Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:05 AM BST

PDB ID	:	5MRW
Title	:	Structure of the KdpFABC complex
Authors	:	Huang, C.; Pedersen, B.P.; Stokes, D.L.
Deposited on	:	2016-12-27
Resolution	:	2.90 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:

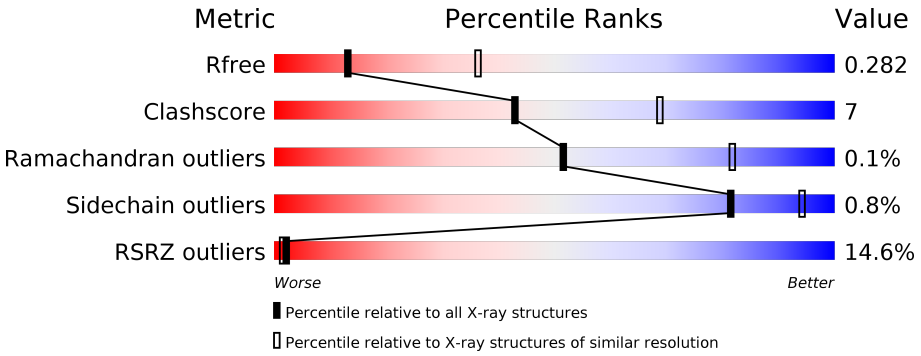
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	557	10% 78% 21%
1	E	557	8% 79% 20%
1	I	557	10% 81% 18%
2	B	674	14% 82% 18%
2	F	674	21% 83% 17%
2	J	674	28% 84% 16%

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Mol	Chain	Length	Quality of chain
3	C	187	5% 83% 17%
3	G	187	9% 86% 14%
3	K	187	8% 86% 14%
4	D	27	7% 96%
4	H	27	7% 96%
4	L	27	15% 96%

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
6	PX4	A	602	-	-	-	X
6	PX4	A	603	-	-	-	X
6	PX4	E	602	-	-	-	X
6	PX4	H	101	-	-	-	X
6	PX4	I	602	-	-	-	X
6	PX4	I	603	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32666 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 Potassium-transporting ATPase potassium-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	E	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	I	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ARG	GLN	engineered mutation	UNP P03959
E	116	ARG	GLN	engineered mutation	UNP P03959
I	116	ARG	GLN	engineered mutation	UNP P03959

- Molecule 2 is a protein called Potassium-transporting ATPase ATP-binding subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			
2	F	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			
2	J	674	Total	C	N	O	P	S	0	0	0
			5008	3187	864	932	1	24			

- Molecule 3 is a protein called Potassium-transporting ATPase KdpC subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			
3	G	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

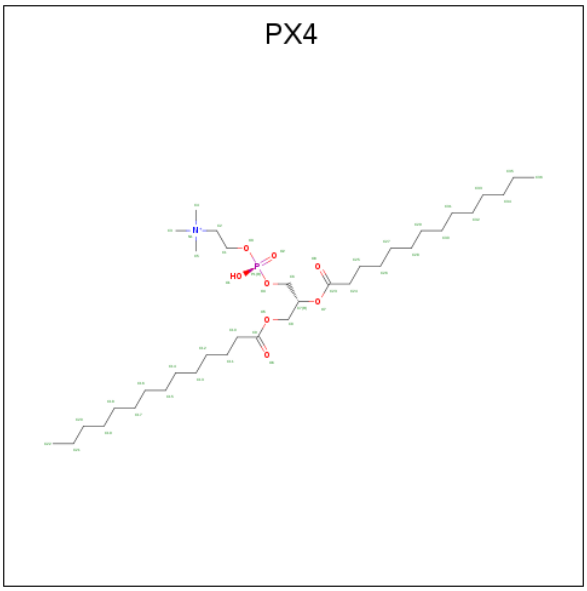
- Molecule 4 is a protein called Potassium-transporting ATPase KdpF subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	H	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	L	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

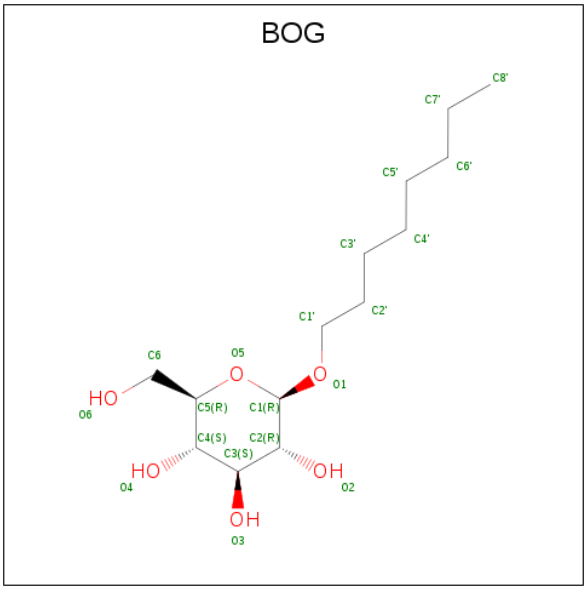
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

- Molecule 6 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	E	1	Total	C	O	P	0	0
			41	32	8	1		
6	H	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		

- Molecule 7 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 8 is water.

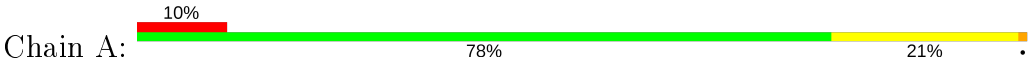
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O 1 1	0	0
8	F	1	Total O 1 1	0	0
8	J	1	Total O 1 1	0	0

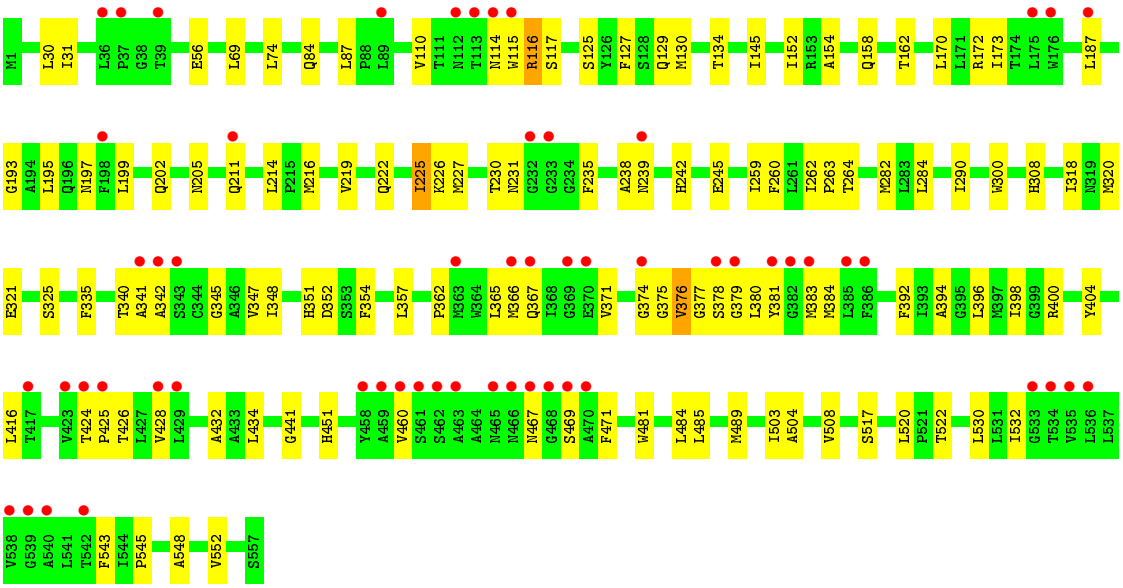
3 Residue-property plots (i)

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: Potassium-transporting ATPase potassium-binding subunit

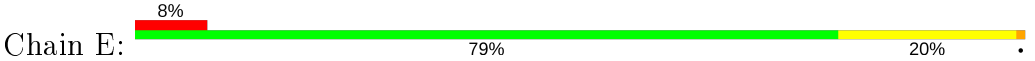
Chain A:

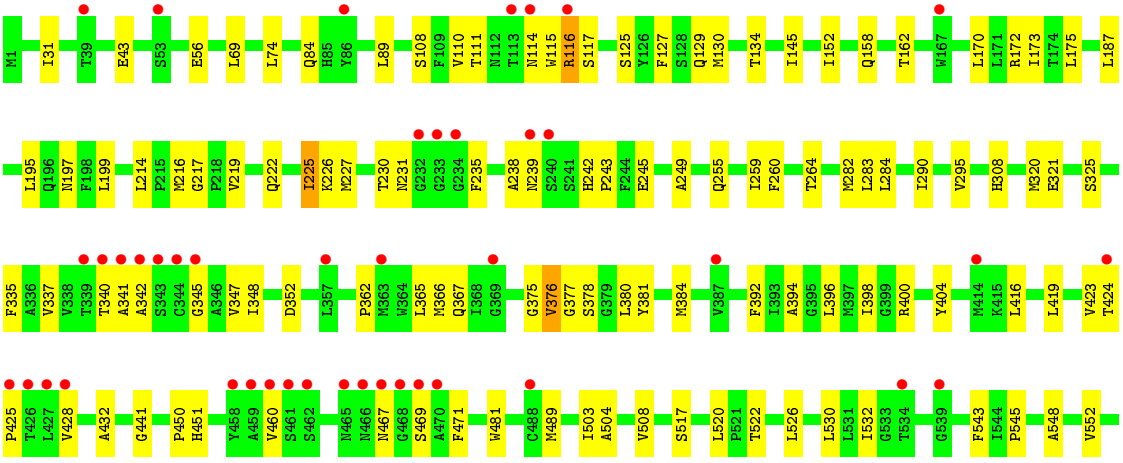




- Molecule 1: Potassium-transporting ATPase potassium-binding subunit

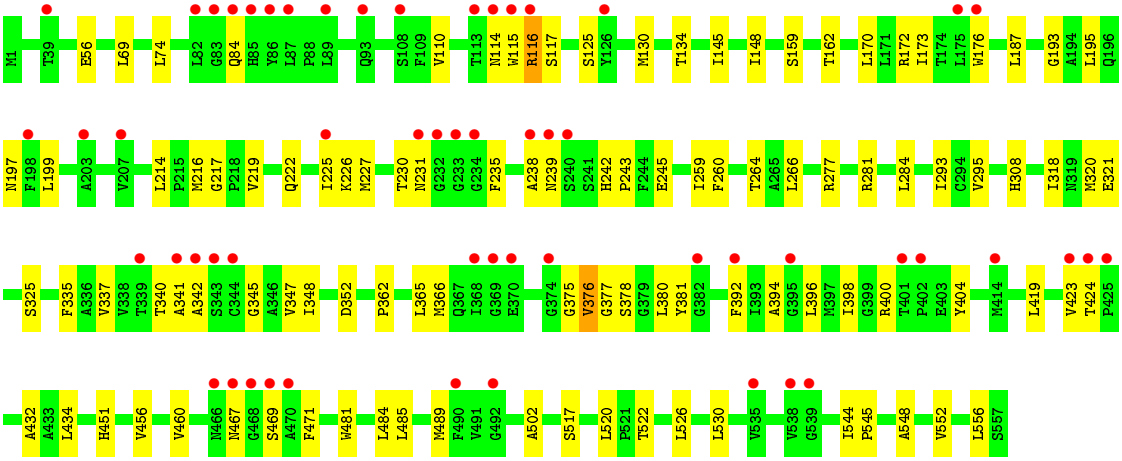
Chain E:





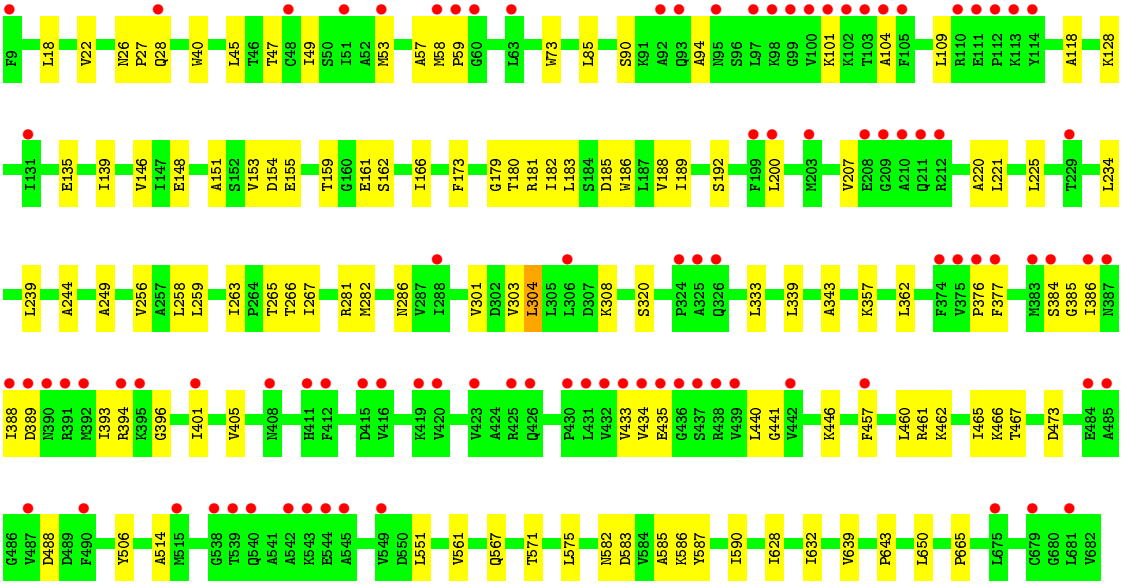
• Molecule 1: Potassium-transporting ATPase potassium-binding subunit

Chain I:



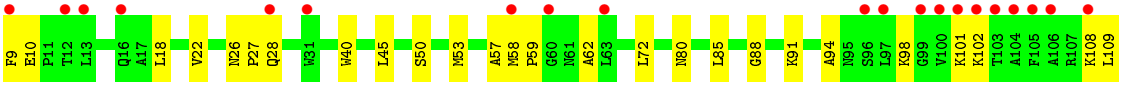
• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

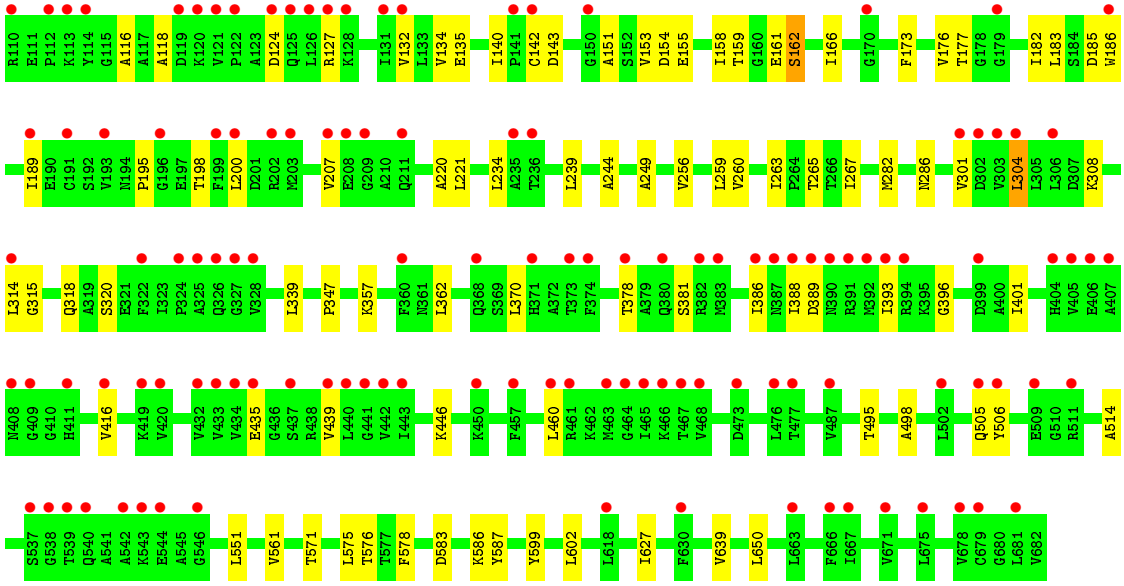
Chain B:



• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

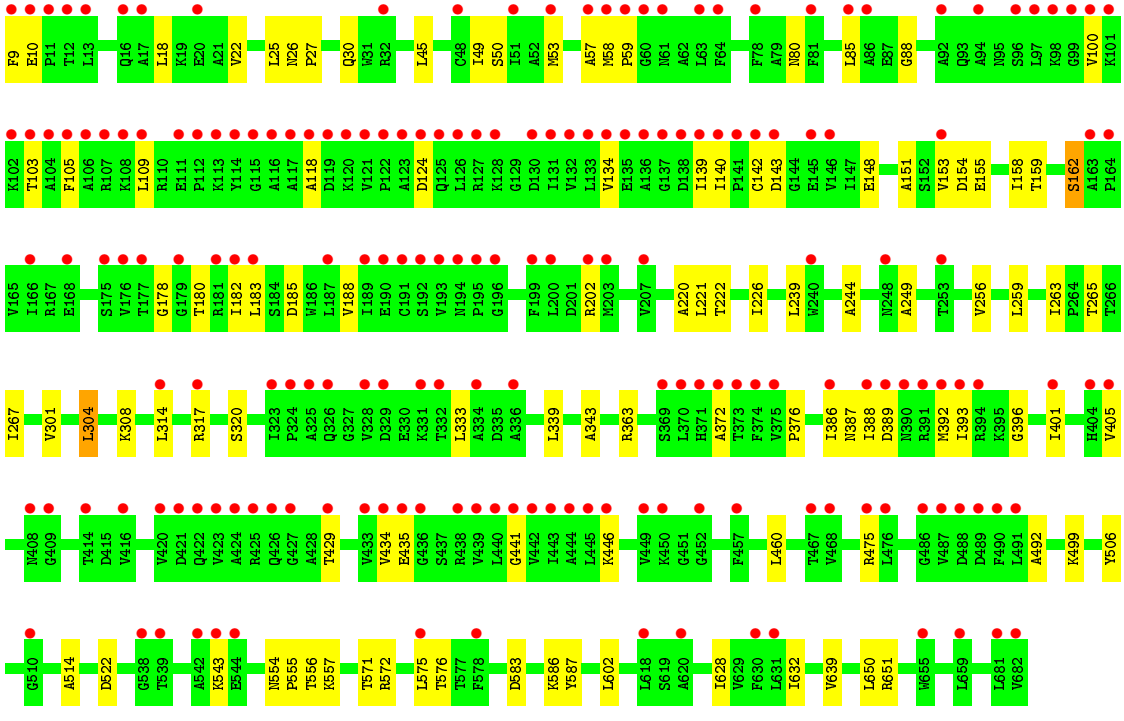
Chain F:





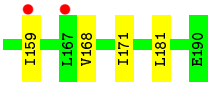
- Molecule 2: Potassium-transporting ATPase ATP-binding subunit

Chain J:



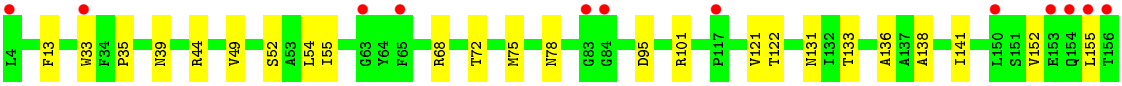
- Molecule 3: Potassium-transporting ATPase KdpC subunit

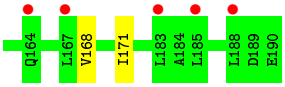
Chain C:



• Molecule 3: Potassium-transporting ATPase KdpC subunit

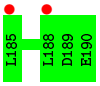
Chain G:





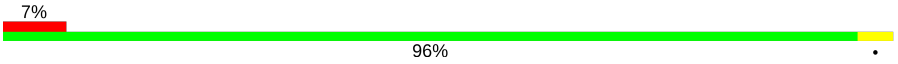
• Molecule 3: Potassium-transporting ATPase KdpC subunit

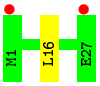
Chain K:



• Molecule 4: Potassium-transporting ATPase KdpF subunit

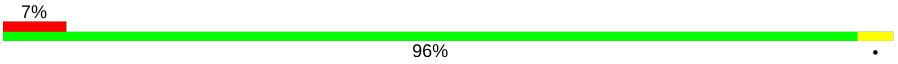
Chain D:

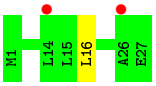




• Molecule 4: Potassium-transporting ATPase KdpF subunit

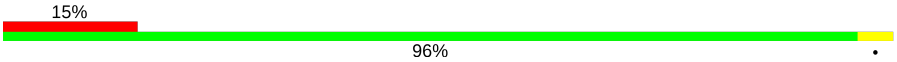
Chain H:

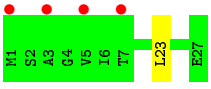




• Molecule 4: Potassium-transporting ATPase KdpF subunit

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.72Å 166.29Å 196.30Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.90) 99.4 (49.88-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.275 0.252 , 0.282	Depositor DCC
R_{free} test set	8397 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	94.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 92.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32666	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: K, BOG, PX4, SEP

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	0.25	0/4249	0.39	0/5784
1	E	0.27	1/4249 (0.0%)	0.39	0/5784
1	I	0.26	1/4249 (0.0%)	0.39	0/5784
2	B	0.24	0/5072	0.40	0/6889
2	F	0.24	0/5072	0.40	0/6889
2	J	0.24	0/5072	0.40	0/6889
3	C	0.24	0/1444	0.40	0/1977
3	G	0.24	0/1444	0.39	0/1977
3	K	0.24	0/1444	0.38	0/1977
4	D	0.23	0/202	0.37	0/275
4	H	0.23	0/202	0.36	0/275
4	L	0.23	0/202	0.37	0/275
All	All	0.25	2/32901 (0.0%)	0.39	0/44775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	217	GLY	C-N	7.48	1.48	1.34
1	I	217	GLY	C-N	5.58	1.44	1.34

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	4157	0	4286	78	0
1	E	4157	0	4286	78	0
1	I	4157	0	4286	70	0
2	B	5008	0	5195	71	0
2	F	5008	0	5195	72	0
2	J	5008	0	5195	66	0
3	C	1413	0	1428	24	0
3	G	1413	0	1428	22	0
3	K	1413	0	1428	21	0
4	D	200	0	221	1	0
4	H	200	0	221	1	0
4	L	200	0	221	1	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	A	82	0	118	1	0
6	E	41	0	59	1	0
6	H	41	0	59	0	0
6	I	82	0	118	3	0
7	A	20	0	28	0	0
7	B	20	0	28	0	0
7	E	20	0	28	1	0
7	I	20	0	28	1	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
8	J	1	0	0	0	0
All	All	32666	0	33856	453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (453) 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:545:PRO:HB2	2:B:239:LEU:HD21	1.65	0.79
1:I:545:PRO:HB2	2:J:239:LEU:HD21	1.65	0.76
1:E:545:PRO:HB2	2:F:239:LEU:HD21	1.69	0.72
1:E:340:THR:HG21	1:E:362:PRO:HB3	1.72	0.72
1:A:116:ARG:NH1	1:A:345:GLY:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:ARG:NH1	2:B:488:ASP:OD1	2.26	0.69
1:A:264:THR:HG23	1:A:284:LEU:HD11	1.75	0.69
2:B:303:VAL:HG22	2:B:466:LYS:HB2	1.75	0.69
1:A:340:THR:HG21	1:A:362:PRO:HB3	1.76	0.68
1:I:264:THR:HG23	1:I:284:LEU:HD11	1.76	0.68
1:I:116:ARG:NH1	1:I:345:GLY:O	2.26	0.67
1:A:214:LEU:HD11	3:C:55:ILE:HD11	1.77	0.67
1:I:398:ILE:HD11	2:J:650:LEU:HB2	1.76	0.66
2:B:385:GLY:HA3	2:B:394:ARG:HD3	1.78	0.66
1:A:195:LEU:HD21	1:A:216:MET:HA	1.78	0.65
2:J:158:ILE:HG13	2:J:159:THR:HG23	1.79	0.65
1:I:130:MET:O	1:I:134:THR:OG1	2.14	0.65
2:B:393:ILE:HG12	2:B:435:GLU:HG2	1.78	0.64
1:E:264:THR:HG23	1:E:284:LEU:HD11	1.79	0.64
1:I:214:LEU:HD11	3:K:55:ILE:HD11	1.79	0.64
2:J:45:LEU:HD11	2:J:256:VAL:HG21	1.80	0.64
2:B:396:GLY:H	2:B:401:ILE:HD11	1.61	0.64
1:E:195:LEU:HD21	1:E:216:MET:HA	1.80	0.64
3:K:35:PRO:O	3:K:39:ASN:ND2	2.31	0.64
2:J:304:LEU:HD21	2:J:460:LEU:HD21	1.80	0.63
3:C:168:VAL:HB	3:C:171:ILE:HG12	1.80	0.63
1:E:214:LEU:HD11	3:G:55:ILE:HD11	1.79	0.63
1:A:130:MET:O	1:A:134:THR:OG1	2.17	0.63
1:A:398:ILE:HD11	2:B:650:LEU:HB2	1.80	0.63
1:E:69:LEU:HD22	1:E:170:LEU:HD13	1.80	0.63
2:J:100:VAL:HG13	2:J:139:ILE:HD12	1.81	0.63
1:E:226:LYS:HA	1:E:231:ASN:HB2	1.81	0.63
1:I:230:THR:HG21	1:I:375:GLY:HA3	1.81	0.63
1:E:398:ILE:HD11	2:F:650:LEU:HB2	1.81	0.63
1:E:341:ALA:HB2	1:E:365:LEU:HD13	1.81	0.62
1:A:366:MET:SD	1:A:467:ASN:ND2	2.67	0.62
1:I:195:LEU:HD21	1:I:216:MET:HA	1.81	0.61
2:B:47:THR:HG21	2:B:73:TRP:HE1	1.63	0.61
1:A:400:ARG:NH2	1:A:517:SER:OG	2.33	0.61
3:G:168:VAL:HB	3:G:171:ILE:HG12	1.81	0.61
1:A:321:GLU:OE2	3:C:85:SER:OG	2.18	0.61
1:E:130:MET:O	1:E:134:THR:OG1	2.18	0.61
1:I:340:THR:HG21	1:I:362:PRO:HB3	1.83	0.61
2:F:45:LEU:HD11	2:F:256:VAL:HG21	1.82	0.61
1:A:226:LYS:HA	1:A:231:ASN:HB2	1.82	0.60
3:C:35:PRO:O	3:C:39:ASN:ND2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:304:LEU:HD21	2:F:460:LEU:HD21	1.83	0.60
2:J:396:GLY:H	2:J:401:ILE:HD11	1.66	0.60
2:B:154:ASP:HB2	2:B:183:LEU:HD11	1.82	0.60
1:I:376:VAL:O	1:I:378:SER:N	2.32	0.60
1:A:376:VAL:O	1:A:378:SER:N	2.33	0.60
1:A:239:ASN:HD21	1:A:347:VAL:H	1.50	0.60
2:F:339:LEU:HB3	2:F:386:ILE:HG21	1.84	0.60
1:I:392:PHE:HZ	2:J:220:ALA:HB1	1.65	0.60
1:I:526:LEU:HD22	2:J:651:ARG:HE	1.67	0.59
2:F:18:LEU:HD11	2:F:88:GLY:HA3	1.84	0.59
1:A:230:THR:HG21	1:A:375:GLY:HA3	1.84	0.59
3:G:35:PRO:O	3:G:39:ASN:ND2	2.33	0.59
3:K:168:VAL:HB	3:K:171:ILE:HG12	1.84	0.59
1:A:227:MET:HE1	1:A:259:ILE:HD11	1.85	0.59
2:B:304:LEU:HD21	2:B:460:LEU:HD21	1.84	0.58
1:I:308:HIS:ND1	3:K:95:ASP:OD2	2.33	0.58
2:B:101:LYS:HD3	2:B:200:LEU:HD12	1.85	0.58
1:I:400:ARG:NH2	1:I:517:SER:OG	2.37	0.58
1:A:341:ALA:HB2	1:A:365:LEU:HD13	1.85	0.58
1:I:239:ASN:HD21	1:I:347:VAL:H	1.50	0.58
1:E:239:ASN:HD21	1:E:347:VAL:H	1.51	0.58
2:F:571:THR:HG22	2:F:639:VAL:HG23	1.86	0.58
1:I:226:LYS:HA	1:I:231:ASN:HB2	1.85	0.57
1:I:239:ASN:HD21	1:I:347:VAL:N	2.02	0.57
1:I:366:MET:SD	1:I:467:ASN:ND2	2.68	0.57
1:A:239:ASN:HD21	1:A:347:VAL:N	2.02	0.57
2:F:315:GLY:O	2:F:318:GLN:NE2	2.36	0.57
1:E:227:MET:HE1	1:E:259:ILE:HD11	1.87	0.57
2:B:18:LEU:HD13	2:B:85:LEU:HA	1.86	0.57
2:J:267:ILE:HD12	2:J:576:THR:HG22	1.85	0.57
2:F:101:LYS:HD2	2:F:200:LEU:HD12	1.86	0.57
2:F:396:GLY:H	2:F:401:ILE:HD11	1.70	0.57
1:E:398:ILE:HD12	1:E:520:LEU:HD11	1.86	0.56
1:E:392:PHE:HZ	2:F:220:ALA:HB1	1.70	0.56
2:B:435:GLU:HG3	2:B:440:LEU:HD11	1.87	0.56
1:E:239:ASN:HD21	1:E:347:VAL:N	2.02	0.56
1:A:290:ILE:HD11	1:A:532:ILE:HG23	1.86	0.56
1:E:404:TYR:HD1	1:E:522:THR:HG21	1.71	0.56
2:J:25:LEU:O	2:J:30:GLN:NE2	2.35	0.56
1:I:197:ASN:HD22	3:K:39:ASN:HA	1.70	0.56
3:G:72:THR:OG1	3:G:75:MET:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HD1	1:A:522:THR:HG21	1.70	0.56
2:B:45:LEU:HD11	2:B:256:VAL:HG21	1.88	0.56
1:E:396:LEU:HD21	2:F:221:LEU:HB3	1.88	0.55
1:I:352:ASP:OD1	1:I:451:HIS:NE2	2.31	0.55
2:J:22:VAL:HG13	2:J:80:ASN:HB2	1.89	0.55
1:A:308:HIS:ND1	3:C:95:ASP:OD2	2.39	0.55
1:A:398:ILE:HD12	1:A:520:LEU:HD11	1.88	0.55
1:E:230:THR:HG21	1:E:375:GLY:HA3	1.88	0.55
3:G:138:ALA:HA	3:G:141:ILE:HG13	1.89	0.55
2:J:554:ASN:HB3	2:J:557:LYS:HG3	1.87	0.55
1:E:295:VAL:HA	1:E:337:VAL:HG21	1.88	0.55
3:G:141:ILE:HG23	3:G:155:LEU:HD23	1.88	0.55
2:J:109:LEU:HD23	2:J:118:ALA:HB2	1.87	0.55
1:A:396:LEU:HD21	2:B:221:LEU:HB3	1.88	0.55
1:E:400:ARG:NH2	1:E:517:SER:OG	2.39	0.55
1:I:260:PHE:HE1	1:I:342:ALA:HB2	1.72	0.55
2:J:339:LEU:HB3	2:J:386:ILE:HG21	1.89	0.55
3:C:72:THR:OG1	3:C:75:MET:O	2.23	0.55
2:F:162:SEP:HB3	2:F:357:LYS:HE2	1.88	0.55
1:A:260:PHE:HE1	1:A:342:ALA:HB2	1.71	0.55
1:E:416:LEU:HB2	1:E:503:ILE:HD11	1.89	0.55
1:A:197:ASN:HB2	1:A:199:LEU:HD13	1.89	0.54
1:I:69:LEU:HD22	1:I:170:LEU:HD13	1.88	0.54
2:J:162:SEP:O1P	2:J:363:ARG:NH2	2.40	0.54
2:F:135:GLU:HA	2:F:186:TRP:HA	1.89	0.54
2:B:571:THR:HG22	2:B:639:VAL:HG23	1.89	0.54
1:E:366:MET:SD	1:E:467:ASN:ND2	2.68	0.54
1:A:548:ALA:HA	1:A:552:VAL:HB	1.90	0.54
1:E:116:ARG:NH1	1:E:345:GLY:O	2.40	0.54
1:I:341:ALA:HB2	1:I:365:LEU:HD13	1.89	0.54
3:K:138:ALA:HA	3:K:141:ILE:HG13	1.89	0.54
1:E:325:SER:HB2	3:G:131:ASN:HB2	1.89	0.54
3:G:101:ARG:HB2	3:G:121:VAL:HG23	1.90	0.54
2:B:179:GLY:HA3	2:B:200:LEU:HD11	1.90	0.54
1:I:396:LEU:HD21	2:J:221:LEU:HB3	1.90	0.54
1:A:416:LEU:HB2	1:A:503:ILE:HD11	1.90	0.53
1:E:376:VAL:O	1:E:378:SER:N	2.33	0.53
3:K:101:ARG:HB2	3:K:121:VAL:HG23	1.89	0.53
2:F:495:THR:HG23	2:F:498:ALA:H	1.74	0.53
1:I:325:SER:HB2	3:K:131:ASN:HB2	1.90	0.53
2:B:339:LEU:HB3	2:B:386:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ILE:HD11	1:E:532:ILE:HG23	1.90	0.53
1:E:260:PHE:HE1	1:E:342:ALA:HB2	1.73	0.53
1:E:548:ALA:HA	1:E:552:VAL:HB	1.90	0.53
1:I:394:ALA:HB2	1:I:530:LEU:HD21	1.90	0.53
3:C:115:SER:HB3	1:E:158:GLN:HG3	1.89	0.53
1:I:227:MET:HE1	1:I:259:ILE:HD11	1.91	0.53
1:A:352:ASP:HB2	1:A:471:PHE:O	2.09	0.53
2:B:153:VAL:HG12	2:B:182:ILE:HG13	1.91	0.53
1:I:398:ILE:HD12	1:I:520:LEU:HD11	1.89	0.53
1:A:352:ASP:OD1	1:A:451:HIS:NE2	2.27	0.53
2:B:433:VAL:HG13	2:B:440:LEU:HB2	1.90	0.53
2:F:18:LEU:HD13	2:F:85:LEU:HA	1.90	0.52
1:A:432:ALA:HB2	1:A:460:VAL:HG21	1.91	0.52
1:A:321:GLU:HA	3:C:122:THR:HB	1.91	0.52
1:I:392:PHE:CZ	2:J:220:ALA:HB1	2.43	0.52
2:J:154:ASP:HB2	2:J:183:LEU:HD11	1.90	0.52
1:E:321:GLU:HA	3:G:122:THR:HB	1.90	0.52
1:E:352:ASP:HB2	1:E:471:PHE:O	2.10	0.52
1:I:335:PHE:HB3	1:I:348:ILE:HG21	1.91	0.52
1:E:197:ASN:HD22	3:G:39:ASN:HA	1.75	0.52
1:E:432:ALA:HB2	1:E:460:VAL:HG21	1.90	0.52
1:A:238:ALA:O	1:A:242:HIS:HB2	2.09	0.52
3:C:138:ALA:HA	3:C:141:ILE:HG13	1.91	0.52
1:I:243:PRO:HB2	3:K:54:LEU:HB3	1.91	0.52
1:A:69:LEU:HD22	1:A:170:LEU:HD13	1.92	0.52
3:C:75:MET:HG3	3:C:78:ASN:HB2	1.92	0.52
1:I:295:VAL:HA	1:I:337:VAL:HG21	1.90	0.52
2:J:103:THR:HG21	2:J:139:ILE:HD11	1.91	0.52
3:K:72:THR:OG1	3:K:75:MET:O	2.26	0.52
1:E:352:ASP:OD1	1:E:451:HIS:NE2	2.28	0.51
1:I:544:ILE:HG22	1:I:545:PRO:HD3	1.92	0.51
2:B:90:SER:HB2	2:B:207:VAL:HG13	1.91	0.51
1:E:378:SER:HA	1:E:381:TYR:CZ	2.44	0.51
1:A:187:LEU:HD13	3:C:33:TRP:HZ3	1.76	0.51
2:F:153:VAL:HG12	2:F:182:ILE:HG13	1.91	0.51
2:F:53:MET:HA	2:F:57:ALA:HB3	1.92	0.51
1:I:548:ALA:HA	1:I:552:VAL:HB	1.91	0.51
2:J:393:ILE:HG12	2:J:435:GLU:HG2	1.93	0.51
2:F:109:LEU:HD22	2:F:116:ALA:HB3	1.92	0.51
2:B:159:THR:HG23	2:B:161:GLU:H	1.74	0.51
1:A:197:ASN:HD22	3:C:39:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:THR:HG21	1:E:489:MET:HB3	1.91	0.51
2:J:49:ILE:O	2:J:53:MET:N	2.34	0.51
1:A:378:SER:HA	1:A:381:TYR:CE2	2.46	0.51
2:B:135:GLU:HA	2:B:186:TRP:HA	1.92	0.51
1:I:84:GLN:OE1	1:I:125:SER:N	2.44	0.51
1:I:321:GLU:HA	3:K:122:THR:HB	1.93	0.51
1:I:432:ALA:HB2	1:I:460:VAL:HG21	1.93	0.51
1:E:43:GLU:OE1	1:E:172:ARG:NH1	2.44	0.50
3:C:44:ARG:HG2	3:C:49:VAL:HA	1.93	0.50
1:E:335:PHE:HB3	1:E:348:ILE:HG21	1.92	0.50
1:I:197:ASN:HB2	1:I:199:LEU:HD13	1.93	0.50
2:F:154:ASP:HB2	2:F:183:LEU:HD11	1.93	0.50
1:I:238:ALA:O	1:I:242:HIS:HB2	2.11	0.50
2:J:571:THR:HG22	2:J:639:VAL:HG23	1.92	0.50
2:B:466:LYS:HD3	3:K:153:GLU:OE2	2.12	0.50
2:B:49:ILE:O	2:B:53:MET:N	2.34	0.50
2:B:18:LEU:O	2:B:22:VAL:HG23	2.12	0.50
1:E:238:ALA:O	1:E:242:HIS:HB2	2.11	0.50
2:J:301:VAL:HG21	2:J:514:ALA:HB2	1.93	0.50
2:F:109:LEU:HD23	2:F:118:ALA:HB2	1.94	0.49
1:E:378:SER:HA	1:E:381:TYR:CE2	2.47	0.49
2:B:281:ARG:NH2	2:B:567:GLN:OE1	2.45	0.49
1:I:114:ASN:ND2	1:I:231:ASN:HB3	2.28	0.49
2:B:583:ASP:HA	2:B:586:LYS:HD3	1.95	0.49
1:E:394:ALA:HB2	1:E:530:LEU:HD21	1.95	0.49
3:K:44:ARG:HG2	3:K:49:VAL:HA	1.95	0.49
1:I:148:ILE:HD13	1:I:381:TYR:HB3	1.95	0.49
2:B:109:LEU:HD23	2:B:118:ALA:HB2	1.94	0.49
1:E:197:ASN:HB2	1:E:199:LEU:HD13	1.93	0.49
6:I:603:PX4:H55	6:I:603:PX4:H16	1.95	0.49
2:B:53:MET:HG3	2:B:59:PRO:HG2	1.95	0.48
3:G:44:ARG:HG2	3:G:49:VAL:HA	1.94	0.48
1:I:378:SER:HA	1:I:381:TYR:CZ	2.47	0.48
2:F:134:VAL:HG11	2:F:140:ILE:HD13	1.95	0.48
2:F:159:THR:HG23	2:F:161:GLU:H	1.79	0.48
1:A:114:ASN:ND2	1:A:231:ASN:HB3	2.28	0.48
2:B:396:GLY:N	2:B:401:ILE:HD11	2.28	0.48
1:I:352:ASP:HB2	1:I:471:PHE:O	2.13	0.48
2:J:103:THR:HB	2:J:105:PHE:CE2	2.48	0.48
3:C:101:ARG:HB2	3:C:121:VAL:HG23	1.96	0.48
2:B:286:ASN:HB3	2:B:551:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HB2	2:B:139:ILE:HD11	1.95	0.48
2:J:405:VAL:HG22	2:J:434:VAL:HG11	1.96	0.48
2:F:98:LYS:HG2	2:F:102:LYS:NZ	2.29	0.48
1:I:404:TYR:HD1	1:I:522:THR:HG21	1.79	0.47
2:F:9:PHE:CD2	2:F:10:GLU:HG3	2.49	0.47
2:J:53:MET:HA	2:J:57:ALA:HB3	1.95	0.47
2:B:357:LYS:HA	2:B:362:LEU:H	1.80	0.47
1:E:219:VAL:HG11	1:E:245:GLU:HG2	1.96	0.47
2:F:98:LYS:HG2	2:F:102:LYS:HZ1	1.78	0.47
2:F:158:ILE:HG21	2:F:177:THR:HG21	1.95	0.47
1:I:502:ALA:HB1	7:I:604:BOG:H2'2	1.96	0.47
1:A:394:ALA:HB2	1:A:530:LEU:HD21	1.96	0.47
1:A:145:ILE:HB	1:A:173:ILE:HD13	1.96	0.47
2:B:282:MET:HE3	2:B:561:VAL:HG22	1.95	0.47
2:J:244:ALA:HB2	2:J:249:ALA:HB2	1.97	0.47
3:K:75:MET:HG3	3:K:78:ASN:HB2	1.96	0.47
1:E:416:LEU:HD11	7:E:603:BOG:H4'2	1.97	0.47
2:J:9:PHE:CD2	2:J:10:GLU:HG3	2.50	0.47
1:E:74:LEU:HB3	1:E:110:VAL:HG21	1.96	0.47
2:F:26:ASN:N	2:F:27:PRO:HD2	2.30	0.47
2:J:343:ALA:HB1	2:J:376:PRO:HA	1.97	0.47
1:A:378:SER:HA	1:A:381:TYR:CZ	2.50	0.47
1:A:434:LEU:HD23	1:A:484:LEU:HD13	1.97	0.47
1:A:335:PHE:HB3	1:A:348:ILE:HG21	1.96	0.47
2:F:108:LYS:HA	2:F:132:VAL:HA	1.96	0.47
2:J:153:VAL:HG12	2:J:182:ILE:HG13	1.97	0.47
2:B:308:LYS:NZ	2:B:473:ASP:OD2	2.40	0.47
2:B:53:MET:HA	2:B:57:ALA:HB3	1.97	0.47
3:G:52:SER:OG	3:G:55:ILE:HG13	2.14	0.47
1:A:345:GLY:HA2	1:A:469:SER:OG	2.15	0.47
2:F:378:THR:HG1	2:F:381:SER:HG	1.55	0.47
1:I:56:GLU:HB3	1:I:162:THR:HB	1.97	0.46
2:J:221:LEU:HD21	2:J:572:ARG:HD3	1.96	0.46
2:J:267:ILE:HG22	2:J:575:LEU:HB3	1.98	0.46
1:A:158:GLN:HG3	3:K:115:SER:HB3	1.96	0.46
2:B:244:ALA:HB2	2:B:249:ALA:HB2	1.98	0.46
2:B:343:ALA:HB1	2:B:376:PRO:HA	1.96	0.46
2:B:146:VAL:HG22	2:B:189:ILE:HG22	1.97	0.46
1:E:392:PHE:CZ	2:F:220:ALA:HB1	2.48	0.46
2:F:357:LYS:HA	2:F:362:LEU:H	1.81	0.46
1:E:345:GLY:HA2	1:E:469:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:LYS:HB2	2:B:643:PRO:HB2	1.97	0.46
2:F:320:SER:HB2	2:F:446:LYS:HG2	1.97	0.46
1:E:114:ASN:ND2	1:E:231:ASN:HB3	2.31	0.46
1:I:345:GLY:HA2	1:I:469:SER:OG	2.15	0.46
2:J:155:GLU:HG2	2:J:180:THR:HG21	1.97	0.46
2:J:26:ASN:N	2:J:27:PRO:HD2	2.30	0.46
1:E:556:LEU:HD12	2:F:602:LEU:HD23	1.98	0.46
2:J:222:THR:O	2:J:226:ILE:HG12	2.16	0.46
1:E:56:GLU:HB3	1:E:162:THR:HB	1.97	0.46
2:F:416:VAL:HG11	2:F:439:VAL:HG11	1.98	0.46
2:B:26:ASN:N	2:B:27:PRO:HD2	2.31	0.45
1:I:187:LEU:HD13	3:K:33:TRP:HZ3	1.81	0.45
2:B:139:ILE:HG22	2:B:181:ARG:HB2	1.99	0.45
2:J:18:LEU:HD11	2:J:88:GLY:HA3	1.98	0.45
3:K:52:SER:OG	3:K:55:ILE:HG13	2.16	0.45
1:A:374:GLY:HA3	1:A:379:GLY:HA3	1.98	0.45
1:A:129:GLN:O	1:A:134:THR:HG23	2.17	0.45
1:E:419:LEU:O	1:E:423:VAL:HG23	2.17	0.45
2:F:53:MET:HG3	2:F:59:PRO:HG2	1.99	0.45
1:E:450:PRO:HG3	2:F:599:TYR:CE1	2.52	0.45
2:J:50:SER:HA	2:J:53:MET:HB3	1.98	0.45
2:B:173:PHE:CE2	2:B:343:ALA:HA	2.51	0.45
1:I:219:VAL:HG22	1:I:235:PHE:CG	2.52	0.45
1:I:219:VAL:HG11	1:I:245:GLU:HG2	1.98	0.45
2:B:263:ILE:O	2:B:265:THR:N	2.49	0.45
1:I:378:SER:HA	1:I:381:TYR:CE2	2.51	0.45
1:I:419:LEU:O	1:I:423:VAL:HG23	2.17	0.45
2:J:124:ASP:N	2:J:124:ASP:OD1	2.50	0.45
2:J:628:ILE:O	2:J:632:ILE:HG13	2.17	0.45
1:A:325:SER:OG	3:C:131:ASN:HB2	2.17	0.45
2:F:318:GLN:HE22	2:F:347:PRO:HB2	1.81	0.45
1:A:56:GLU:HB3	1:A:162:THR:HB	1.99	0.45
2:J:388:ILE:HG23	2:J:389:ASP:H	1.80	0.45
1:I:193:GLY:HA2	3:K:37:GLN:HB3	1.98	0.44
2:J:317:ARG:HH11	2:J:429:THR:HG23	1.82	0.44
2:J:320:SER:HB2	2:J:446:LYS:HG2	1.98	0.44
2:B:155:GLU:O	2:B:159:THR:HG22	2.17	0.44
2:B:148:GLU:HB2	2:B:188:VAL:HB	1.99	0.44
1:E:89:LEU:HB2	1:E:127:PHE:HB2	1.99	0.44
2:F:393:ILE:HG12	2:F:435:GLU:HG2	1.98	0.44
2:F:22:VAL:HG13	2:F:80:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:PRO:HB2	3:G:54:LEU:HB3	1.99	0.44
3:C:141:ILE:HG23	3:C:155:LEU:HD23	2.00	0.44
2:F:301:VAL:HG21	2:F:514:ALA:HB2	2.00	0.44
2:J:18:LEU:HD13	2:J:85:LEU:HA	1.99	0.44
2:J:583:ASP:HA	2:J:586:LYS:HD3	1.99	0.44
1:A:74:LEU:HB3	1:A:110:VAL:HG21	1.98	0.44
2:F:124:ASP:OD1	2:F:124:ASP:N	2.49	0.44
2:J:134:VAL:HG11	2:J:140:ILE:HD13	2.00	0.44
1:A:318:ILE:HG22	1:A:320:MET:HG2	2.00	0.44
2:B:234:LEU:HD21	4:D:16:LEU:HD11	1.99	0.44
2:B:320:SER:HB2	2:B:446:LYS:HG2	1.98	0.44
2:B:388:ILE:HG23	2:B:389:ASP:H	1.83	0.44
1:E:129:GLN:O	1:E:134:THR:HG23	2.17	0.44
2:F:263:ILE:O	2:F:265:THR:N	2.50	0.44
2:J:499:LYS:NZ	2:J:522:ASP:OD1	2.48	0.44
2:J:53:MET:HG3	2:J:59:PRO:HG2	2.00	0.44
1:A:205:ASN:OD1	1:A:211:GLN:NE2	2.51	0.44
2:F:176:VAL:HG11	2:F:189:ILE:HG21	1.99	0.44
1:I:197:ASN:ND2	3:K:39:ASN:HA	2.33	0.44
2:F:583:ASP:HA	2:F:586:LYS:HD3	1.99	0.44
3:K:141:ILE:HG21	3:K:152:VAL:HG13	2.00	0.44
1:A:219:VAL:HG11	1:A:245:GLU:HG2	1.99	0.44
1:A:351:HIS:HA	1:A:354:PHE:CD1	2.53	0.44
2:B:151:ALA:HB2	2:B:185:ASP:HB2	2.00	0.44
3:C:133:THR:HG23	3:C:136:ALA:H	1.83	0.44
3:C:159:ILE:HG12	3:C:181:LEU:HD21	2.00	0.44
2:F:282:MET:HE3	2:F:561:VAL:HG22	1.99	0.44
3:G:75:MET:HG3	3:G:78:ASN:HB2	1.99	0.44
2:J:148:GLU:HB2	2:J:188:VAL:HB	2.00	0.44
2:J:18:LEU:O	2:J:22:VAL:HG23	2.18	0.44
2:J:333:LEU:HD11	2:J:441:GLY:HA3	2.00	0.44
1:A:371:VAL:HG13	1:A:383:MET:HB2	2.00	0.43
2:B:377:PHE:HB2	2:B:384:SER:HB3	2.00	0.43
2:F:388:ILE:HG23	2:F:389:ASP:H	1.82	0.43
2:F:58:MET:N	2:F:59:PRO:HD2	2.33	0.43
2:J:314:LEU:O	2:J:555:PRO:HG2	2.18	0.43
2:B:457:PHE:CE1	2:B:467:THR:HG21	2.53	0.43
1:E:249:ALA:HB1	3:G:171:ILE:HG22	2.00	0.43
1:I:222:GLN:HA	1:I:225:ILE:HD12	1.99	0.43
1:A:115:TRP:HE1	1:A:117:SER:HB3	1.82	0.43
1:A:84:GLN:OE1	1:A:125:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HD13	1:E:152:ILE:HG21	1.99	0.43
1:I:434:LEU:HD23	1:I:484:LEU:HD13	1.99	0.43
1:I:544:ILE:HA	1:I:544:ILE:HD12	1.86	0.43
2:J:308:LYS:HG3	2:J:314:LEU:HD23	2.00	0.43
2:J:372:ALA:HB2	2:J:388:ILE:HA	2.00	0.43
1:A:154:ALA:HA	1:A:508:VAL:HG22	2.00	0.43
2:F:244:ALA:HB2	2:F:249:ALA:HB2	2.01	0.43
1:A:441:GLY:HA2	1:A:481:TRP:HE1	1.83	0.43
2:B:128:LYS:HG3	2:B:192:SER:HA	2.01	0.43
1:A:392:PHE:CZ	2:B:220:ALA:HB1	2.54	0.43
2:F:91:LYS:HD2	2:F:94:ALA:HB3	1.99	0.43
2:J:314:LEU:O	2:J:556:THR:OG1	2.37	0.43
2:J:475:ARG:HG2	2:J:492:ALA:HB3	2.00	0.43
1:A:441:GLY:HA2	1:A:481:TRP:NE1	2.33	0.43
3:C:52:SER:OG	3:C:55:ILE:HG13	2.18	0.43
2:F:127:ARG:NH1	2:F:195:PRO:HG2	2.34	0.43
2:F:18:LEU:O	2:F:22:VAL:HG23	2.17	0.43
2:J:58:MET:N	2:J:59:PRO:HD2	2.33	0.43
2:B:155:GLU:HG2	2:B:180:THR:HG21	2.01	0.43
1:I:556:LEU:HD12	2:J:602:LEU:HD23	2.01	0.43
2:B:301:VAL:HG21	2:B:514:ALA:HB2	2.00	0.43
1:E:222:GLN:HA	1:E:225:ILE:HD12	2.00	0.43
1:E:441:GLY:HA2	1:E:481:TRP:NE1	2.34	0.43
1:E:84:GLN:OE1	1:E:125:SER:N	2.52	0.43
1:I:115:TRP:HE1	1:I:117:SER:HB3	1.84	0.43
1:A:260:PHE:CE1	1:A:342:ALA:HB2	2.52	0.43
1:A:380:LEU:O	1:A:384:MET:HG2	2.18	0.43
2:F:578:PHE:HE2	2:F:627:ILE:HD11	1.83	0.43
2:J:263:ILE:O	2:J:265:THR:N	2.51	0.43
2:B:258:LEU:HB2	2:B:590:ILE:HG21	2.00	0.42
1:E:425:PRO:HA	1:E:428:VAL:HG22	2.00	0.42
1:I:485:LEU:O	1:I:489:MET:HG3	2.19	0.42
1:I:293:ILE:HG22	6:I:603:PX4:H48	2.01	0.42
2:J:202:ARG:HH22	2:J:543:LYS:HD3	1.84	0.42
2:B:333:LEU:HD11	2:B:441:GLY:HA3	2.01	0.42
1:E:115:TRP:HE1	1:E:117:SER:HB3	1.83	0.42
1:E:197:ASN:ND2	3:G:39:ASN:HA	2.33	0.42
3:G:133:THR:HG23	3:G:136:ALA:H	1.84	0.42
3:G:141:ILE:HG21	3:G:152:VAL:HG13	2.00	0.42
1:E:260:PHE:CE1	1:E:342:ALA:HB2	2.54	0.42
1:I:145:ILE:HB	1:I:173:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:159:ILE:HG12	3:K:181:LEU:HD21	2.01	0.42
2:B:58:MET:N	2:B:59:PRO:HD2	2.33	0.42
1:I:74:LEU:HB3	1:I:110:VAL:HG21	2.00	0.42
3:C:156:THR:HG21	2:F:505:GLN:HG2	2.00	0.42
2:F:155:GLU:O	2:F:159:THR:HG22	2.18	0.42
1:I:266:LEU:HB3	1:I:380:LEU:HD22	2.01	0.42
2:F:101:LYS:NZ	2:F:198:THR:HG21	2.35	0.42
1:I:456:VAL:HG13	1:I:481:TRP:HH2	1.84	0.42
1:A:426:THR:HG21	6:A:602:PX4:H48	2.00	0.42
2:B:28:GLN:HG2	2:B:40:TRP:CH2	2.54	0.42
1:E:219:VAL:HG22	1:E:235:PHE:CG	2.54	0.42
2:J:142:CYS:SG	2:J:143:ASP:N	2.92	0.42
1:A:300:TRP:HZ3	1:A:357:LEU:HD12	1.84	0.42
1:A:31:ILE:HD13	1:A:152:ILE:HG21	2.01	0.42
2:B:225:LEU:HD21	2:B:267:ILE:HD11	2.02	0.42
2:B:460:LEU:HG	2:B:465:ILE:HB	2.01	0.42
2:J:226:ILE:HG21	4:L:23:LEU:HB2	2.02	0.42
2:B:166:ILE:HG13	2:B:173:PHE:HD2	1.84	0.42
2:B:94:ALA:HB2	2:B:207:VAL:HG11	2.02	0.42
1:E:504:ALA:O	1:E:508:VAL:HG23	2.19	0.42
2:J:143:ASP:OD1	2:J:178:GLY:N	2.35	0.42
1:E:108:SER:HB3	1:E:115:TRP:H	1.85	0.41
1:A:367:GLN:HB3	1:A:543:PHE:CE2	2.54	0.41
1:E:255:GLN:O	1:E:259:ILE:HG13	2.20	0.41
1:I:318:ILE:HG22	1:I:320:MET:HG2	2.01	0.41
2:J:387:ASN:CG	2:J:392:MET:HG2	2.40	0.41
1:A:222:GLN:HA	1:A:225:ILE:HD12	2.03	0.41
1:A:197:ASN:ND2	3:C:39:ASN:HA	2.34	0.41
1:E:145:ILE:HB	1:E:173:ILE:HD13	2.03	0.41
2:F:142:CYS:SG	2:F:143:ASP:N	2.93	0.41
2:F:308:LYS:HG3	2:F:314:LEU:HD23	2.01	0.41
2:J:26:ASN:N	2:J:27:PRO:CD	2.84	0.41
2:F:151:ALA:HB2	2:F:185:ASP:HB2	2.02	0.41
1:E:175:LEU:HD11	3:G:13:PHE:HE2	1.85	0.41
1:I:260:PHE:CE1	1:I:342:ALA:HB2	2.52	0.41
6:I:602:PX4:H62	6:I:602:PX4:H69	1.92	0.41
2:J:151:ALA:HB2	2:J:185:ASP:HB2	2.02	0.41
2:F:28:GLN:HG2	2:F:40:TRP:CH2	2.56	0.41
1:A:219:VAL:HG22	1:A:235:PHE:CG	2.56	0.41
1:A:504:ALA:O	1:A:508:VAL:HG23	2.20	0.41
2:B:628:ILE:O	2:B:632:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:HD13	3:G:33:TRP:HZ3	1.86	0.41
2:F:26:ASN:N	2:F:27:PRO:CD	2.83	0.41
1:I:214:LEU:HA	1:I:214:LEU:HD23	1.93	0.41
2:B:582:ASN:HA	2:B:665:PRO:HG3	2.01	0.41
2:F:94:ALA:HB2	2:F:207:VAL:HG11	2.03	0.41
2:F:267:ILE:HD12	2:F:576:THR:HG22	2.03	0.41
1:E:308:HIS:ND1	3:G:95:ASP:OD2	2.53	0.41
1:A:202:GLN:HB3	1:A:214:LEU:HB2	2.03	0.41
2:B:405:VAL:HG22	2:B:434:VAL:HG11	2.03	0.41
1:E:441:GLY:HA2	1:E:481:TRP:HE1	1.84	0.41
1:E:367:GLN:HB3	1:E:543:PHE:CZ	2.56	0.41
1:I:172:ARG:HG2	1:I:176:TRP:CZ3	2.55	0.41
1:A:87:LEU:HD13	1:A:127:PHE:CE2	2.55	0.41
1:A:425:PRO:HA	1:A:428:VAL:HG22	2.03	0.41
6:E:602:PX4:H54	6:E:602:PX4:H49	1.81	0.41
2:F:370:LEU:HB3	2:F:388:ILE:HG13	2.03	0.41
2:F:50:SER:HA	2:F:53:MET:HB3	2.03	0.41
1:I:277:ARG:HB3	1:I:281:ARG:NH1	2.35	0.41
2:B:585:ALA:HB3	2:B:665:PRO:HB2	2.02	0.41
3:C:69:PRO:HG2	3:C:123:ALA:HA	2.02	0.41
1:E:526:LEU:HD21	2:F:650:LEU:HD23	2.02	0.41
2:F:234:LEU:HD21	4:H:16:LEU:HD11	2.02	0.41
1:A:485:LEU:O	1:A:489:MET:HG3	2.21	0.41
2:B:267:ILE:HG22	2:B:575:LEU:HB3	2.03	0.41
2:B:26:ASN:N	2:B:27:PRO:CD	2.84	0.41
1:E:380:LEU:O	1:E:384:MET:HG2	2.21	0.41
2:F:72:LEU:HD22	2:F:260:VAL:HG11	2.03	0.41
3:C:50:ARG:HA	3:C:50:ARG:HD3	1.89	0.40
2:F:53:MET:SD	2:F:62:ALA:HA	2.61	0.40
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.95	0.40
1:A:193:GLY:HA2	3:C:37:GLN:HB3	2.04	0.40
1:E:283:LEU:HA	1:E:283:LEU:HD12	1.92	0.40
1:A:30:LEU:HD22	1:A:172:ARG:HD2	2.03	0.40
1:E:320:MET:O	3:G:68:ARG:NH2	2.53	0.40
2:F:166:ILE:HG13	2:F:173:PHE:HD2	1.86	0.40
2:F:286:ASN:HB3	2:F:551:LEU:HB2	2.04	0.40
2:F:575:LEU:HD23	2:F:575:LEU:HA	1.93	0.40
1:A:262:ILE:N	1:A:263:PRO:HD2	2.37	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	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	34	66
1	E	555/557 (100%)	531 (96%)	22 (4%)	2 (0%)	34	66
1	I	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	34	66
2	B	671/674 (100%)	648 (97%)	23 (3%)	0	100	100
2	F	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
2	J	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
3	C	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
3	G	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
3	K	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
4	D	25/27 (93%)	25 (100%)	0	0	100	100
4	H	25/27 (93%)	25 (100%)	0	0	100	100
4	L	25/27 (93%)	25 (100%)	0	0	100	100
All	All	4308/4335 (99%)	4129 (96%)	173 (4%)	6 (0%)	51	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	GLY
1	I	377	GLY
1	E	377	GLY
1	A	376	VAL
1	E	376	VAL
1	I	376	VAL

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	439/439 (100%)	435 (99%)	4 (1%)	78 93
1	E	439/439 (100%)	435 (99%)	4 (1%)	78 93
1	I	439/439 (100%)	436 (99%)	3 (1%)	84 95
2	B	523/523 (100%)	518 (99%)	5 (1%)	76 92
2	F	523/523 (100%)	519 (99%)	4 (1%)	81 94
2	J	523/523 (100%)	519 (99%)	4 (1%)	81 94
3	C	149/149 (100%)	148 (99%)	1 (1%)	84 95
3	G	149/149 (100%)	149 (100%)	0	100 100
3	K	149/149 (100%)	148 (99%)	1 (1%)	84 95
4	D	21/21 (100%)	21 (100%)	0	100 100
4	H	21/21 (100%)	21 (100%)	0	100 100
4	L	21/21 (100%)	21 (100%)	0	100 100
All	All	3396/3396 (100%)	3370 (99%)	26 (1%)	81 94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	225	ILE
1	A	282	MET
1	A	424	THR
2	B	259	LEU
2	B	266	THR
2	B	304	LEU
2	B	506	TYR
2	B	587	TYR
3	C	34	PHE
1	E	116	ARG
1	E	225	ILE
1	E	282	MET
1	E	424	THR
2	F	259	LEU
2	F	304	LEU
2	F	506	TYR
2	F	587	TYR

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Mol	Chain	Res	Type
1	I	116	ARG
1	I	159	SER
1	I	424	THR
2	J	259	LEU
2	J	304	LEU
2	J	506	TYR
2	J	587	TYR
3	K	34	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	114	ASN
1	A	211	GLN
1	A	239	ASN
1	E	114	ASN
1	E	239	ASN
2	F	624	ASN
2	J	624	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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	SEP	F	162	2	8,9,10	1.56	1 (12%)	8,12,14	1.66	2 (25%)
2	SEP	B	162	2	8,9,10	1.55	1 (12%)	8,12,14	1.82	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SEP	J	162	2	8,9,10	1.56	1 (12%)	8,12,14	1.79	2 (25%)

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	SEP	F	162	2	-	0/5/8/10	-
2	SEP	B	162	2	-	1/5/8/10	-
2	SEP	J	162	2	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	162	SEP	P-O1P	3.39	1.61	1.50
2	B	162	SEP	P-O1P	3.37	1.61	1.50
2	F	162	SEP	P-O1P	3.36	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	162	SEP	OG-CB-CA	3.41	111.46	108.14
2	J	162	SEP	OG-CB-CA	3.36	111.42	108.14
2	B	162	SEP	P-OG-CB	-3.36	109.03	118.30
2	J	162	SEP	P-OG-CB	-3.26	109.30	118.30
2	F	162	SEP	P-OG-CB	-3.18	109.54	118.30
2	F	162	SEP	OG-CB-CA	2.94	111.01	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	162	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	162	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	162	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
7	BOG	B	701	-	20,20,20	1.22	1 (5%)	25,25,25	0.80	0
7	BOG	E	603	-	20,20,20	1.22	1 (5%)	25,25,25	0.82	0
6	PX4	I	603	-	40,40,45	1.26	5 (12%)	43,45,53	1.15	2 (4%)
6	PX4	H	101	-	40,40,45	1.27	5 (12%)	43,45,53	1.12	2 (4%)
6	PX4	I	602	-	40,40,45	1.27	5 (12%)	43,45,53	1.07	2 (4%)
6	PX4	A	603	-	40,40,45	1.27	5 (12%)	43,45,53	1.10	2 (4%)
7	BOG	I	604	-	20,20,20	1.21	1 (5%)	25,25,25	0.82	0
6	PX4	A	602	-	40,40,45	1.26	5 (12%)	43,45,53	1.15	2 (4%)
7	BOG	A	604	-	20,20,20	1.21	1 (5%)	25,25,25	0.79	0
6	PX4	E	602	-	40,40,45	1.26	5 (12%)	43,45,53	1.11	2 (4%)

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
7	BOG	B	701	-	-	1/11/31/31	0/1/1/1
7	BOG	E	603	-	-	3/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PX4	I	603	-	-	15/44/44/49	-
6	PX4	H	101	-	-	19/44/44/49	-
6	PX4	I	602	-	-	8/44/44/49	-
6	PX4	A	603	-	-	18/44/44/49	-
7	BOG	I	604	-	-	4/11/31/31	0/1/1/1
6	PX4	A	602	-	-	22/44/44/49	-
7	BOG	A	604	-	-	3/11/31/31	0/1/1/1
6	PX4	E	602	-	-	17/44/44/49	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	604	BOG	O5-C1	3.56	1.50	1.41
7	A	604	BOG	O5-C1	3.53	1.50	1.41
7	E	603	BOG	O5-C1	3.53	1.50	1.41
7	B	701	BOG	O5-C1	3.51	1.50	1.41
6	H	101	PX4	O5-C9	3.29	1.43	1.33
6	A	602	PX4	O5-C9	3.29	1.42	1.33
6	A	603	PX4	O5-C9	3.26	1.42	1.33
6	I	602	PX4	O5-C9	3.22	1.42	1.33
6	E	602	PX4	O5-C9	3.21	1.42	1.33
6	I	603	PX4	O5-C9	3.19	1.42	1.33
6	I	603	PX4	O7-C23	3.15	1.43	1.34
6	A	602	PX4	O7-C23	3.10	1.43	1.34
6	I	602	PX4	O7-C23	3.06	1.42	1.34
6	A	603	PX4	O7-C23	3.06	1.42	1.34
6	H	101	PX4	O7-C23	3.05	1.42	1.34
6	E	602	PX4	O7-C23	3.02	1.42	1.34
6	H	101	PX4	O7-C7	-2.60	1.40	1.46
6	E	602	PX4	O7-C7	-2.58	1.40	1.46
6	A	603	PX4	O7-C7	-2.58	1.40	1.46
6	I	602	PX4	O7-C7	-2.54	1.40	1.46
6	A	602	PX4	O7-C7	-2.48	1.40	1.46
6	I	603	PX4	O7-C7	-2.34	1.40	1.46
6	E	602	PX4	P1-O3	2.32	1.67	1.59
6	A	603	PX4	P1-O3	2.32	1.67	1.59
6	H	101	PX4	P1-O3	2.31	1.67	1.59
6	I	603	PX4	P1-O3	2.30	1.67	1.59
6	I	602	PX4	P1-O3	2.30	1.67	1.59
6	A	602	PX4	P1-O3	2.26	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	602	PX4	P1-O4	2.10	1.67	1.59
6	A	603	PX4	P1-O4	2.10	1.67	1.59
6	E	602	PX4	P1-O4	2.07	1.67	1.59
6	H	101	PX4	P1-O4	2.06	1.67	1.59
6	A	602	PX4	P1-O4	2.04	1.67	1.59
6	I	603	PX4	P1-O4	2.03	1.67	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	603	PX4	O7-C23-C24	4.49	121.19	111.50
6	A	602	PX4	O7-C23-C24	4.05	120.24	111.50
6	H	101	PX4	O7-C23-C24	3.90	119.90	111.50
6	A	603	PX4	O7-C23-C24	3.81	119.72	111.50
6	E	602	PX4	O7-C23-C24	3.81	119.71	111.50
6	I	602	PX4	O7-C23-C24	3.67	119.41	111.50
6	A	602	PX4	O5-C9-C10	2.71	120.41	111.91
6	A	603	PX4	O5-C9-C10	2.64	120.18	111.91
6	I	603	PX4	O5-C9-C10	2.61	120.08	111.91
6	E	602	PX4	O5-C9-C10	2.60	120.07	111.91
6	H	101	PX4	O5-C9-C10	2.56	119.94	111.91
6	I	602	PX4	O5-C9-C10	2.51	119.77	111.91

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	603	PX4	O8-C23-O7-C7
6	I	603	PX4	C24-C23-O7-C7
6	H	101	PX4	C1-O3-P1-O1
6	A	603	PX4	C1-O3-P1-O1
7	I	604	BOG	O5-C1-O1-C1'
6	A	602	PX4	C6-O4-P1-O1
6	A	602	PX4	O8-C23-O7-C7
6	A	602	PX4	C24-C23-O7-C7
7	A	604	BOG	O5-C1-O1-C1'
6	E	602	PX4	C1-O3-P1-O1
6	E	602	PX4	C1-O3-P1-O2
6	E	602	PX4	C6-O4-P1-O3
6	A	602	PX4	O6-C9-O5-C8
6	H	101	PX4	O8-C23-O7-C7
6	H	101	PX4	C24-C23-O7-C7

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Mol	Chain	Res	Type	Atoms
6	A	602	PX4	C10-C9-O5-C8
7	I	604	BOG	O5-C5-C6-O6
7	I	604	BOG	C4-C5-C6-O6
6	E	602	PX4	C9-C10-C11-C12
6	A	603	PX4	C9-C10-C11-C12
6	I	603	PX4	C23-C24-C25-C26
6	A	603	PX4	C24-C23-O7-C7
6	H	101	PX4	C6-O4-P1-O3
6	A	602	PX4	C6-O4-P1-O3
6	A	603	PX4	O8-C23-O7-C7
6	A	603	PX4	C11-C12-C13-C14
6	A	602	PX4	C10-C11-C12-C13
6	E	602	PX4	C11-C12-C13-C14
6	H	101	PX4	C1-O3-P1-O2
6	A	603	PX4	C1-O3-P1-O2
6	H	101	PX4	C24-C25-C26-C27
6	I	603	PX4	C12-C13-C14-C15
6	H	101	PX4	C27-C28-C29-C30
6	I	602	PX4	C9-C10-C11-C12
6	I	603	PX4	C10-C11-C12-C13
6	A	603	PX4	C27-C28-C29-C30
6	I	602	PX4	C25-C26-C27-C28
6	H	101	PX4	C31-C32-C33-C34
6	H	101	PX4	C10-C11-C12-C13
6	A	602	PX4	C17-C18-C19-C20
6	A	602	PX4	C29-C30-C31-C32
7	A	604	BOG	C3'-C4'-C5'-C6'
6	E	602	PX4	C10-C9-O5-C8
7	E	603	BOG	C1'-C2'-C3'-C4'
6	E	602	PX4	O6-C9-O5-C8
6	H	101	PX4	C29-C30-C31-C32
6	I	603	PX4	C25-C26-C27-C28
6	A	602	PX4	C14-C15-C16-C17
7	E	603	BOG	O5-C1-O1-C1'
6	H	101	PX4	C25-C26-C27-C28
6	H	101	PX4	C32-C33-C34-C35
6	A	602	PX4	C18-C19-C20-C21
6	E	602	PX4	O7-C7-C8-O5
6	A	602	PX4	C1-O3-P1-O2
6	E	602	PX4	C23-C24-C25-C26
6	A	603	PX4	C25-C26-C27-C28
6	E	602	PX4	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
7	A	604	BOG	C2'-C1'-O1-C1
7	B	701	BOG	C3'-C4'-C5'-C6'
6	A	603	PX4	C10-C9-O5-C8
6	I	602	PX4	C26-C27-C28-C29
6	A	602	PX4	C25-C26-C27-C28
6	A	602	PX4	C26-C27-C28-C29
6	A	602	PX4	C24-C25-C26-C27
6	A	603	PX4	C6-C7-C8-O5
6	A	603	PX4	O6-C9-O5-C8
6	A	602	PX4	C27-C28-C29-C30
6	H	101	PX4	C6-O4-P1-O2
6	E	602	PX4	C6-O4-P1-O1
6	I	602	PX4	C32-C33-C34-C35
6	A	602	PX4	C11-C12-C13-C14
6	E	602	PX4	C6-C7-C8-O5
6	A	603	PX4	O7-C7-C8-O5
6	I	603	PX4	C11-C12-C13-C14
6	A	602	PX4	C31-C32-C33-C34
6	I	603	PX4	C6-C7-O7-C23
6	I	602	PX4	C7-C6-O4-P1
6	A	602	PX4	C7-C6-O4-P1
6	I	602	PX4	C16-C17-C18-C19
6	I	603	PX4	C6-O4-P1-O3
6	A	603	PX4	C6-O4-P1-O3
7	E	603	BOG	C3'-C4'-C5'-C6'
6	I	603	PX4	C13-C14-C15-C16
6	A	602	PX4	C28-C29-C30-C31
6	I	603	PX4	O7-C7-C8-O5
6	E	602	PX4	C1-O3-P1-O4
6	I	602	PX4	C1-O3-P1-O1
6	A	603	PX4	C24-C25-C26-C27
6	A	603	PX4	C6-C7-O7-C23
6	A	603	PX4	C8-C7-O7-C23
6	A	602	PX4	C30-C31-C32-C33
6	A	603	PX4	C17-C18-C19-C20
6	I	603	PX4	O7-C23-C24-C25
6	I	602	PX4	C28-C29-C30-C31
6	E	602	PX4	C14-C15-C16-C17
6	E	602	PX4	C24-C25-C26-C27
6	H	101	PX4	O7-C23-C24-C25
6	I	603	PX4	C6-C7-C8-O5
6	A	603	PX4	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
6	E	602	PX4	C17-C18-C19-C20
6	H	101	PX4	C11-C10-C9-O5
6	H	101	PX4	O7-C7-C8-O5
6	I	603	PX4	C18-C19-C20-C21
7	I	604	BOG	C4'-C5'-C6'-C7'
6	H	101	PX4	O8-C23-C24-C25
6	A	602	PX4	C13-C14-C15-C16
6	H	101	PX4	C11-C10-C9-O6
6	E	602	PX4	C25-C26-C27-C28
6	H	101	PX4	C14-C15-C16-C17
6	I	603	PX4	C26-C27-C28-C29

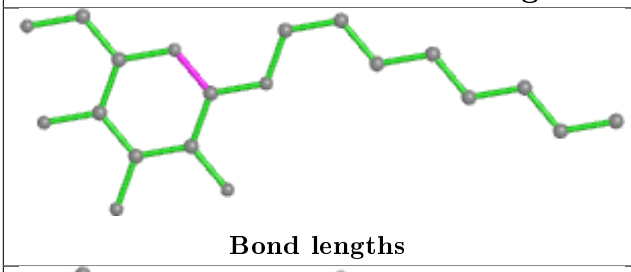
There are no ring outliers.

6 monomers are involved in 7 short contacts:

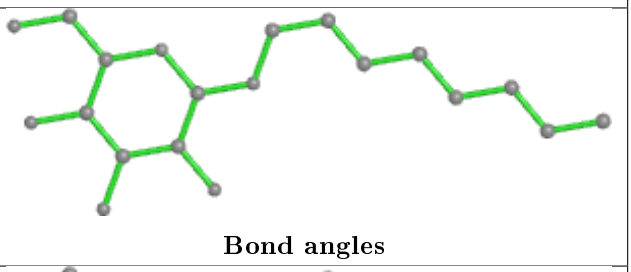
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	603	BOG	1	0
6	I	603	PX4	2	0
6	I	602	PX4	1	0
7	I	604	BOG	1	0
6	A	602	PX4	1	0
6	E	602	PX4	1	0

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 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.

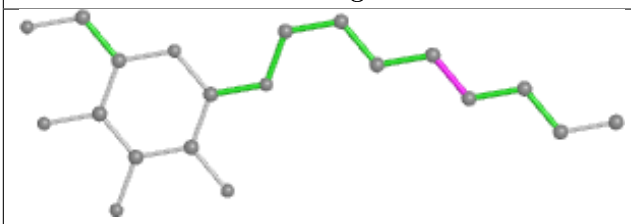
Ligand BOG B 701



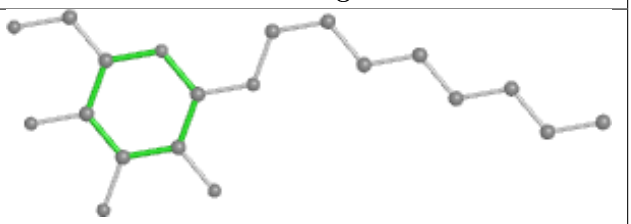
Bond lengths



Bond angles

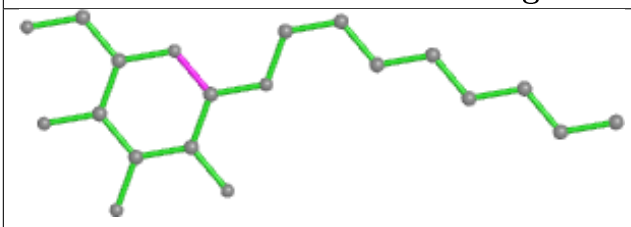


Torsions



Rings

Ligand BOG E 603



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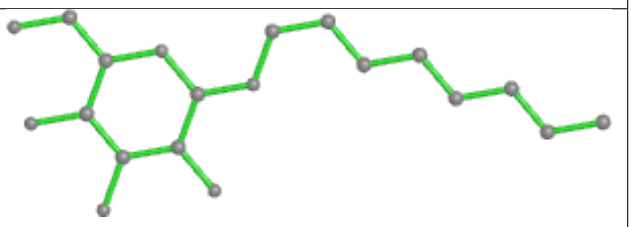
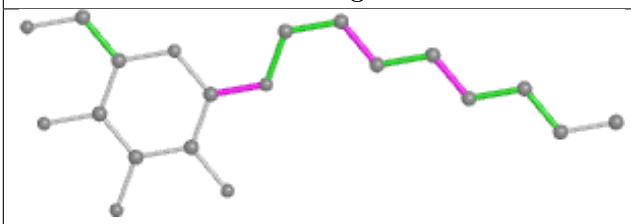
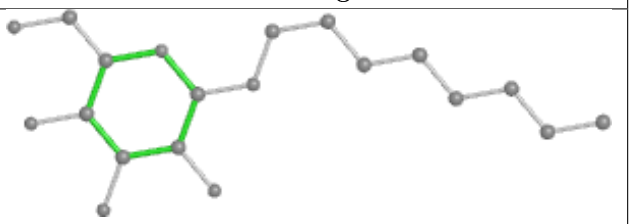


Bond angles

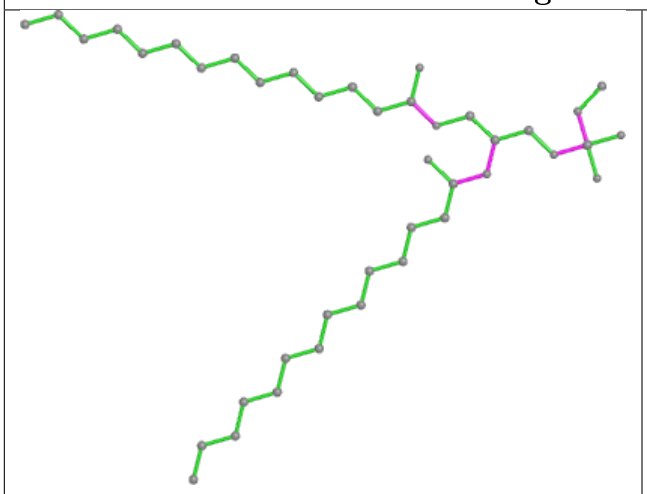


Torsions

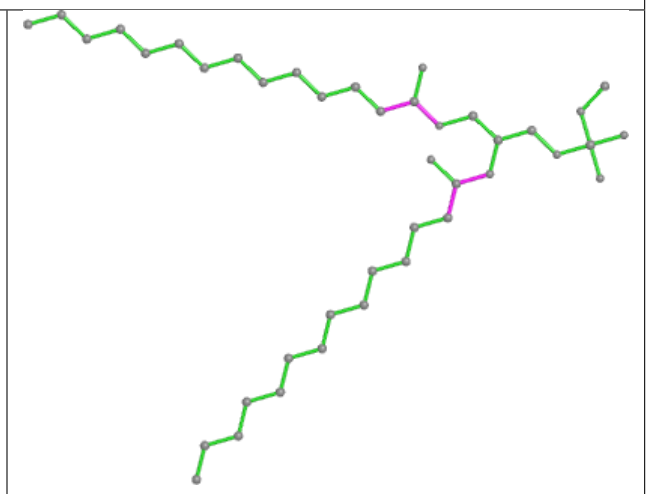


Rings

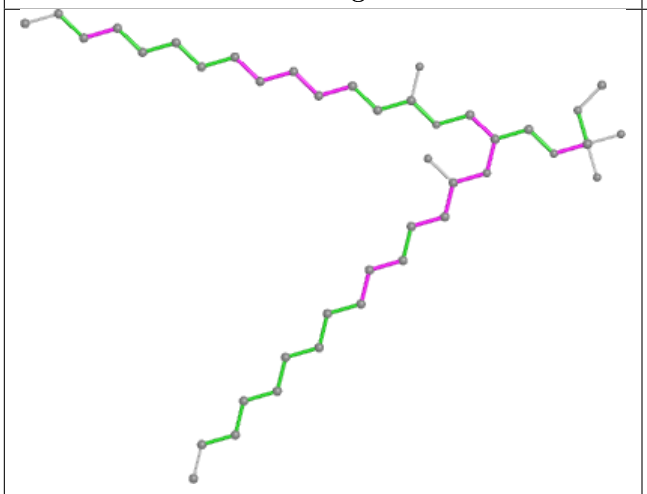
Ligand PX4 I 603



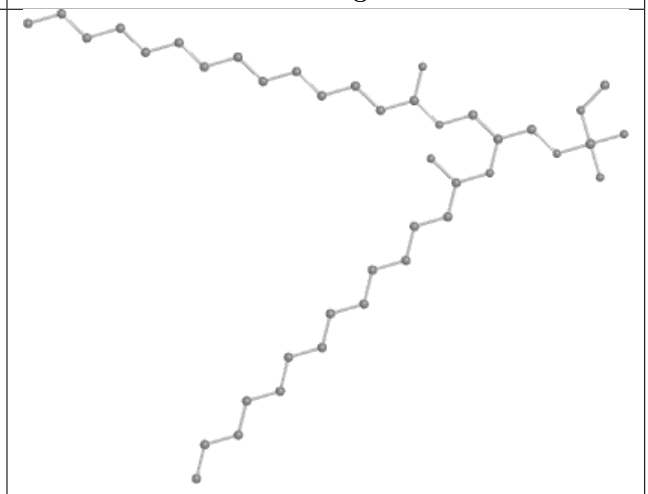
Bond lengths



Bond angles

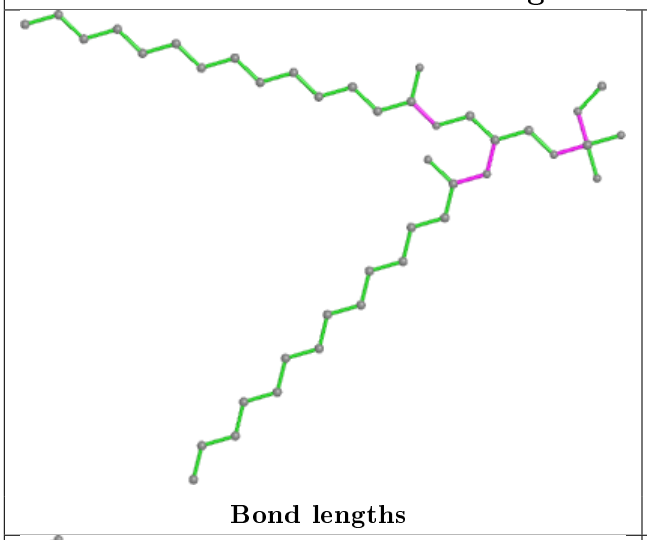


Torsions

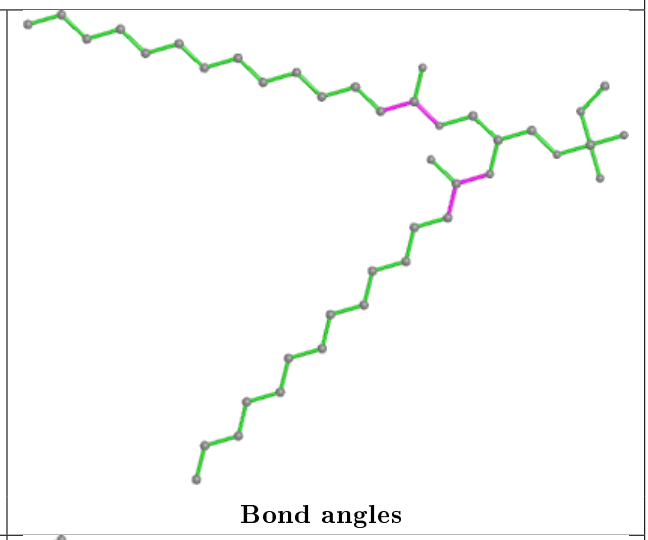


Rings

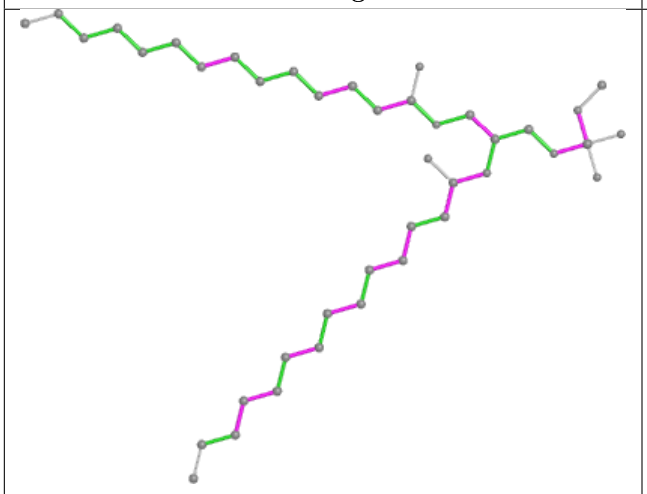
Ligand PX4 H 101



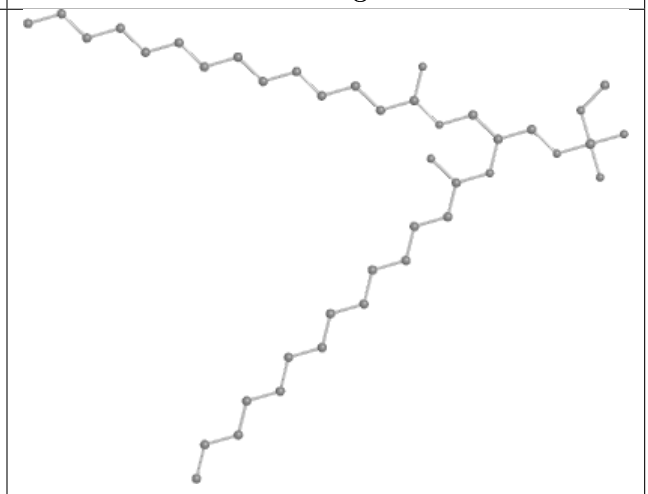
Bond lengths



Bond angles

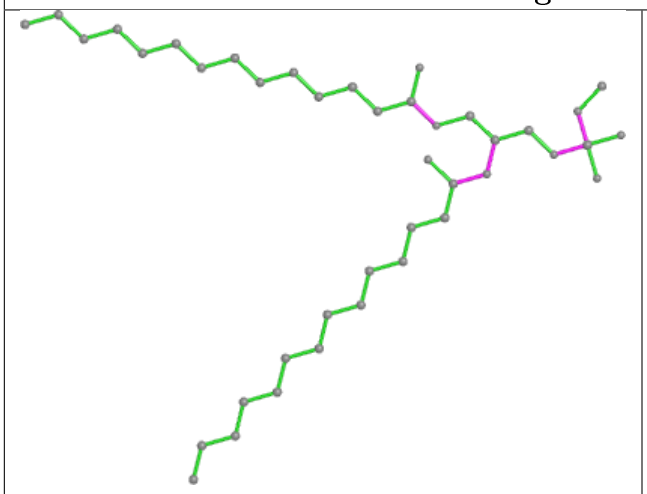


Torsions

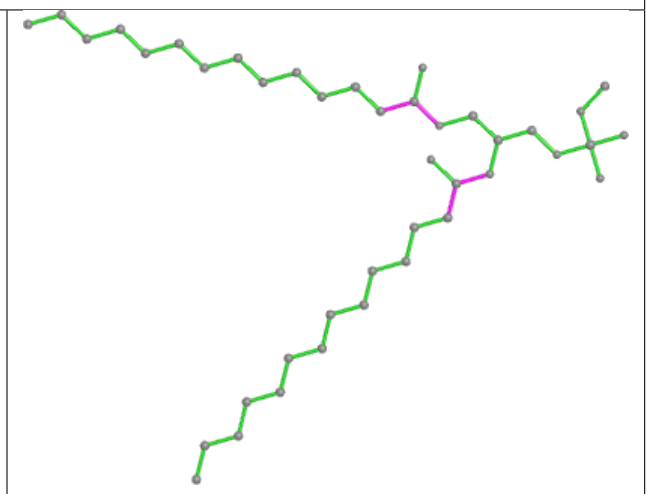


Rings

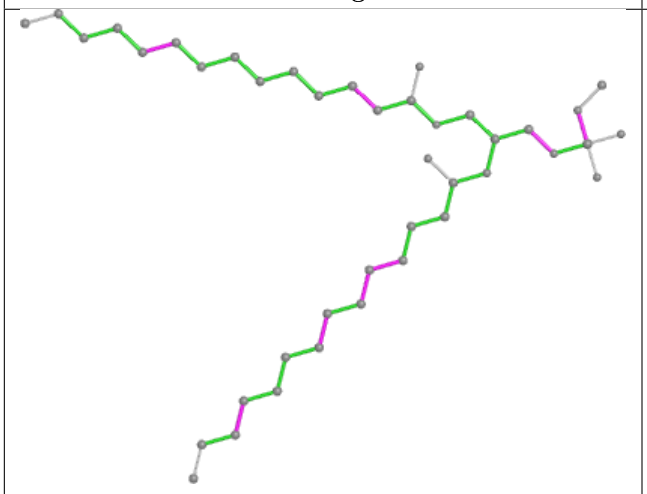
Ligand PX4 I 602



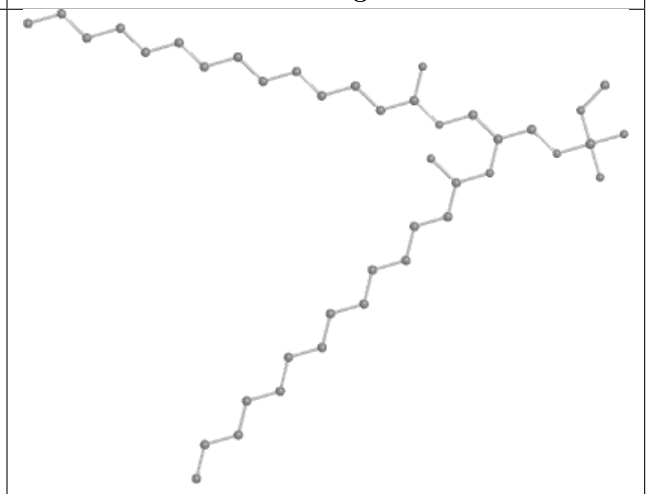
Bond lengths



Bond angles

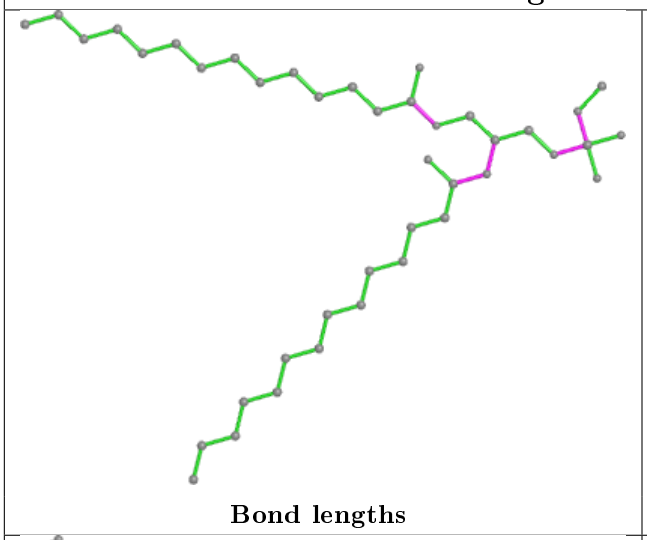


Torsions

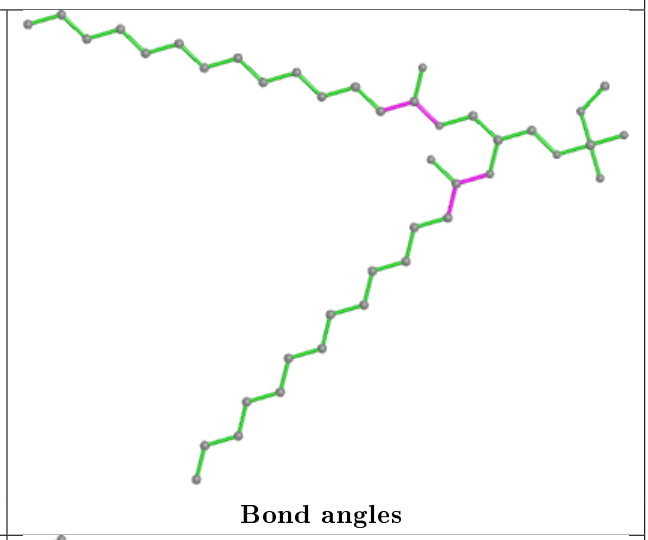


Rings

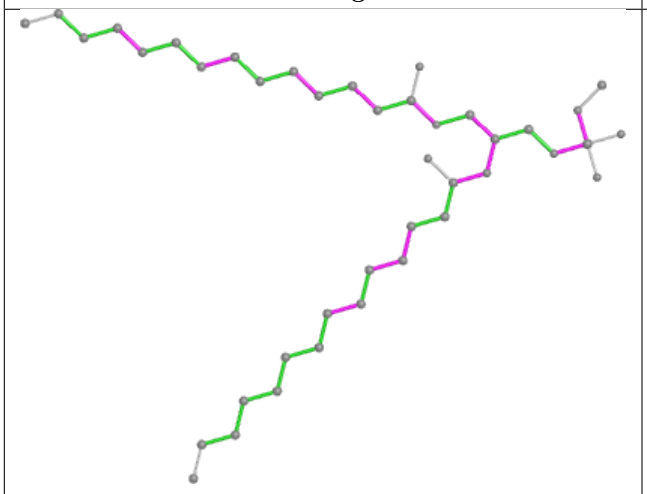
Ligand PX4 A 603



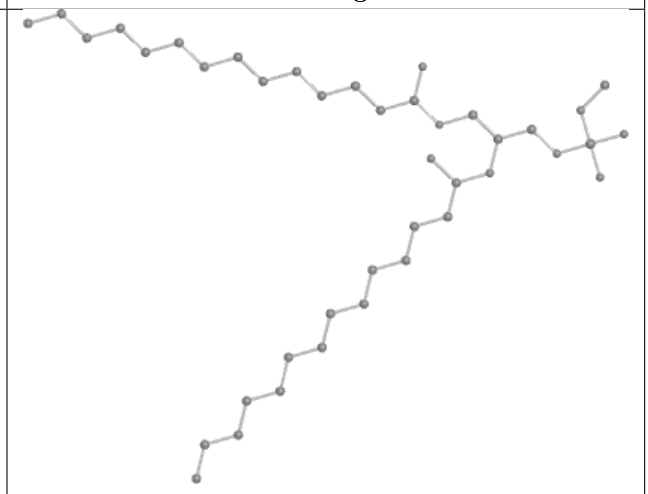
Bond lengths



Bond angles

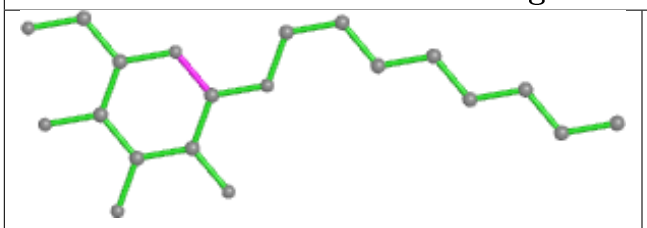


Torsions

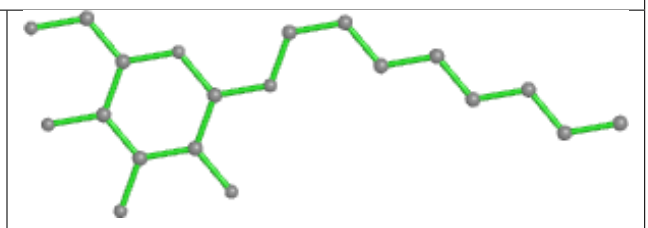


Rings

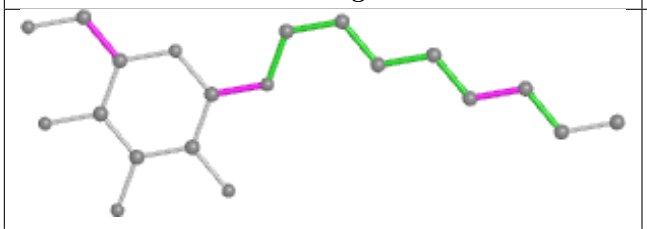
Ligand BOG I 604



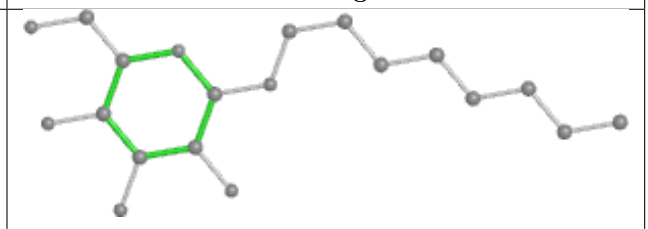
Bond lengths



Bond angles

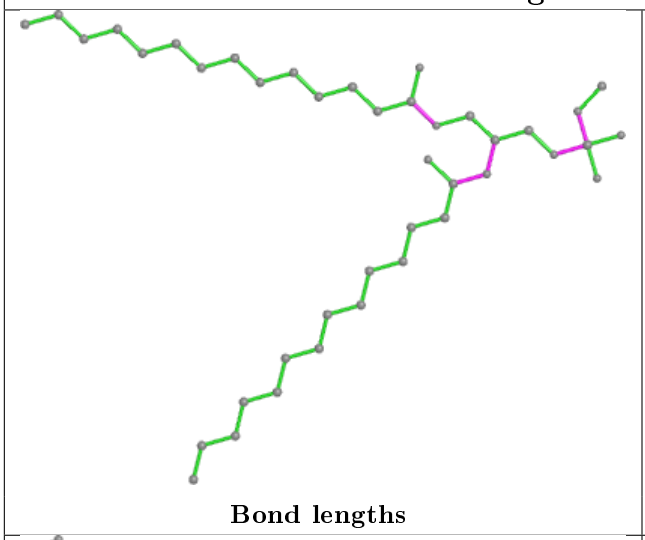


Torsions

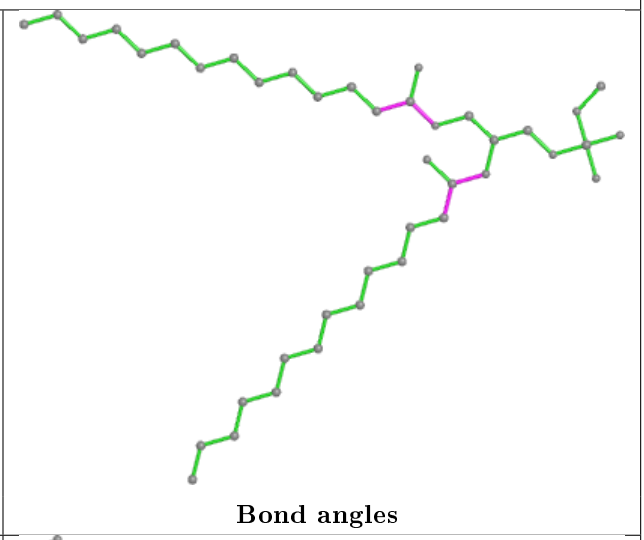


Rings

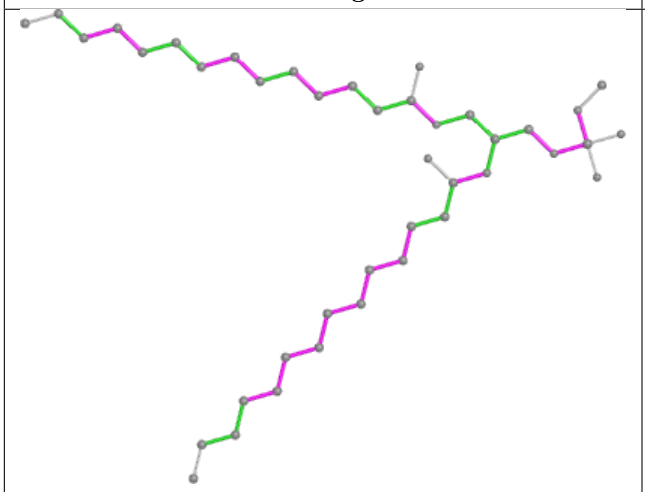
Ligand PX4 A 602



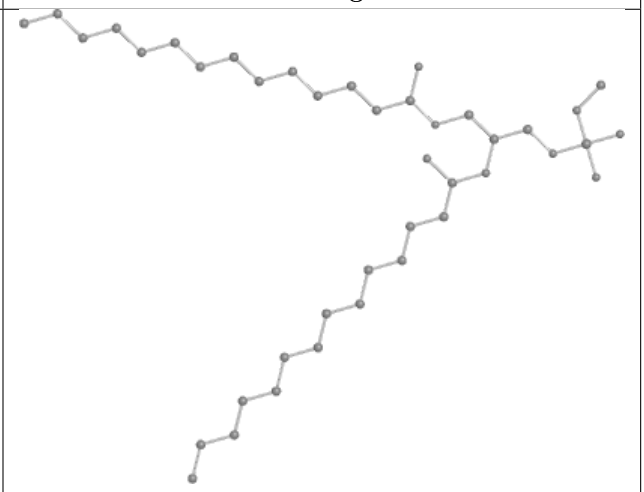
Bond lengths



Bond angles

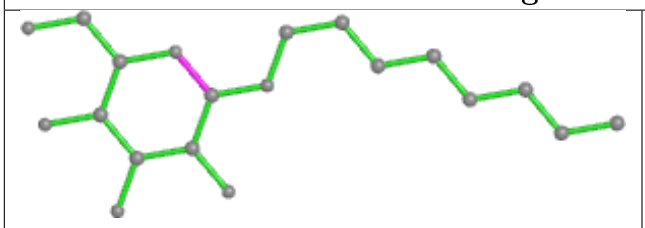


Torsions

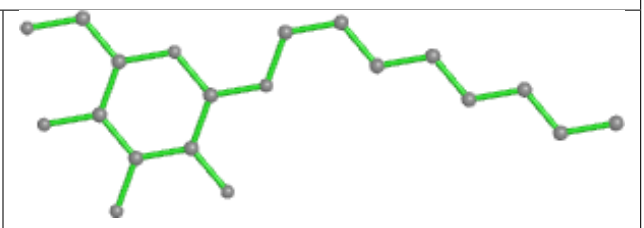


Rings

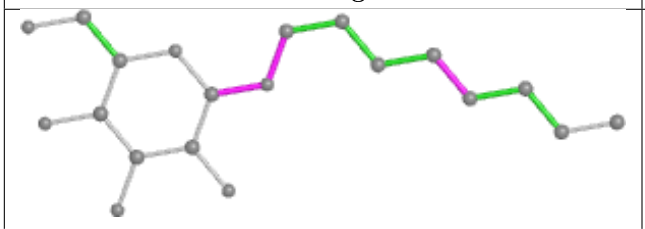
Ligand BOG A 604



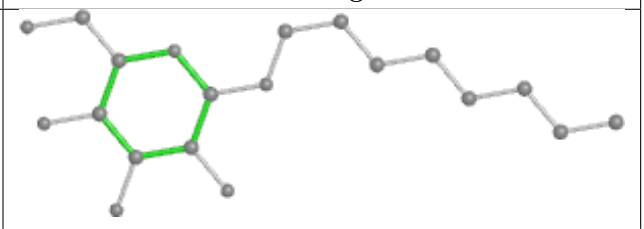
Bond lengths



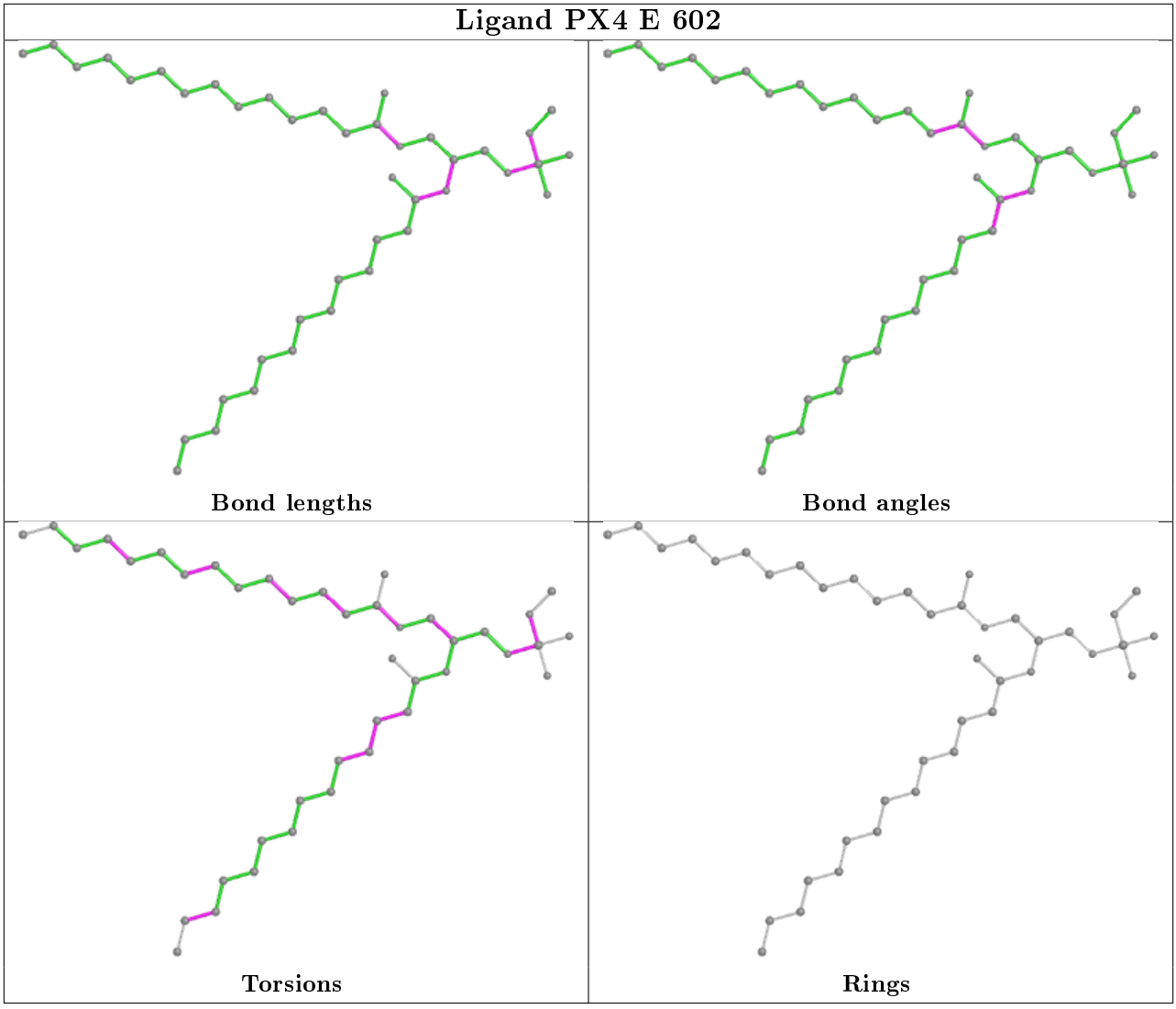
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	557/557 (100%)	0.53	58 (10%) 6 5	84, 115, 153, 208	0
1	E	557/557 (100%)	0.43	43 (7%) 13 10	83, 116, 151, 232	0
1	I	557/557 (100%)	0.54	56 (10%) 7 5	92, 121, 160, 225	0
2	B	673/674 (99%)	0.71	95 (14%) 2 2	107, 152, 241, 371	0
2	F	673/674 (99%)	0.99	143 (21%) 0 0	108, 162, 253, 364	0
2	J	673/674 (99%)	1.39	188 (27%) 0 0	117, 184, 310, 484	0
3	C	187/187 (100%)	0.37	9 (4%) 30 27	102, 128, 169, 226	0
3	G	187/187 (100%)	0.40	17 (9%) 9 6	109, 134, 184, 250	0
3	K	187/187 (100%)	0.36	15 (8%) 12 9	103, 134, 191, 267	0
4	D	27/27 (100%)	0.21	2 (7%) 14 11	122, 149, 186, 203	0
4	H	27/27 (100%)	-0.02	2 (7%) 14 11	118, 143, 187, 212	0
4	L	27/27 (100%)	0.43	4 (14%) 2 1	132, 158, 231, 255	0
All	All	4332/4335 (99%)	0.73	632 (14%) 2 1	83, 138, 246, 484	0

All (632) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	388	ILE	11.9
2	B	539	THR	11.4
2	J	12	THR	11.2
2	J	388	ILE	11.1
2	J	103	THR	11.1
2	J	120	LYS	10.6
2	J	60	GLY	10.1
2	J	106	ALA	10.0
2	J	389	ASP	9.9
2	J	97	LEU	9.7
2	J	121	VAL	9.5

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Mol	Chain	Res	Type	RSRZ
2	B	540	GLN	9.3
2	J	112	PRO	9.3
2	B	543	LYS	9.0
2	J	126	LEU	8.8
2	J	391	ARG	8.6
2	B	388	ILE	8.5
2	J	390	ASN	8.5
2	J	392	MET	8.1
2	J	433	VAL	8.0
2	F	465	ILE	8.0
2	J	16	GLN	7.9
2	F	539	THR	7.9
2	J	408	ASN	7.8
2	F	390	ASN	7.7
2	F	105	PHE	7.6
2	J	113	LYS	7.6
2	F	416	VAL	7.5
2	J	9	PHE	7.4
2	J	58	MET	7.3
2	J	488	ASP	7.3
2	B	439	VAL	7.3
2	J	119	ASP	7.3
2	B	436	GLY	7.2
2	J	435	GLU	7.2
2	J	141	PRO	7.1
2	J	189	ILE	7.1
2	B	538	GLY	7.1
2	F	131	ILE	7.0
2	J	131	ILE	7.0
2	J	100	VAL	7.0
2	J	59	PRO	7.0
2	J	10	GLU	6.8
2	F	374	PHE	6.8
2	J	203	MET	6.7
2	B	411	HIS	6.7
2	F	391	ARG	6.7
2	F	433	VAL	6.6
2	J	436	GLY	6.6
2	F	325	ALA	6.5
2	B	437	SER	6.4
2	J	476	LEU	6.4
2	J	122	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
2	B	432	VAL	6.3
2	B	99	GLY	6.2
1	E	469	SER	6.2
2	J	164	PRO	6.2
2	J	543	LYS	6.2
2	J	372	ALA	6.1
2	B	102	LYS	6.0
2	F	392	MET	6.0
2	F	543	LYS	6.0
2	F	394	ARG	6.0
2	J	163	ALA	5.9
2	J	145	GLU	5.9
2	J	202	ARG	5.9
2	B	544	GLU	5.8
2	B	58	MET	5.8
2	F	411	HIS	5.8
2	F	324	PRO	5.8
2	J	182	ILE	5.8
1	A	424	THR	5.8
2	J	183	LEU	5.7
2	J	13	LEU	5.7
2	B	374	PHE	5.7
2	J	105	PHE	5.7
2	J	371	HIS	5.7
2	F	466	LYS	5.7
2	J	439	VAL	5.6
2	F	407	ALA	5.6
2	F	439	VAL	5.6
2	J	181	ARG	5.5
1	A	176	TRP	5.5
2	B	110	ARG	5.5
2	B	101	LYS	5.5
2	B	390	ASN	5.4
2	B	100	VAL	5.3
2	J	393	ILE	5.3
2	F	208	GLU	5.3
2	J	132	VAL	5.2
2	F	442	VAL	5.2
1	E	424	THR	5.2
2	F	12	THR	5.2
2	F	386	ILE	5.2
2	B	435	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	679	CYS	5.1
2	J	123	ALA	5.1
2	F	409	GLY	5.1
1	I	468	GLY	5.0
2	B	114	TYR	5.0
2	F	408	ASN	5.0
2	F	538	GLY	5.0
2	J	429	THR	5.0
2	J	434	VAL	5.0
2	F	28	GLN	4.9
2	F	211	GLN	4.9
1	I	424	THR	4.9
2	J	153	VAL	4.9
2	B	324	PRO	4.9
1	I	470	ALA	4.8
2	B	210	ALA	4.8
2	J	104	ALA	4.8
2	F	373	THR	4.8
1	A	89	LEU	4.8
2	F	380	GLN	4.8
2	J	176	VAL	4.8
1	I	401	THR	4.8
1	A	36	LEU	4.8
2	J	325	ALA	4.8
1	I	232	GLY	4.8
2	J	111	GLU	4.8
2	F	387	ASN	4.8
2	J	118	ALA	4.8
2	F	440	LEU	4.7
1	I	113	THR	4.7
2	J	98	LYS	4.7
1	E	468	GLY	4.7
2	F	114	TYR	4.7
2	F	681	LEU	4.7
2	B	434	VAL	4.7
2	B	103	THR	4.6
2	F	112	PRO	4.6
1	E	53	SER	4.6
2	F	419	LYS	4.6
2	B	377	PHE	4.6
2	J	192	SER	4.5
2	J	442	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	F	126	LEU	4.5
2	F	97	LEU	4.5
2	F	406	GLU	4.5
2	J	441	GLY	4.5
2	F	678	VAL	4.5
2	B	9	PHE	4.5
2	B	375	VAL	4.5
2	J	115	GLY	4.4
2	F	434	VAL	4.4
2	J	127	ARG	4.4
2	J	191	CYS	4.4
2	J	424	ALA	4.4
1	I	239	ASN	4.4
2	B	211	GLN	4.4
2	J	207	VAL	4.4
2	J	416	VAL	4.4
2	B	542	ALA	4.3
2	J	140	ILE	4.3
2	F	328	VAL	4.3
2	F	326	GLN	4.3
2	B	92	ALA	4.3
2	B	325	ALA	4.3
1	I	86	TYR	4.3
2	F	101	LYS	4.3
2	J	199	PHE	4.3
2	F	191	CYS	4.2
2	B	389	ASP	4.2
2	J	114	TYR	4.2
2	B	416	VAL	4.2
2	F	202	ARG	4.2
2	J	374	PHE	4.2
1	I	469	SER	4.2
2	F	460	LEU	4.1
2	J	444	ALA	4.1
2	J	125	GLN	4.1
2	F	303	VAL	4.1
1	A	369	GLY	4.1
1	I	539	GLY	4.1
2	F	104	ALA	4.1
2	F	199	PHE	4.1
2	B	392	MET	4.1
2	J	404	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	441	GLY	4.1
1	E	470	ALA	4.0
2	F	437	SER	4.0
2	J	324	PRO	4.0
2	J	618	LEU	4.0
2	J	101	LYS	4.0
2	F	666	PHE	4.0
2	J	440	LEU	4.0
1	A	382	GLY	4.0
1	I	114	ASN	4.0
1	I	343	SER	4.0
2	F	630	PHE	4.0
1	I	89	LEU	3.9
2	B	391	ARG	3.9
2	J	117	ALA	3.9
2	B	98	LYS	3.9
1	A	468	GLY	3.9
2	J	48	CYS	3.9
2	F	16	GLN	3.9
2	F	360	PHE	3.9
2	J	681	LEU	3.9
2	J	329	ASP	3.9
1	I	87	LEU	3.9
1	A	39	THR	3.9
1	A	113	THR	3.9
2	J	130	ASP	3.8
3	C	116	VAL	3.8
2	J	142	CYS	3.8
2	B	97	LEU	3.8
2	J	487	VAL	3.8
2	F	675	LEU	3.8
1	A	466	ASN	3.8
2	F	63	LEU	3.8
2	J	139	ILE	3.8
2	J	373	THR	3.8
2	J	468	VAL	3.8
2	B	326	GLN	3.8
1	E	240	SER	3.8
2	J	542	ALA	3.8
2	F	203	MET	3.8
2	J	336	ALA	3.8
2	J	443	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	425	PRO	3.7
1	I	234	GLY	3.7
2	J	490	PHE	3.7
1	A	469	SER	3.7
2	F	506	TYR	3.7
2	J	457	PHE	3.7
2	B	438	ARG	3.7
2	B	60	GLY	3.7
1	I	240	SER	3.7
1	I	83	GLY	3.6
2	F	389	ASP	3.6
2	J	53	MET	3.6
2	J	539	THR	3.6
2	J	370	LEU	3.6
2	J	438	ARG	3.6
2	F	119	ASP	3.6
2	J	133	LEU	3.6
2	J	538	GLY	3.6
2	B	415	ASP	3.6
2	J	240	TRP	3.6
2	J	426	GLN	3.6
2	F	304	LEU	3.6
2	F	306	LEU	3.6
3	G	188	LEU	3.6
2	F	393	ILE	3.6
2	J	193	VAL	3.5
2	J	491	LEU	3.5
2	J	108	LYS	3.5
1	E	233	GLY	3.5
1	I	176	TRP	3.5
2	J	107	ARG	3.5
2	J	446	LYS	3.5
1	A	175	LEU	3.5
2	B	549	VAL	3.5
2	B	431	LEU	3.5
2	J	96	SER	3.5
2	F	124	ASP	3.5
3	C	47	ASP	3.5
3	G	155	LEU	3.5
2	J	425	ARG	3.5
2	F	108	LYS	3.4
1	A	428	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	466	ASN	3.4
2	F	540	GLN	3.4
2	J	332	THR	3.4
2	J	405	VAL	3.4
2	B	545	ALA	3.4
2	B	209	GLY	3.4
2	J	630	PHE	3.4
2	B	430	PRO	3.4
2	F	509	GLU	3.4
2	B	112	PRO	3.4
2	J	94	ALA	3.4
2	F	113	LYS	3.3
1	I	203	ALA	3.3
3	K	158	LEU	3.3
3	K	188	LEU	3.3
2	B	105	PHE	3.3
1	A	461	SER	3.3
2	F	383	MET	3.3
2	F	120	LYS	3.3
2	F	13	LEU	3.3
3	K	154	GLN	3.3
1	A	459	ALA	3.3
1	I	93	GLN	3.3
2	J	200	LEU	3.3
2	F	9	PHE	3.3
2	J	369	SER	3.3
3	G	154	GLN	3.3
1	A	367	GLN	3.3
2	J	78	PHE	3.3
2	B	386	ILE	3.3
2	F	463	MET	3.3
4	L	3	ALA	3.2
2	F	327	GLY	3.2
1	E	461	SER	3.2
2	J	194	ASN	3.2
1	I	369	GLY	3.2
1	A	538	VAL	3.2
2	J	116	ALA	3.2
2	J	109	LEU	3.2
2	B	426	GLN	3.2
3	G	185	LEU	3.2
3	K	50	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	433	VAL	3.2
2	F	432	VAL	3.2
2	F	546	GLY	3.2
2	B	394	ARG	3.2
2	B	425	ARG	3.2
2	B	199	PHE	3.2
2	J	136	ALA	3.1
2	F	60	GLY	3.1
2	J	175	SER	3.1
2	B	412	PHE	3.1
1	E	428	VAL	3.1
1	E	459	ALA	3.1
2	J	420	VAL	3.1
1	A	379	GLY	3.1
2	J	489	ASP	3.1
1	A	343	SER	3.1
1	A	370	GLU	3.1
1	I	233	GLY	3.1
1	E	341	ALA	3.1
2	B	63	LEU	3.1
3	K	4	LEU	3.1
1	E	342	ALA	3.1
2	F	200	LEU	3.1
2	F	457	PHE	3.1
1	A	470	ALA	3.0
2	F	100	VAL	3.0
2	J	445	LEU	3.0
3	C	167	LEU	3.0
1	I	85	HIS	3.0
1	A	458	TYR	3.0
1	I	84	GLN	3.0
2	J	179	GLY	3.0
2	J	409	GLY	3.0
1	E	239	ASN	3.0
1	A	211	GLN	3.0
2	B	515	MET	3.0
2	B	387	ASN	3.0
4	L	7	THR	3.0
1	E	234	GLY	3.0
2	J	510	GLY	3.0
2	J	86	ALA	3.0
2	F	322	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	450	LYS	3.0
3	C	117	PRO	3.0
2	B	200	LEU	3.0
1	E	232	GLY	3.0
1	I	344	CYS	3.0
1	E	539	GLY	3.0
2	F	477	THR	3.0
3	K	55	ILE	3.0
2	B	95	ASN	2.9
2	J	331	LYS	2.9
1	A	423	VAL	2.9
1	A	37	PRO	2.9
1	A	539	GLY	2.9
2	F	467	THR	2.9
2	B	203	MET	2.9
1	E	458	TYR	2.9
2	J	20	GLU	2.9
2	F	667	ILE	2.9
1	I	39	THR	2.9
2	F	121	VAL	2.9
2	F	235	ALA	2.9
2	F	537	SER	2.9
2	B	111	GLU	2.9
2	F	502	LEU	2.9
2	F	122	PRO	2.8
2	B	51	ILE	2.8
2	F	435	GLU	2.8
2	J	134	VAL	2.8
2	B	59	PRO	2.8
2	B	208	GLU	2.8
2	F	420	VAL	2.8
2	J	128	LYS	2.8
1	I	341	ALA	2.8
2	F	128	LYS	2.8
2	J	138	ASP	2.8
1	I	392	PHE	2.8
2	J	64	PHE	2.8
2	F	186	TRP	2.8
4	D	27	GLU	2.8
2	F	96	SER	2.8
2	B	442	VAL	2.8
2	J	450	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	681	LEU	2.8
2	F	464	GLY	2.7
2	F	544	GLU	2.7
2	F	404	HIS	2.7
1	A	232	GLY	2.7
1	I	116	ARG	2.7
2	J	11	PRO	2.7
1	A	342	ALA	2.7
2	J	414	THR	2.7
3	G	183	LEU	2.7
1	I	207	VAL	2.7
2	F	618	LEU	2.7
2	F	170	GLY	2.7
2	F	196	GLY	2.7
2	J	190	GLU	2.7
2	J	427	GLY	2.7
2	J	486	GLY	2.7
2	F	511	ARG	2.7
3	K	155	LEU	2.7
1	A	366	MET	2.7
1	E	340	THR	2.7
2	J	323	ILE	2.7
2	F	193	VAL	2.7
3	K	45	GLU	2.7
2	F	127	ARG	2.7
1	A	114	ASN	2.7
3	K	185	LEU	2.7
2	B	288	ILE	2.7
1	I	175	LEU	2.7
1	I	467	ASN	2.7
2	J	177	THR	2.6
2	F	542	ALA	2.6
4	H	26	ALA	2.6
1	E	343	SER	2.6
1	E	460	VAL	2.6
1	A	533	GLY	2.6
2	B	485	ALA	2.6
2	B	490	PHE	2.6
1	A	378	SER	2.6
2	J	401	ILE	2.6
2	J	187	LEU	2.6
1	E	86	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	104	ALA	2.6
2	F	141	PRO	2.6
2	J	168	GLU	2.6
2	F	443	ILE	2.6
2	J	386	ILE	2.6
2	J	85	LEU	2.6
1	E	345	GLY	2.6
2	F	132	VAL	2.6
2	F	301	VAL	2.6
1	E	488	CYS	2.6
1	E	534	THR	2.6
1	I	423	VAL	2.6
2	F	461	ARG	2.6
2	J	682	VAL	2.6
2	F	110	ARG	2.6
3	C	5	ARG	2.6
2	J	253	THR	2.5
3	C	159	ILE	2.5
1	I	82	LEU	2.5
2	F	487	VAL	2.5
2	F	106	ALA	2.5
1	A	233	GLY	2.5
1	A	425	PRO	2.5
2	J	137	GLY	2.5
1	A	460	VAL	2.5
1	I	414	MET	2.5
2	J	544	GLU	2.5
1	I	368	ILE	2.5
2	B	420	VAL	2.5
3	G	156	THR	2.5
1	I	425	PRO	2.5
2	B	306	LEU	2.5
2	F	476	LEU	2.5
2	B	395	LYS	2.5
2	J	51	ILE	2.5
1	A	465	ASN	2.5
2	B	423	VAL	2.5
1	A	187	LEU	2.5
1	E	363	MET	2.4
3	G	83	GLY	2.4
1	A	462	SER	2.4
2	J	81	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	93	GLN	2.4
2	J	655	TRP	2.4
1	E	114	ASN	2.4
1	A	463	ALA	2.4
2	B	376	PRO	2.4
1	E	369	GLY	2.4
2	F	58	MET	2.4
1	E	113	THR	2.4
2	F	468	VAL	2.4
2	F	382	ARG	2.4
1	A	540	ALA	2.4
2	F	142	CYS	2.4
3	G	150	LEU	2.4
3	K	148	ARG	2.4
1	A	363	MET	2.4
1	E	462	SER	2.4
2	F	505	GLN	2.4
2	F	663	LEU	2.4
2	B	113	LYS	2.4
1	I	492	GLY	2.4
3	G	164	GLN	2.4
2	B	383	MET	2.4
1	I	490	PHE	2.4
2	F	209	GLY	2.4
2	J	328	VAL	2.4
2	F	302	ASP	2.4
2	F	473	ASP	2.4
2	J	143	ASP	2.4
4	D	1	MET	2.4
1	E	466	ASN	2.3
1	E	467	ASN	2.3
3	C	120	LEU	2.3
3	G	84	GLY	2.3
2	J	449	VAL	2.3
1	I	342	ALA	2.3
2	J	659	LEU	2.3
1	I	535	VAL	2.3
2	B	484	GLU	2.3
3	G	4	LEU	2.3
2	B	384	SER	2.3
1	I	395	GLY	2.3
2	F	368	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	16	LEU	2.3
1	A	534	THR	2.3
1	E	426	THR	2.3
3	G	63	GLY	2.3
1	E	167	TRP	2.3
1	I	538	VAL	2.3
2	J	421	ASP	2.3
1	E	427	LEU	2.3
2	J	99	GLY	2.3
2	J	135	GLU	2.3
2	B	487	VAL	2.3
4	H	14	LEU	2.3
1	A	374	GLY	2.3
2	F	150	GLY	2.3
2	J	166	ILE	2.3
2	F	102	LYS	2.3
2	F	405	VAL	2.3
2	J	248	ASN	2.3
3	K	33	TRP	2.3
1	A	385	LEU	2.3
2	J	631	LEU	2.3
1	A	112	ASN	2.2
1	E	339	THR	2.2
2	F	103	THR	2.2
1	A	341	ALA	2.2
2	J	63	LEU	2.2
2	J	195	PRO	2.2
1	A	381	TYR	2.2
2	F	125	GLN	2.2
2	J	146	VAL	2.2
2	B	679	CYS	2.2
1	I	374	GLY	2.2
1	A	115	TRP	2.2
2	B	131	ILE	2.2
2	J	422	GLN	2.2
1	A	535	VAL	2.2
1	I	238	ALA	2.2
2	J	620	ALA	2.2
1	A	536	LEU	2.2
2	F	314	LEU	2.2
2	J	467	THR	2.2
2	J	375	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	PHE	2.2
1	A	417	THR	2.2
2	B	28	GLN	2.2
1	I	382	GLY	2.2
2	B	212	ARG	2.2
2	J	578	PHE	2.2
2	J	423	VAL	2.2
2	B	48	CYS	2.2
2	B	408	ASN	2.2
2	F	189	ILE	2.2
2	J	17	ALA	2.2
2	J	57	ALA	2.2
3	G	65	PHE	2.2
1	A	383	MET	2.2
4	L	5	VAL	2.2
2	J	196	GLY	2.2
1	E	39	THR	2.2
2	J	452	GLY	2.1
1	I	225	ILE	2.1
4	L	1	MET	2.1
1	E	387	VAL	2.1
1	E	357	LEU	2.1
2	B	457	PHE	2.1
2	J	575	LEU	2.1
3	K	150	LEU	2.1
2	J	334	ALA	2.1
2	J	317	ARG	2.1
3	G	153	GLU	2.1
2	F	207	VAL	2.1
2	F	399	ASP	2.1
2	F	31	TRP	2.1
1	I	198	PHE	2.1
2	J	326	GLN	2.1
1	I	231	ASN	2.1
1	I	339	THR	2.1
2	J	92	ALA	2.1
3	G	117	PRO	2.1
2	F	371	HIS	2.1
2	J	394	ARG	2.1
1	I	370	GLU	2.1
2	B	675	LEU	2.1
2	J	61	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	149	ASN	2.1
2	J	475	ARG	2.1
1	I	115	TRP	2.1
3	G	33	TRP	2.1
1	A	429	LEU	2.1
1	I	126	TYR	2.1
3	K	51	GLY	2.1
1	E	116	ARG	2.1
3	K	152	VAL	2.1
3	C	139	TRP	2.1
2	F	378	THR	2.1
2	F	99	GLY	2.1
1	E	465	ASN	2.1
1	I	402	PRO	2.1
2	F	671	VAL	2.0
2	B	401	ILE	2.0
1	A	542	THR	2.0
1	E	344	CYS	2.0
1	A	386	PHE	2.0
1	A	467	ASN	2.0
2	J	32	ARG	2.0
1	I	108	SER	2.0
2	J	102	LYS	2.0
2	J	124	ASP	2.0
2	B	229	THR	2.0
1	E	414	MET	2.0
2	B	53	MET	2.0
2	J	314	LEU	2.0
2	B	419	LYS	2.0
2	F	179	GLY	2.0
2	F	236	THR	2.0
3	G	167	LEU	2.0
1	A	239	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	SEP	J	162	10/11	0.68	0.19	218,226,232,235	0
2	SEP	F	162	10/11	0.79	0.35	169,175,199,205	0
2	SEP	B	162	10/11	0.94	0.20	153,163,177,182	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

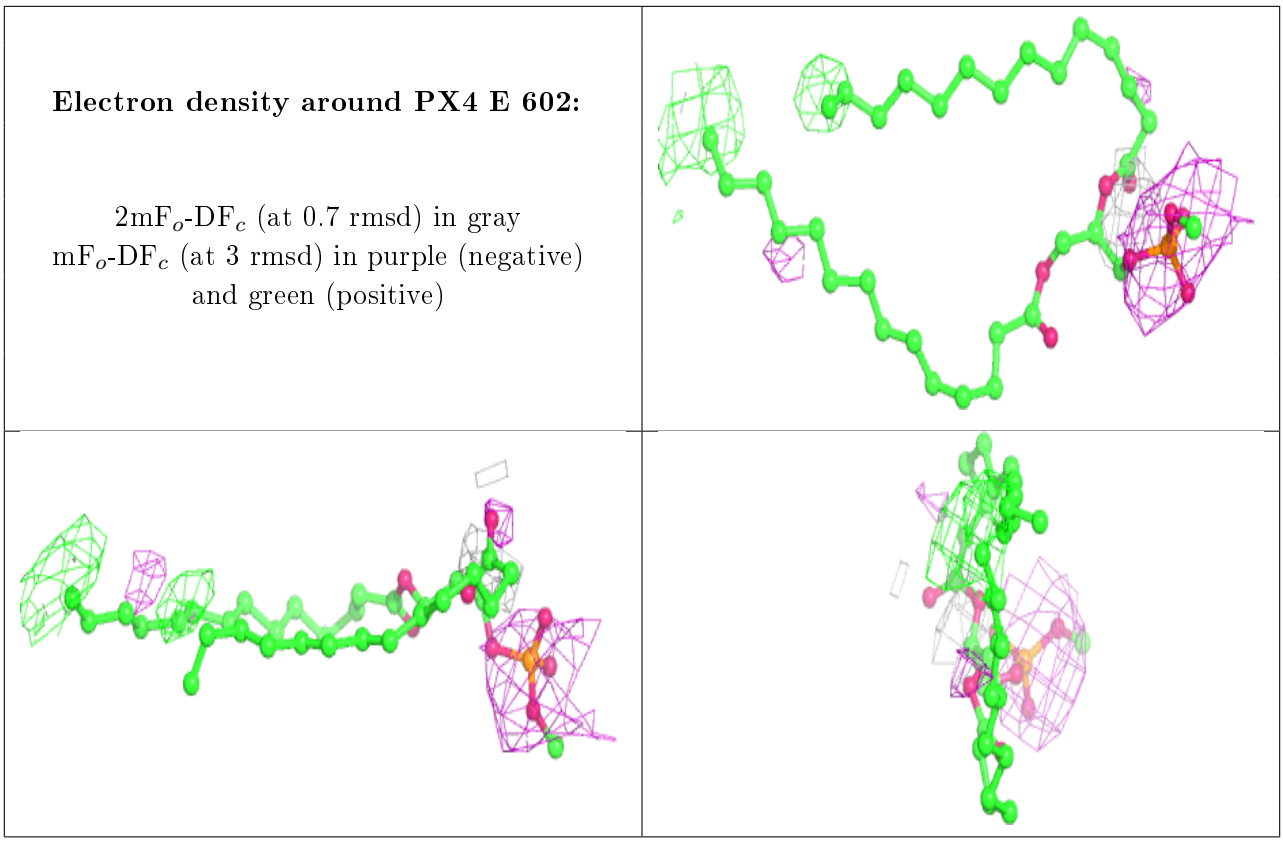
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	PX4	E	602	41/46	0.31	0.75	199,227,281,284	0
6	PX4	I	602	41/46	0.48	0.67	167,183,225,228	0
6	PX4	A	602	41/46	0.59	0.46	156,188,203,205	0
6	PX4	A	603	41/46	0.67	0.44	130,169,230,232	0
6	PX4	H	101	41/46	0.69	0.42	171,197,211,214	0
5	K	E	601	1/1	0.72	0.34	124,124,124,124	0
6	PX4	I	603	41/46	0.73	0.46	164,204,226,228	0
5	K	I	601	1/1	0.77	0.37	123,123,123,123	0
7	BOG	E	603	20/20	0.78	0.23	154,184,190,194	0
7	BOG	B	701	20/20	0.78	0.33	173,185,194,195	0
7	BOG	A	604	20/20	0.85	0.32	178,191,198,198	0
5	K	A	601	1/1	0.86	0.36	123,123,123,123	0
7	BOG	I	604	20/20	0.88	0.41	205,221,224,227	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.

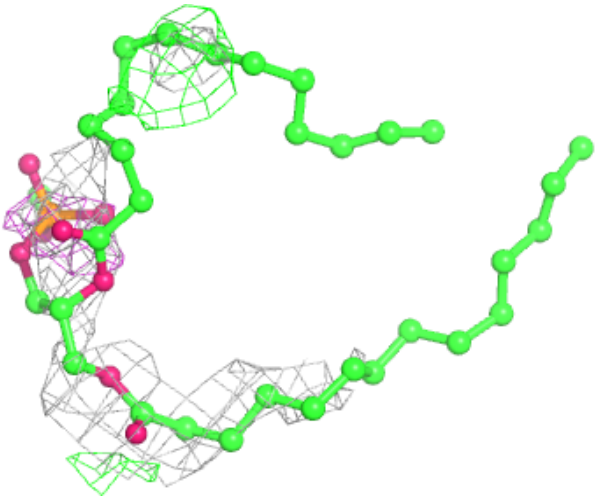
Electron density around PX4 E 602:

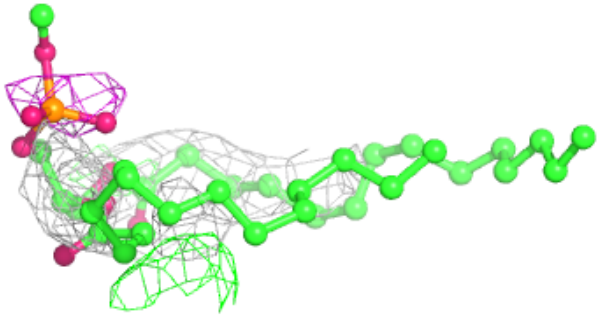
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

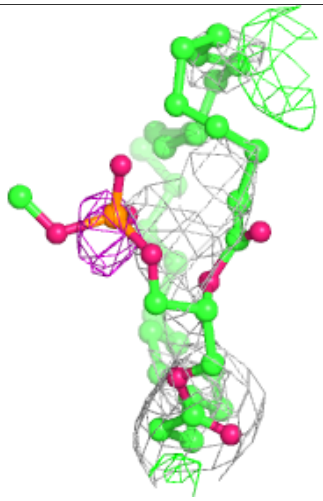


Electron density around PX4 I 602:

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

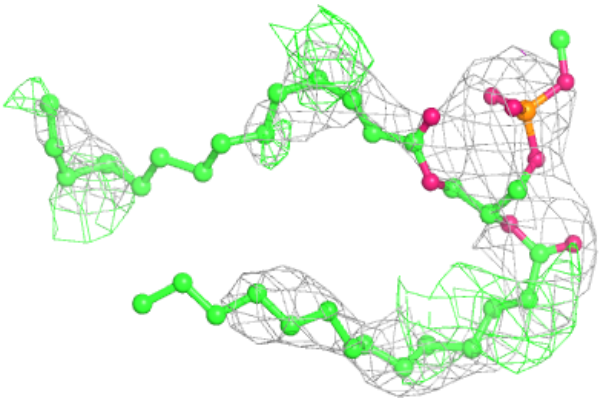


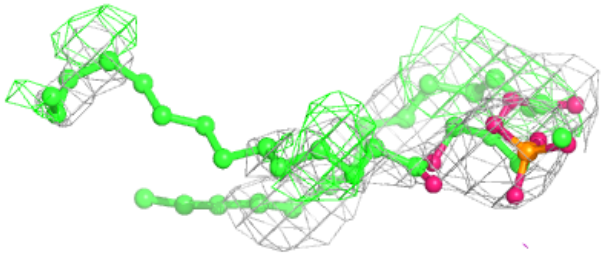


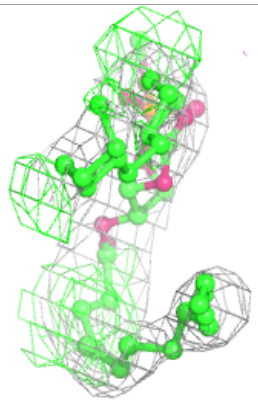


Electron density around PX4 A 602:

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

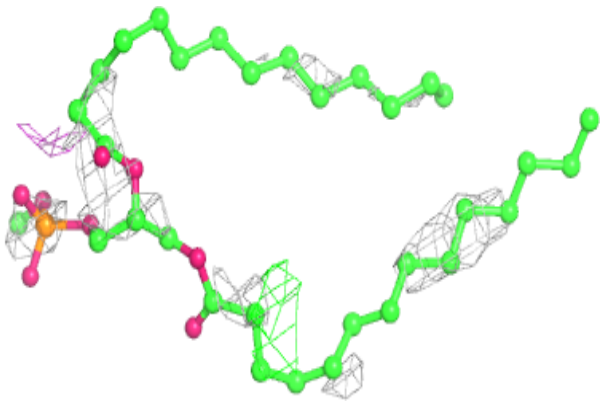


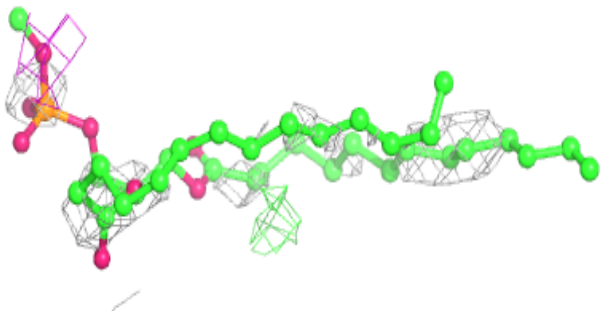


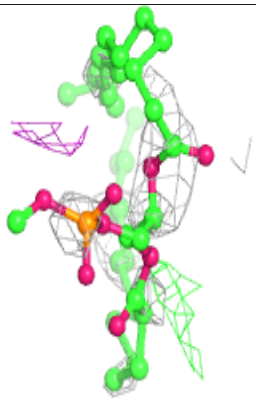


Electron density around PX4 A 603:

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

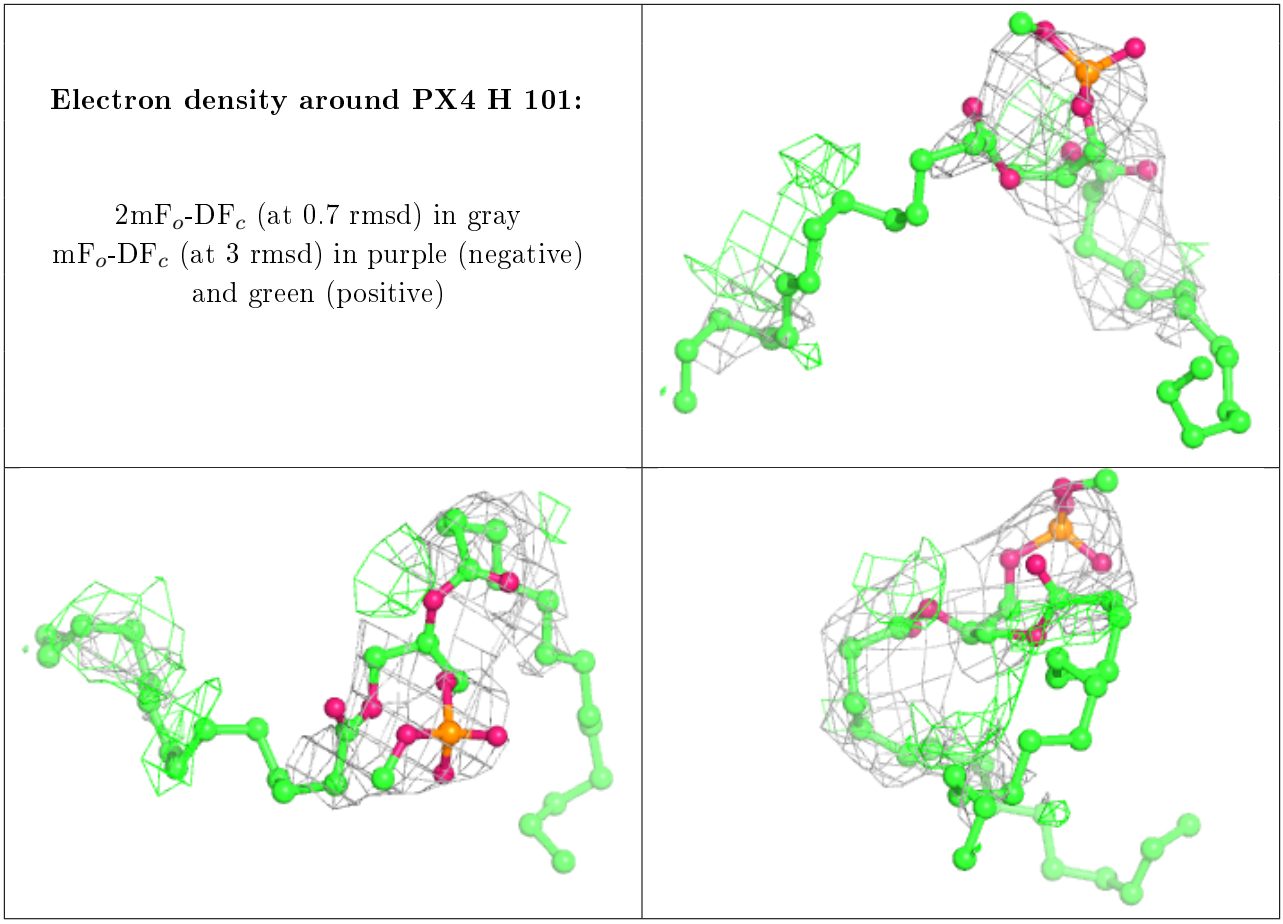






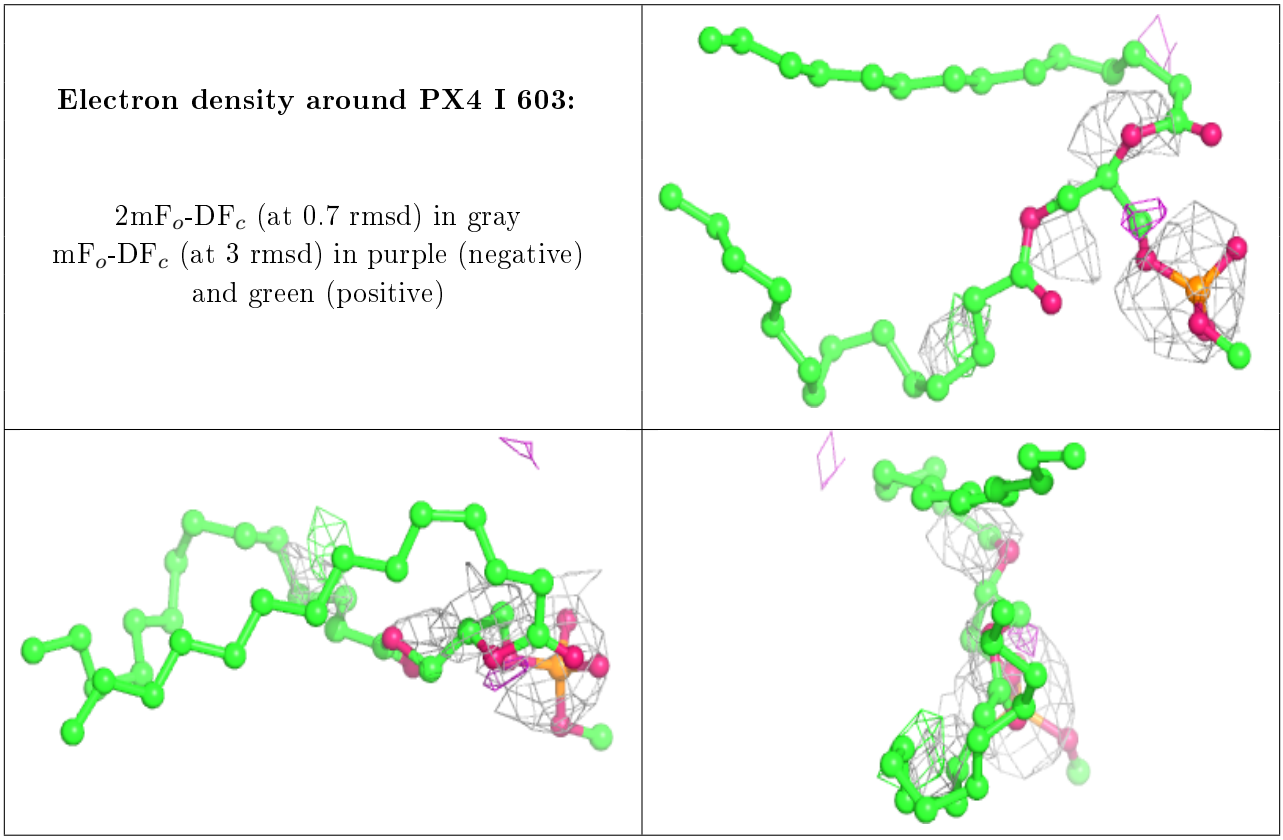
Electron density around PX4 H 101:

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



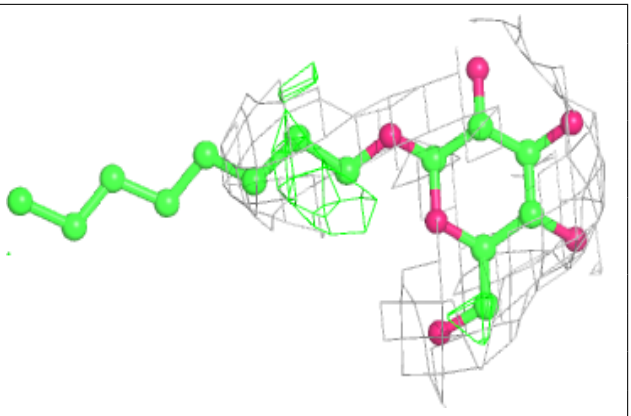
Electron density around PX4 I 603:

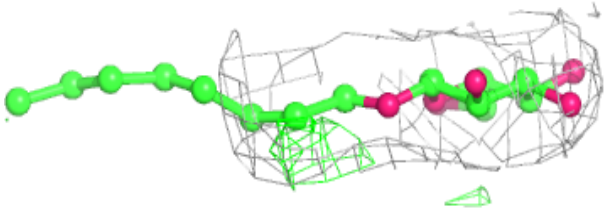
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

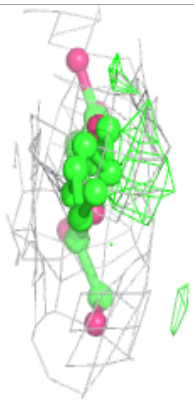


Electron density around BOG E 603:

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

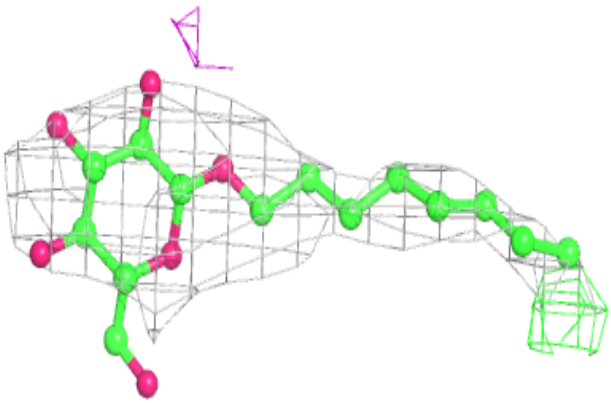


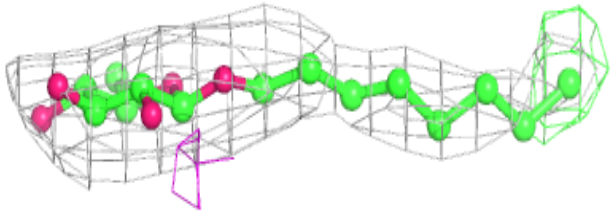


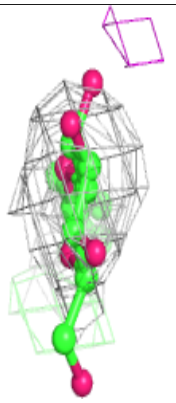


Electron density around BOG B 701:

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

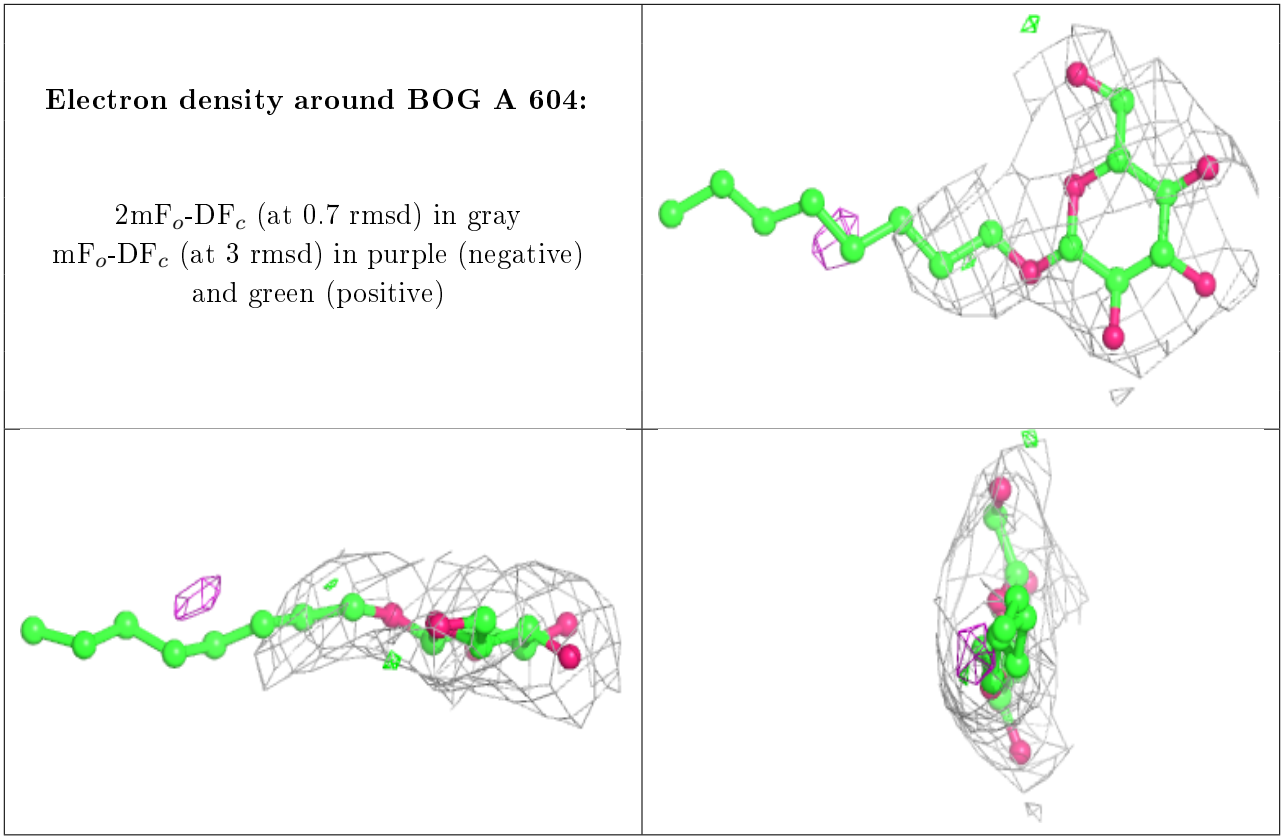






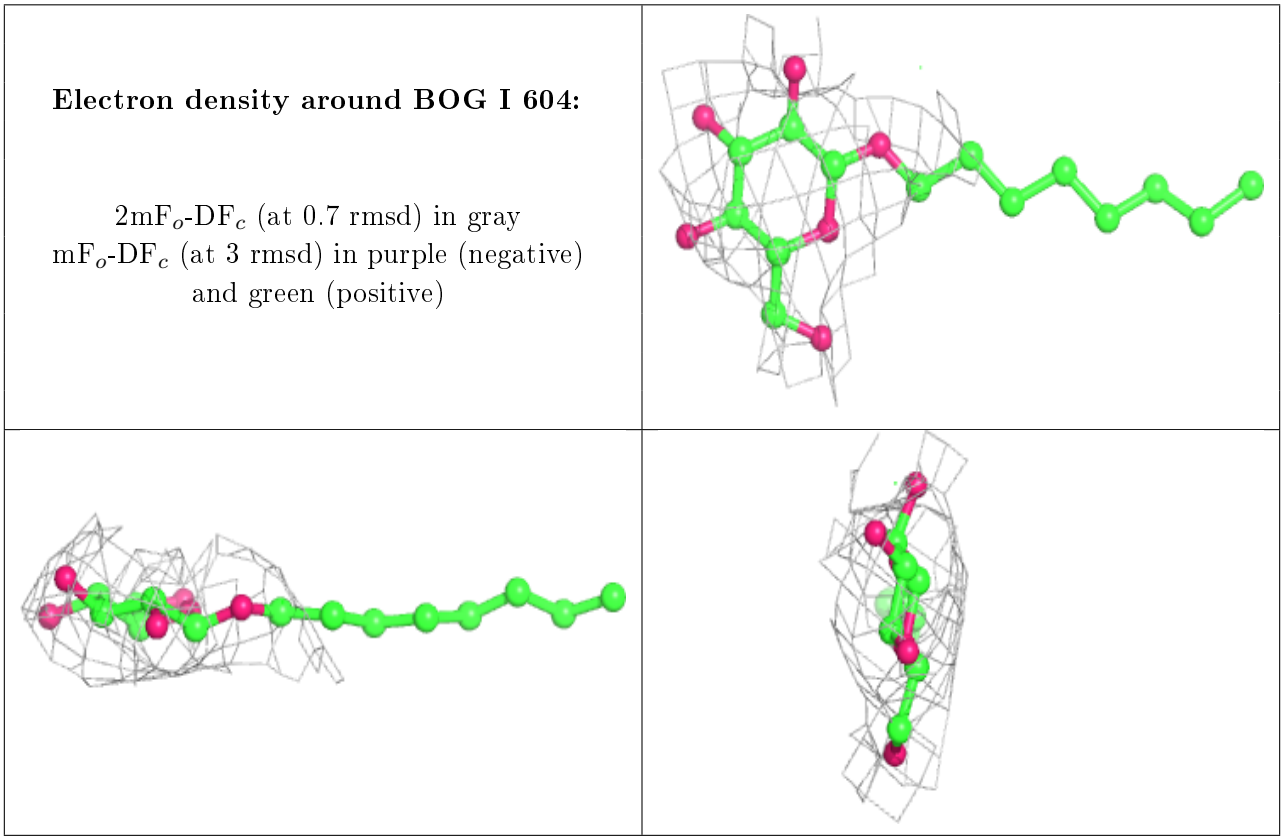
Electron density around BOG A 604:

$2mF_o$-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 I 604:

$2mF_o$-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.