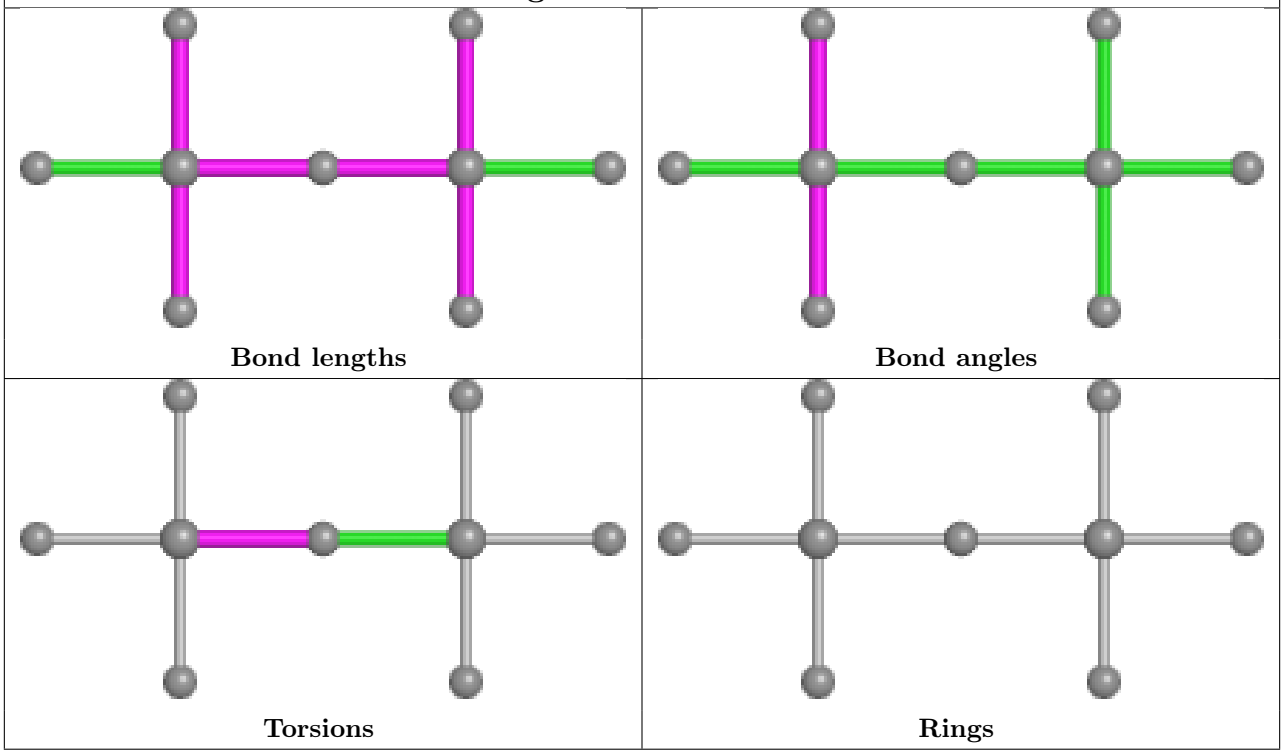


Torsions



Rings

Ligand 2PN B 806



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, 95^{th} 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	676/729 (92%)	-0.53	2 (0%)	94	91	64, 103, 128, 141	0
1	B	681/729 (93%)	-0.41	2 (0%)	94	91	68, 111, 138, 150	0
All	All	1357/1458 (93%)	-0.47	4 (0%)	94	91	64, 107, 135, 150	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	GLY	3.0
1	B	162	ASP	2.8
1	A	158	SER	2.8
1	A	320	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
2	MG	B	803	1/1	0.86	0.17	95,95,95,95	0

Continued on next page...

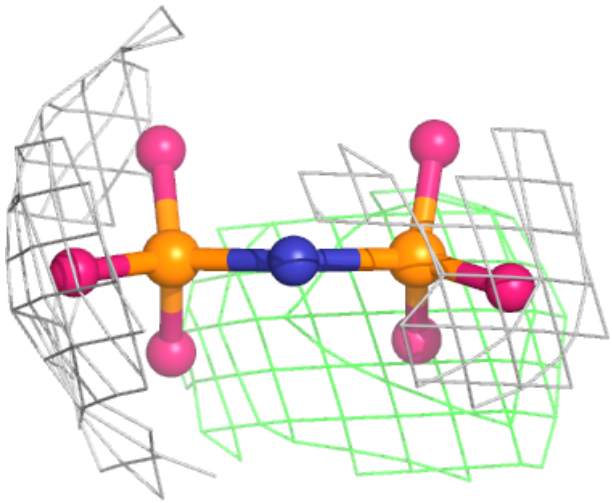
Continued from previous page...

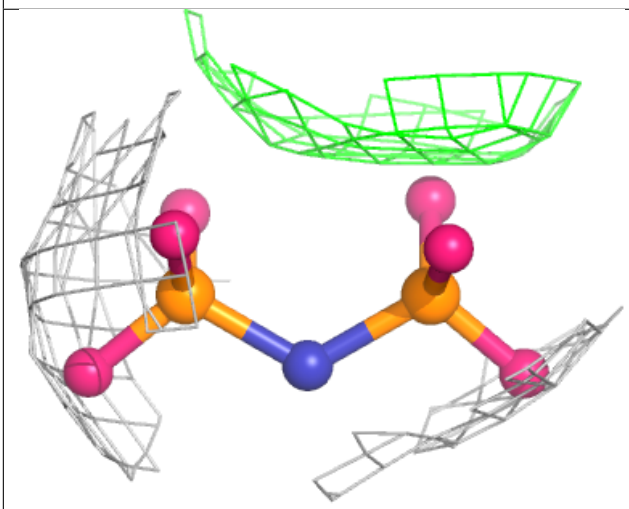
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	801	1/1	0.87	0.25	88,88,88,88	0
2	MG	A	802	1/1	0.89	0.16	103,103,103,103	0
2	MG	A	805	1/1	0.90	0.22	91,91,91,91	0
2	MG	A	801	1/1	0.93	0.23	83,83,83,83	0
3	2PN	B	806	9/9	0.93	0.13	107,108,109,111	0
2	MG	B	804	1/1	0.94	0.10	106,106,106,106	0
2	MG	A	804	1/1	0.94	0.11	101,101,101,101	0
2	MG	B	802	1/1	0.95	0.07	108,108,108,108	0
3	2PN	A	806	9/9	0.96	0.15	96,98,100,100	0
2	MG	B	805	1/1	0.96	0.21	101,101,101,101	0
4	SO4	B	807	5/5	0.97	0.20	89,90,90,90	0
2	MG	A	803	1/1	0.98	0.14	87,87,87,87	0

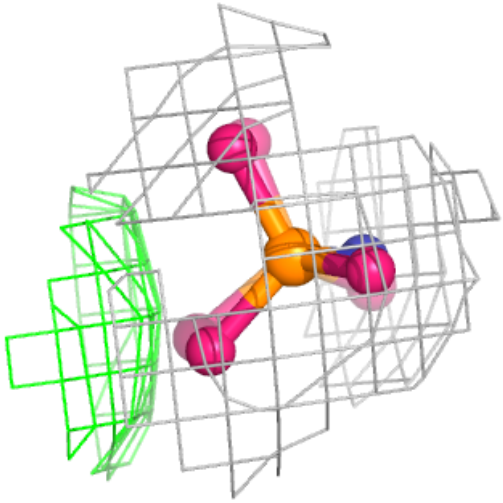
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PN 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)

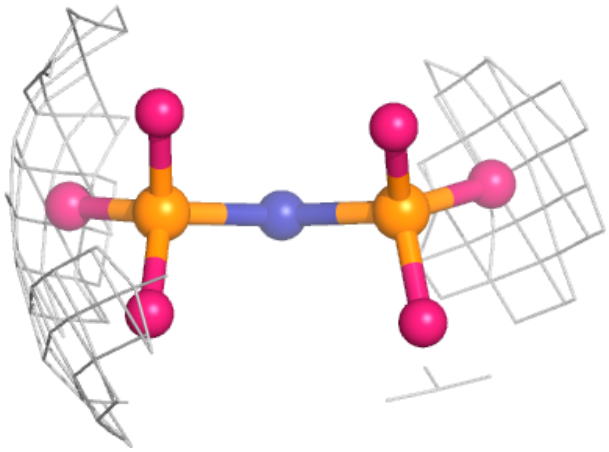


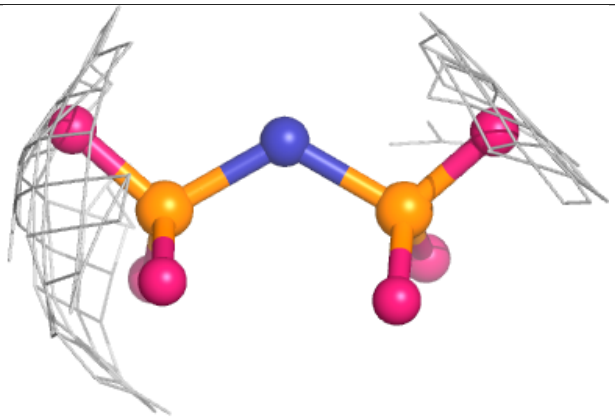


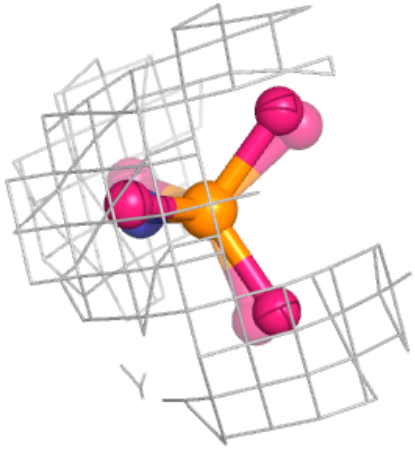


Electron density around 2PN A 806:

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

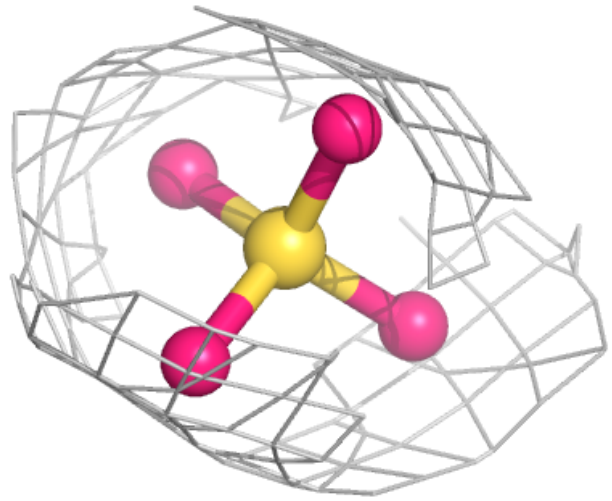


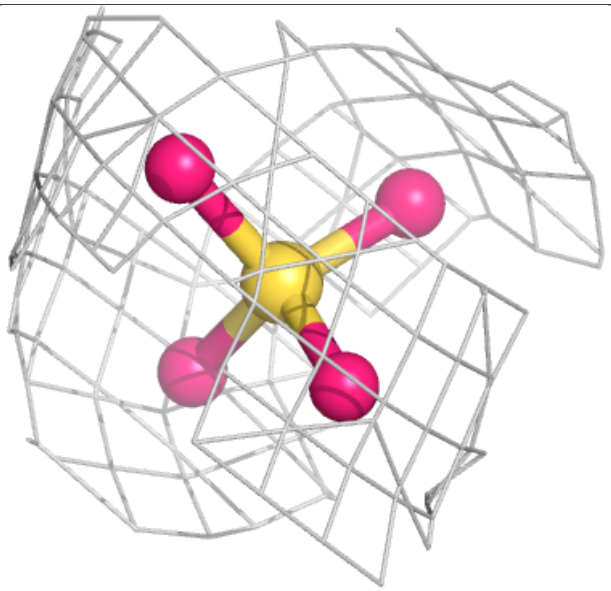


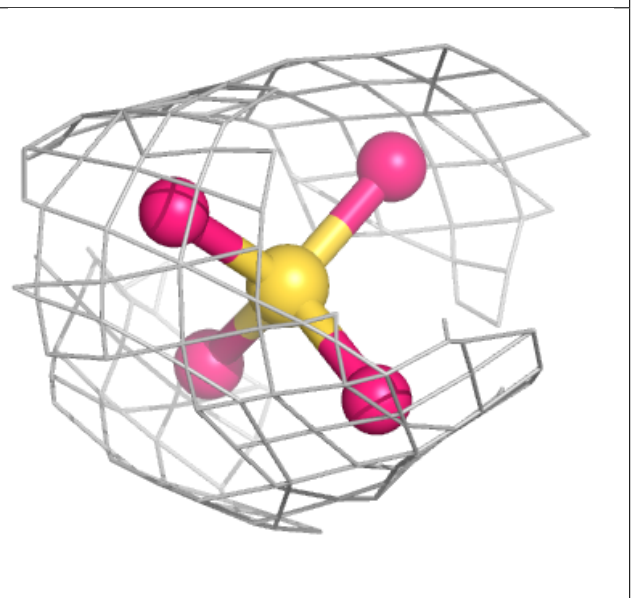


Electron density around SO4 B 807:

$2mF_o$-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.