Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2026 – 10:19 PM UTC

PDB ID	:	6JUH / pdb_00006juh
Title	:	structure of CavAb in complex with efonidipine
Authors	:	Tang, L.; Xu, F.
Deposited on	:	2019-04-13
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

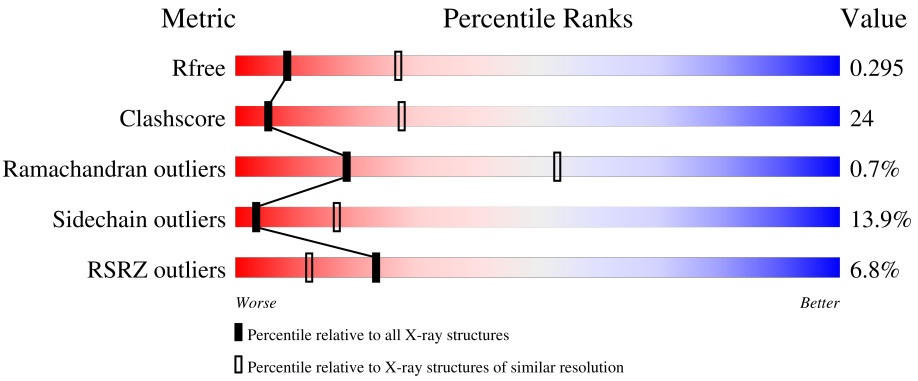
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	267	5% 57% 34% 8%
1	B	267	7% 55% 37% 6%
1	C	267	8% 51% 35% 12%
1	D	267	7% 58% 31% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8851 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.

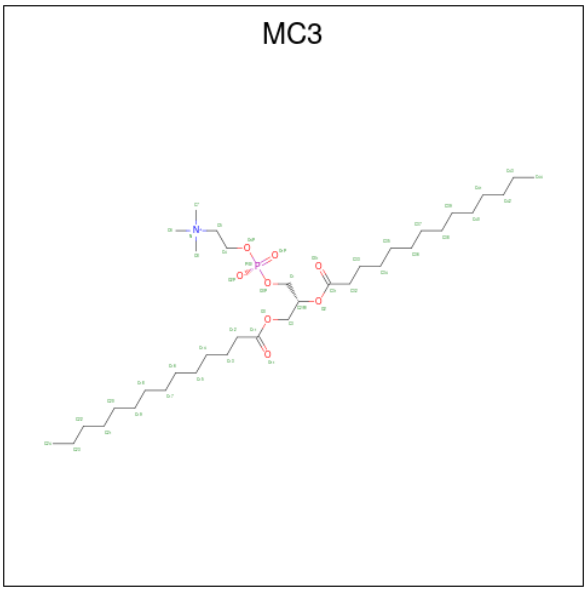
- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2164	1453	331	369	11			
1	B	263	Total	C	N	O	S	0	0	0
			2164	1453	331	369	11			
1	C	261	Total	C	N	O	S	0	0	0
			2148	1443	328	366	11			
1	D	263	Total	C	N	O	S	0	0	0
			2164	1453	331	369	11			

There are 12 discrepancies between the modelled and reference sequences:

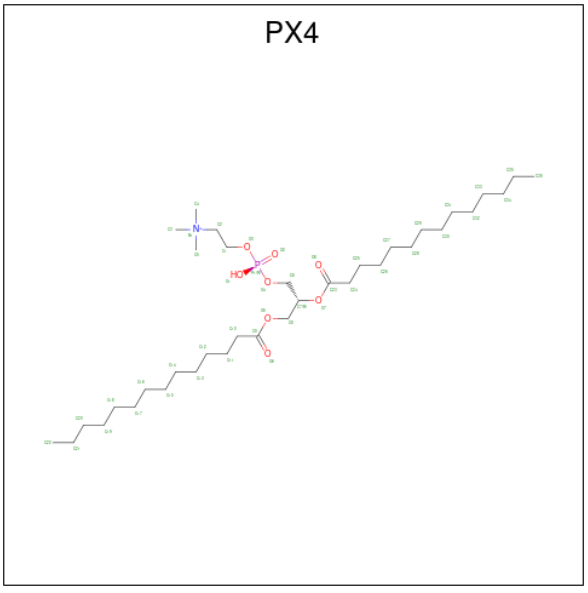
Chain	Residue	Modelled	Actual	Comment	Reference
A	1177	ASP	GLU	engineered mutation	UNP A8EVM5
A	1178	ASP	SER	engineered mutation	UNP A8EVM5
A	1181	ASN	MET	engineered mutation	UNP A8EVM5
B	1177	ASP	GLU	engineered mutation	UNP A8EVM5
B	1178	ASP	SER	engineered mutation	UNP A8EVM5
B	1181	ASN	MET	engineered mutation	UNP A8EVM5
C	1177	ASP	GLU	engineered mutation	UNP A8EVM5
C	1178	ASP	SER	engineered mutation	UNP A8EVM5
C	1181	ASN	MET	engineered mutation	UNP A8EVM5
D	1177	ASP	GLU	engineered mutation	UNP A8EVM5
D	1178	ASP	SER	engineered mutation	UNP A8EVM5
D	1181	ASN	MET	engineered mutation	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: $C_{36}H_{72}NO_8P$).



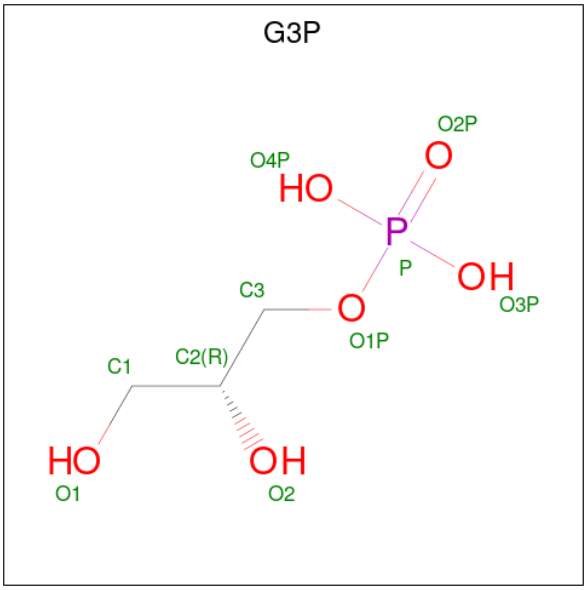
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	13	7	1		
2	B	1	Total	C	O	P	0	0
			21	13	7	1		
2	C	1	Total	C	O	P	0	0
			21	13	7	1		
2	D	1	Total	C	O	P	0	0
			21	13	7	1		

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



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

- Molecule 4 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$).

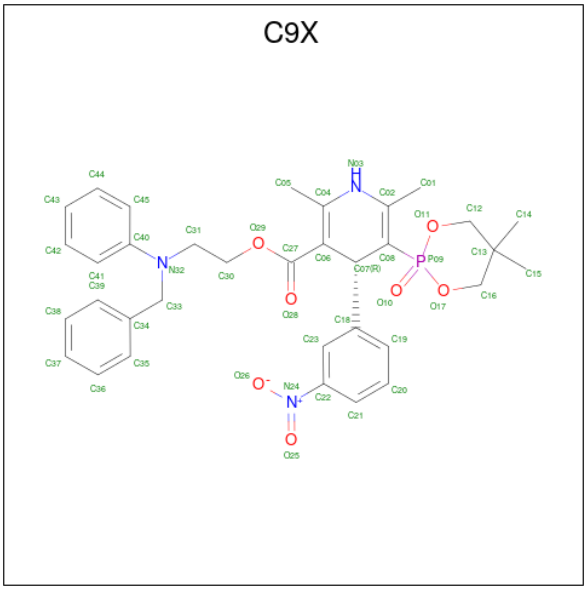


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 10 3 6 1	0	0
4	C	1	Total C O P 10 3 6 1	0	0
4	C	1	Total C O P 10 3 6 1	0	0
4	D	1	Total C O P 10 3 6 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

- Molecule 6 is 2-[phenyl-(phenylmethyl)amino]ethyl (4 {R})-5-(5,5-dimethyl-2-oxidanylidene -1,3,2$l^{5}-dioxaphosphinan-2-yl)-2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3-ca rboxylate (CCD ID: C9X) (formula: $C_{34}H_{38}N_3O_7P$).



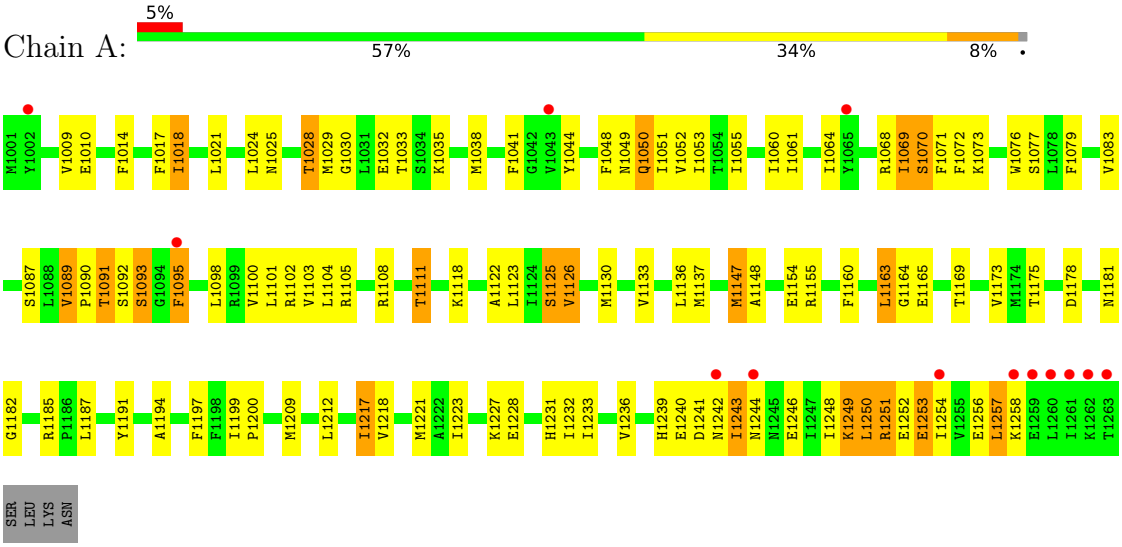
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	D	1	45	34	3	7	1	0	0

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.

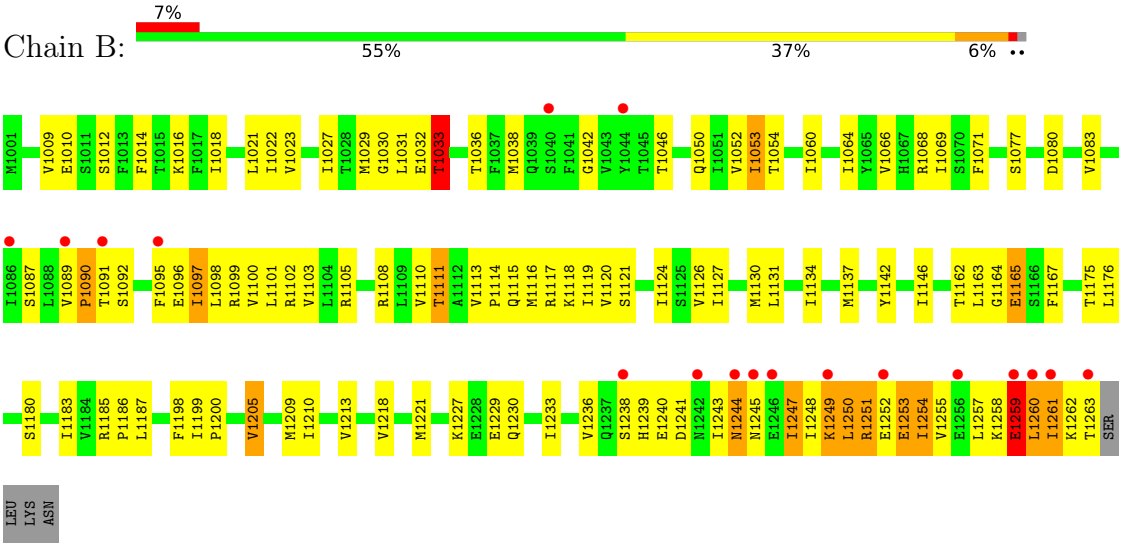
• Molecule 1: Ion transport protein

Chain A:



• Molecule 1: Ion transport protein

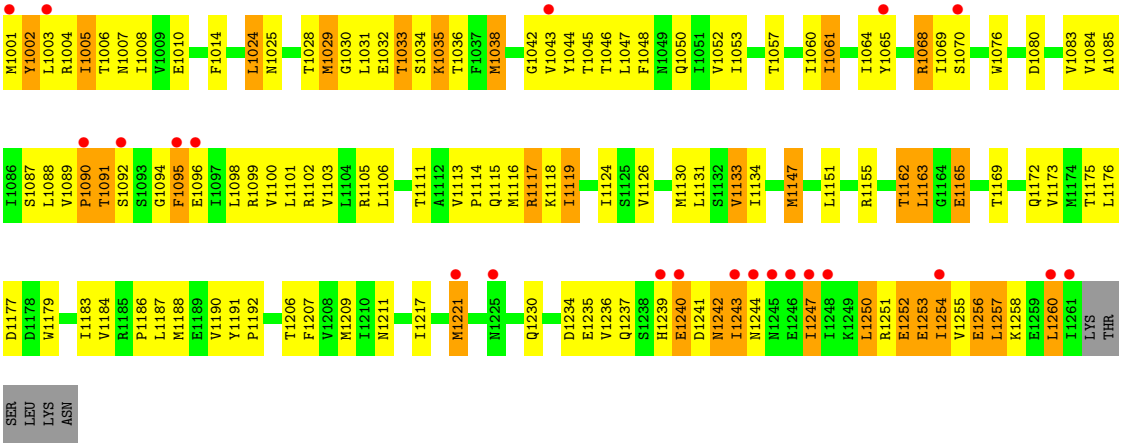
Chain B:



• Molecule 1: Ion transport protein

Chain C:

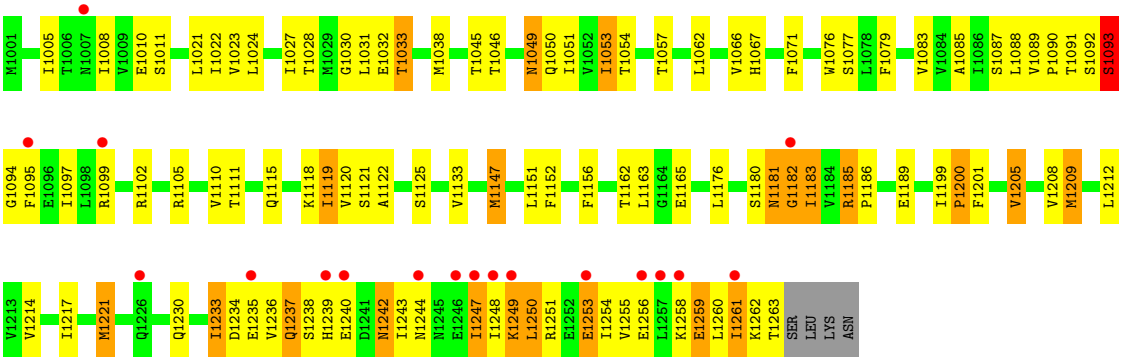




• Molecule 1: Ion transport protein

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	124.86Å 125.52Å 191.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.00 29.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (29.82-3.00) 88.5 (29.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.00Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.235 , 0.291 0.241 , 0.295	Depositor DCC
R_{free} test set	2666 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8851	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: G3P, C9X, PX4, MC3, CA

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	0.70	0/2217	1.03	5/3012 (0.2%)
1	B	0.72	0/2217	1.03	7/3012 (0.2%)
1	C	0.77	1/2201 (0.0%)	1.00	8/2991 (0.3%)
1	D	0.69	0/2217	1.00	3/3012 (0.1%)
All	All	0.72	1/8852 (0.0%)	1.02	23/12027 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1241	ASP	CA-C	5.98	1.60	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1089	VAL	CA-C-N	10.80	133.34	119.84
1	B	1089	VAL	C-N-CA	10.80	133.34	119.84
1	A	1242	ASN	N-CA-C	-10.00	101.86	114.56
1	B	1248	ILE	N-CA-C	-9.51	101.12	110.72
1	D	1181	ASN	N-CA-C	-9.18	99.82	111.02
1	A	1089	VAL	CA-C-N	7.72	127.77	119.89
1	A	1089	VAL	C-N-CA	7.72	127.77	119.89
1	C	1254	ILE	N-CA-C	-7.43	104.25	112.80
1	A	1243	ILE	N-CA-C	-6.66	106.03	112.29
1	C	1240	GLU	N-CA-C	-6.41	104.34	111.71
1	A	1250	LEU	N-CA-C	-5.90	104.92	111.36
1	C	1241	ASP	CA-C-O	5.76	126.49	119.11
1	D	1209	MET	N-CA-C	-5.76	104.91	111.07
1	B	1033	THR	N-CA-C	-5.61	106.28	113.23
1	B	1241	ASP	N-CA-C	-5.52	106.54	113.28
1	C	1253	GLU	N-CA-C	-5.43	104.93	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1198	PHE	N-CA-C	5.25	117.91	111.82
1	D	1247	ILE	N-CA-C	-5.18	108.07	113.10
1	C	1124	ILE	CB-CA-C	-5.17	105.26	112.04
1	B	1247	ILE	N-CA-C	-5.14	108.49	113.53
1	C	1250	LEU	N-CA-C	-5.13	106.42	113.30
1	C	1098	LEU	N-CA-C	-5.07	106.94	113.23
1	C	1190	VAL	CB-CA-C	-5.05	106.45	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2164	0	2239	119	0
1	B	2164	0	2239	105	0
1	C	2148	0	2219	146	0
1	D	2164	0	2239	119	0
2	A	21	0	19	1	0
2	B	21	0	19	0	0
2	C	21	0	19	1	0
2	D	21	0	19	0	0
3	A	10	0	5	1	0
3	B	10	0	5	0	0
3	C	20	0	10	0	0
4	A	10	0	7	0	0
4	C	20	0	14	0	0
4	D	10	0	7	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	D	45	0	0	0	0
All	All	8851	0	9060	428	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 24.

All (428) 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:D:1259:GLU:OE1	1:D:1260:LEU:HD12	1.34	1.24
1:C:1115:GLN:O	1:C:1119:ILE:HG22	1.37	1.23
1:C:1076:TRP:CE2	1:C:1117:ARG:HD3	1.81	1.15
1:B:1239:HIS:CE1	1:C:1237:GLN:HG2	1.85	1.09
1:D:1099:ARG:HD3	1:D:1102:ARG:NH1	1.67	1.09
1:D:1261:ILE:HD11	1:D:1262:LYS:HE2	1.35	1.07
1:A:1240:GLU:HB3	1:D:1239:HIS:HD2	1.17	1.06
1:A:1240:GLU:HB3	1:D:1239:HIS:CD2	1.91	1.04
1:C:1076:TRP:CZ2	1:C:1117:ARG:HD3	1.90	1.04
1:D:1259:GLU:OE1	1:D:1260:LEU:CD1	2.10	0.98
1:B:1239:HIS:HE1	1:C:1237:GLN:HG2	1.27	0.98
1:C:1076:TRP:CD2	1:C:1117:ARG:HD3	1.99	0.98
1:D:1256:GLU:O	1:D:1260:LEU:HD13	1.64	0.96
1:D:1237:GLN:HE21	1:D:1237:GLN:HA	1.28	0.95
1:C:1089:VAL:O	1:C:1090:PRO:O	1.85	0.94
1:A:1250:LEU:O	1:A:1254:ILE:HD13	1.69	0.93
1:C:1113:VAL:HG12	1:C:1114:PRO:O	1.69	0.92
1:B:1090:PRO:HB2	1:B:1092:SER:O	1.70	0.92
1:D:1182:GLY:O	1:D:1186:PRO:HD2	1.69	0.92
1:B:1251:ARG:HB3	1:B:1251:ARG:NH1	1.86	0.91
1:D:1261:ILE:HD11	1:D:1262:LYS:CE	2.04	0.88
1:C:1076:TRP:CH2	1:C:1117:ARG:HD3	2.09	0.86
1:C:1091:THR:O	1:C:1092:SER:OG	1.93	0.86
1:C:1244:ASN:HA	1:C:1247:ILE:HG22	1.57	0.86
1:D:1091:THR:O	1:D:1092:SER:OG	1.95	0.83
1:A:1249:LYS:CB	1:A:1249:LYS:NZ	2.41	0.83
1:C:1076:TRP:CE2	1:C:1117:ARG:CD	2.61	0.83
1:A:1249:LYS:NZ	1:A:1249:LYS:HB3	1.95	0.82
1:C:1057:THR:O	1:C:1061:ILE:HG13	1.80	0.81
1:C:1239:HIS:HA	1:C:1242:ASN:HB2	1.61	0.80
1:D:1261:ILE:CD1	1:D:1262:LYS:HE2	2.13	0.79
1:D:1053:ILE:HD12	1:D:1088:LEU:HD23	1.65	0.79
1:A:1254:ILE:HA	1:B:1254:ILE:HD12	1.64	0.78
1:D:1099:ARG:CD	1:D:1102:ARG:NH1	2.45	0.77
1:C:1005:ILE:HD11	1:C:1065:TYR:CE2	2.20	0.77
1:C:1244:ASN:HA	1:C:1247:ILE:CG2	2.14	0.77
1:B:1249:LYS:O	1:B:1252:GLU:HG2	1.85	0.77
1:D:1181:ASN:O	1:D:1186:PRO:HD2	1.85	0.76
1:B:1221:MET:HE2	1:C:1221:MET:HB2	1.68	0.76
1:C:1076:TRP:CD2	1:C:1117:ARG:CD	2.68	0.75
1:C:1247:ILE:O	1:C:1247:ILE:HD13	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:TRP:CE3	1:C:1117:ARG:HD3	2.22	0.74
1:D:1256:GLU:O	1:D:1260:LEU:CD1	2.34	0.74
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.51	0.74
1:A:1092:SER:O	1:A:1093:SER:OG	2.04	0.73
1:C:1115:GLN:O	1:C:1119:ILE:CG2	2.29	0.73
1:D:1094:GLY:O	1:D:1095:PHE:HD1	1.71	0.72
1:A:1251:ARG:NH1	1:D:1250:LEU:HD23	2.04	0.72
1:C:1060:ILE:O	1:C:1064:ILE:HG12	1.87	0.72
1:A:1250:LEU:HG	1:A:1254:ILE:HD13	1.71	0.72
1:B:1251:ARG:HB3	1:B:1251:ARG:HH11	1.50	0.72
1:C:1076:TRP:CZ3	1:C:1117:ARG:HD3	2.25	0.71
1:A:1069:ILE:CD1	1:A:1073:LYS:HE2	2.20	0.71
1:B:1119:ILE:HD11	1:C:1133:VAL:HG13	1.70	0.71
1:D:1085:ALA:O	1:D:1088:LEU:HB2	1.91	0.71
1:B:1260:LEU:HD23	1:B:1260:LEU:C	2.16	0.71
1:C:1005:ILE:HD11	1:C:1065:TYR:HE2	1.56	0.71
1:A:1251:ARG:CB	1:A:1251:ARG:HH11	2.03	0.70
1:D:1261:ILE:HG13	1:D:1262:LYS:N	2.06	0.70
1:B:1252:GLU:HG3	1:B:1253:GLU:OE2	1.92	0.70
1:B:1258:LYS:O	1:B:1261:ILE:N	2.22	0.70
1:D:1089:VAL:HG13	1:D:1090:PRO:HD2	1.73	0.70
1:A:1069:ILE:HD12	1:A:1073:LYS:HE2	1.73	0.70
1:A:1079:PHE:CE1	1:A:1083:VAL:HG21	2.27	0.70
1:D:1182:GLY:O	1:D:1186:PRO:CD	2.40	0.69
1:C:1003:LEU:O	1:C:1007:ASN:ND2	2.25	0.69
1:C:1004:ARG:HE	1:C:1004:ARG:HA	1.57	0.69
1:C:1239:HIS:O	1:C:1242:ASN:N	2.26	0.69
1:A:1069:ILE:O	1:A:1070:SER:C	2.35	0.68
1:C:1244:ASN:CA	1:C:1247:ILE:HG22	2.24	0.68
1:A:1069:ILE:HG13	1:A:1070:SER:N	2.09	0.68
1:D:1237:GLN:HA	1:D:1237:GLN:NE2	2.04	0.68
1:C:1184:VAL:HG12	1:C:1188:MET:HE2	1.75	0.68
1:D:1242:ASN:O	1:D:1242:ASN:OD1	2.12	0.67
1:A:1069:ILE:HG13	1:A:1070:SER:H	1.59	0.67
1:A:1250:LEU:HG	1:A:1254:ILE:CD1	2.24	0.67
1:C:1239:HIS:C	1:C:1242:ASN:H	2.03	0.67
1:D:1087:SER:HA	1:D:1102:ARG:HG2	1.75	0.67
1:C:1239:HIS:O	1:C:1242:ASN:HB2	1.94	0.67
1:B:1250:LEU:HD11	1:C:1251:ARG:HG3	1.77	0.67
1:D:1180:SER:O	1:D:1185:ARG:HB2	1.94	0.67
1:A:1249:LYS:HB3	1:A:1249:LYS:HZ2	1.58	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1091:THR:C	1:C:1092:SER:HG	1.99	0.66
1:C:1076:TRP:CG	1:C:1117:ARG:HE	2.12	0.66
1:B:1100:VAL:HG11	1:C:1151:LEU:HG	1.77	0.66
1:C:1114:PRO:O	1:C:1116:MET:N	2.27	0.66
1:D:1180:SER:O	1:D:1181:ASN:C	2.37	0.66
1:D:1248:ILE:HD12	1:D:1251:ARG:HD3	1.78	0.66
1:C:1247:ILE:HD13	1:C:1247:ILE:C	2.21	0.65
1:C:1068:ARG:HD2	1:C:1069:ILE:HG12	1.79	0.65
1:A:1069:ILE:HD12	1:A:1073:LYS:CE	2.26	0.65
1:C:1239:HIS:CA	1:C:1242:ASN:HB2	2.26	0.65
1:B:1243:ILE:HD11	1:C:1240:GLU:OE1	1.95	0.65
1:C:1239:HIS:O	1:C:1242:ASN:CB	2.44	0.64
1:D:1182:GLY:O	1:D:1186:PRO:HG2	1.96	0.64
1:C:1076:TRP:CZ2	1:C:1117:ARG:CD	2.77	0.64
1:C:1004:ARG:HA	1:C:1004:ARG:NE	2.13	0.64
1:C:1235:GLU:HG2	1:D:1233:ILE:HG12	1.79	0.64
1:D:1089:VAL:O	1:D:1102:ARG:NH2	2.31	0.64
1:A:1243:ILE:HD12	1:B:1244:ASN:HB3	1.80	0.64
1:D:1180:SER:O	1:D:1185:ARG:N	2.30	0.63
1:B:1239:HIS:HE1	1:C:1237:GLN:CG	2.06	0.63
1:A:1249:LYS:CB	1:A:1249:LYS:HZ1	2.11	0.63
1:C:1076:TRP:CZ3	1:C:1117:ARG:HG2	2.33	0.63
1:D:1083:VAL:HG11	1:D:1105:ARG:HA	1.81	0.63
1:A:1250:LEU:O	1:A:1254:ILE:CD1	2.46	0.63
1:B:1115:GLN:N	1:B:1115:GLN:OE1	2.29	0.62
1:C:1117:ARG:HH11	1:C:1117:ARG:CB	2.13	0.62
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.35	0.62
1:D:1099:ARG:CD	1:D:1102:ARG:HH11	2.13	0.62
1:D:1183:ILE:N	1:D:1183:ILE:HD13	2.14	0.61
1:B:1244:ASN:HA	1:B:1247:ILE:HG22	1.81	0.61
1:C:1162:THR:HG22	1:C:1165:GLU:HB2	1.81	0.61
1:A:1257:LEU:HD11	1:B:1257:LEU:O	1.99	0.61
1:B:1239:HIS:CE1	1:C:1237:GLN:CG	2.75	0.61
1:D:1238:SER:O	1:D:1242:ASN:HB3	2.01	0.61
1:B:1261:ILE:HG13	1:B:1261:ILE:O	1.99	0.61
1:C:1114:PRO:O	1:C:1115:GLN:HB2	2.00	0.61
1:C:1217:ILE:HG12	1:D:1214:VAL:HG13	1.82	0.61
1:C:1096:GLU:HG3	1:C:1099:ARG:HE	1.67	0.60
1:A:1061:ILE:HA	1:A:1064:ILE:HD12	1.82	0.60
1:B:1116:MET:O	1:B:1119:ILE:HG22	2.02	0.60
1:C:1244:ASN:C	1:C:1247:ILE:HG22	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:TRP:CD2	1:C:1117:ARG:NE	2.70	0.59
1:C:1116:MET:O	1:C:1119:ILE:HG23	2.03	0.59
1:C:1236:VAL:O	1:C:1240:GLU:HG2	2.02	0.59
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.31	0.59
1:A:1217:ILE:HD11	1:D:1217:ILE:HG23	1.85	0.59
1:A:1163:LEU:HB2	1:D:1033:THR:HG21	1.85	0.59
1:C:1002:TYR:HE1	1:C:1006:THR:OG1	1.85	0.59
1:C:1087:SER:HB3	1:C:1105:ARG:HH21	1.68	0.59
1:B:1120:VAL:HG12	1:B:1124:ILE:HD11	1.85	0.58
1:A:1251:ARG:HH11	1:A:1251:ARG:CG	2.16	0.58
1:D:1051:ILE:O	1:D:1054:THR:OG1	2.22	0.58
1:A:1068:ARG:O	1:A:1069:ILE:HG13	2.04	0.58
1:D:1053:ILE:HD12	1:D:1088:LEU:CD2	2.34	0.58
1:C:1068:ARG:HD3	1:C:1068:ARG:C	2.28	0.58
1:B:1262:LYS:HG3	1:B:1263:THR:N	2.19	0.57
1:D:1254:ILE:O	1:D:1258:LYS:HG2	2.04	0.57
1:A:1130:MET:HE2	1:A:1212:LEU:HD21	1.86	0.57
1:B:1244:ASN:HA	1:B:1247:ILE:CG2	2.35	0.57
1:A:1240:GLU:CB	1:D:1239:HIS:CD2	2.79	0.57
1:B:1162:THR:HG22	1:B:1164:GLY:N	2.20	0.57
1:D:1099:ARG:HD3	1:D:1102:ARG:HH11	1.65	0.57
1:D:1094:GLY:O	1:D:1095:PHE:CD1	2.56	0.57
1:D:1028:THR:HA	1:D:1031:LEU:HD12	1.87	0.56
1:A:1122:ALA:O	1:A:1125:SER:OG	2.21	0.56
1:A:1148:ALA:HB1	1:A:1160:PHE:CD1	2.40	0.56
1:A:1024:LEU:HD13	1:A:1048:PHE:HZ	1.69	0.56
1:C:1031:LEU:C	1:C:1033:THR:H	2.14	0.56
1:D:1263:THR:HG23	1:D:1263:THR:O	2.06	0.56
1:A:1217:ILE:HG13	1:A:1218:VAL:N	2.20	0.56
1:A:1221:MET:SD	1:B:1221:MET:SD	3.03	0.56
1:A:1024:LEU:HD13	1:A:1048:PHE:CZ	2.41	0.56
1:C:1096:GLU:O	1:C:1096:GLU:HG2	2.06	0.56
1:A:1217:ILE:HD12	1:A:1221:MET:HE3	1.88	0.55
1:B:1127:ILE:O	1:B:1130:MET:N	2.38	0.55
1:C:1002:TYR:CE1	1:C:1006:THR:OG1	2.59	0.55
1:A:1249:LYS:NZ	1:A:1249:LYS:HB2	2.20	0.55
1:B:1091:THR:HA	1:B:1102:ARG:HH22	1.72	0.54
1:C:1130:MET:HE2	1:C:1134:ILE:HD11	1.89	0.54
1:D:1182:GLY:O	1:D:1186:PRO:CG	2.55	0.54
1:A:1248:ILE:HA	1:A:1251:ARG:HB3	1.90	0.54
1:A:1249:LYS:HZ1	1:A:1249:LYS:HB2	1.70	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1002:TYR:CD1	1:C:1002:TYR:C	2.85	0.54
1:A:1092:SER:C	1:A:1093:SER:HG	2.11	0.54
1:D:1092:SER:O	1:D:1093:SER:OG	2.24	0.53
1:B:1087:SER:HB3	1:B:1105:ARG:HH21	1.73	0.53
1:B:1080:ASP:OD1	1:B:1111:THR:HG21	2.09	0.53
1:B:1131:LEU:HA	1:B:1134:ILE:HD12	1.89	0.53
1:A:1091:THR:HG23	1:A:1102:ARG:HH12	1.74	0.53
1:C:1094:GLY:C	1:C:1095:PHE:CG	2.86	0.53
1:C:1173:VAL:HG13	1:C:1179:TRP:HB2	1.91	0.53
1:C:1235:GLU:OE2	1:D:1236:VAL:HG11	2.09	0.53
1:D:1199:ILE:HB	1:D:1200:PRO:HD3	1.90	0.53
1:B:1162:THR:HG22	1:B:1164:GLY:H	1.74	0.53
1:B:1221:MET:HE2	1:C:1221:MET:CB	2.37	0.53
1:C:1076:TRP:CE3	1:C:1117:ARG:CD	2.89	0.53
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.08	0.53
1:D:1181:ASN:O	1:D:1186:PRO:CD	2.56	0.53
1:C:1089:VAL:HG13	1:C:1090:PRO:HD2	1.89	0.53
1:A:1095:PHE:CD1	1:A:1095:PHE:N	2.76	0.53
1:D:1030:GLY:O	1:D:1033:THR:HB	2.08	0.53
1:B:1258:LYS:O	1:B:1261:ILE:HG22	2.09	0.52
1:A:1191:TYR:HB3	3:A:1302:PX4:H18	1.90	0.52
1:B:1244:ASN:C	1:B:1247:ILE:HG22	2.35	0.52
1:D:1099:ARG:NH1	1:D:1102:ARG:HH11	2.07	0.52
1:C:1117:ARG:HH11	1:C:1117:ARG:CG	2.22	0.52
1:A:1068:ARG:HG2	1:A:1069:ILE:HG23	1.91	0.52
1:A:1241:ASP:HA	1:A:1244:ASN:CB	2.40	0.52
1:B:1259:GLU:HA	1:B:1261:ILE:HG22	1.92	0.52
1:A:1087:SER:HA	1:A:1102:ARG:HG2	1.92	0.52
1:C:1252:GLU:HA	1:C:1255:VAL:HG13	1.92	0.52
1:A:1083:VAL:CG1	1:A:1105:ARG:HA	2.40	0.51
1:B:1110:VAL:HG13	1:B:1116:MET:HB3	1.92	0.51
1:A:1251:ARG:HH11	1:A:1251:ARG:CA	2.23	0.51
1:C:1253:GLU:O	1:D:1258:LYS:NZ	2.42	0.51
1:C:1068:ARG:HD3	1:C:1069:ILE:N	2.25	0.51
1:A:1249:LYS:O	1:A:1253:GLU:HB2	2.09	0.51
1:A:1217:ILE:HD11	1:D:1217:ILE:CG2	2.40	0.51
1:D:1008:ILE:O	1:D:1011:SER:HB3	2.11	0.51
1:B:1162:THR:HB	1:B:1165:GLU:HB2	1.92	0.51
1:C:1257:LEU:HB3	1:D:1258:LYS:HZ2	1.76	0.51
1:A:1254:ILE:HA	1:B:1254:ILE:CD1	2.37	0.51
1:B:1012:SER:O	1:B:1016:LYS:HG3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1239:HIS:C	1:C:1242:ASN:HB2	2.36	0.51
1:D:1180:SER:O	1:D:1181:ASN:O	2.28	0.51
1:A:1254:ILE:HD12	1:B:1254:ILE:HD12	1.93	0.51
1:C:1089:VAL:O	1:C:1090:PRO:C	2.54	0.51
1:A:1240:GLU:CB	1:D:1239:HIS:HD2	2.06	0.51
1:A:1248:ILE:O	1:A:1251:ARG:HB3	2.10	0.50
1:A:1243:ILE:HD12	1:B:1244:ASN:CB	2.41	0.50
1:C:1256:GLU:CB	1:D:1258:LYS:HE3	2.40	0.50
1:D:1260:LEU:CD1	1:D:1260:LEU:N	2.75	0.50
1:A:1032:GLU:HG2	1:A:1038:MET:HE3	1.93	0.50
1:A:1253:GLU:HA	1:A:1256:GLU:HB2	1.92	0.50
1:B:1180:SER:O	1:B:1185:ARG:HG3	2.11	0.50
1:C:1162:THR:HG22	1:C:1165:GLU:N	2.24	0.50
1:C:1235:GLU:OE2	1:D:1236:VAL:CG1	2.60	0.50
1:C:1068:ARG:CD	1:C:1069:ILE:N	2.75	0.50
1:A:1249:LYS:HG3	1:B:1251:ARG:HD3	1.92	0.50
1:A:1251:ARG:NH1	1:D:1250:LEU:CD2	2.75	0.50
1:A:1241:ASP:HA	1:A:1244:ASN:HB3	1.93	0.49
1:B:1250:LEU:CD1	1:C:1251:ARG:HG3	2.40	0.49
1:B:1251:ARG:HB3	1:B:1251:ARG:CZ	2.41	0.49
1:C:1005:ILE:HD11	1:C:1065:TYR:CD2	2.46	0.49
1:C:1103:VAL:HG11	1:D:1147:MET:SD	2.52	0.49
1:C:1250:LEU:HD12	1:D:1251:ARG:HG2	1.95	0.49
1:C:1004:ARG:O	1:C:1004:ARG:HD3	2.11	0.49
1:A:1250:LEU:C	1:A:1254:ILE:HD13	2.36	0.49
1:C:1025:ASN:HB2	1:C:1052:VAL:HG21	1.93	0.49
1:C:1236:VAL:O	1:C:1240:GLU:CG	2.61	0.49
1:D:1062:LEU:O	1:D:1066:VAL:HG23	2.12	0.49
1:C:1030:GLY:O	1:C:1033:THR:HB	2.13	0.49
1:A:1251:ARG:NH1	1:A:1251:ARG:CG	2.75	0.49
1:A:1024:LEU:HD12	1:A:1025:ASN:N	2.27	0.48
1:D:1240:GLU:N	1:D:1240:GLU:OE1	2.46	0.48
1:A:1253:GLU:OE1	1:B:1255:VAL:HG22	2.13	0.48
1:B:1221:MET:CE	1:C:1221:MET:HB2	2.41	0.48
1:D:1079:PHE:CZ	1:D:1083:VAL:HG21	2.48	0.48
1:D:1099:ARG:HH11	1:D:1102:ARG:HH11	1.61	0.48
1:A:1137:MET:HE2	1:A:1209:MET:HE2	1.95	0.48
1:B:1090:PRO:O	1:B:1102:ARG:NH2	2.46	0.48
1:D:1118:LYS:O	1:D:1121:SER:HB2	2.12	0.48
1:B:1029:MET:SD	1:B:1103:VAL:HG23	2.53	0.48
1:C:1029:MET:HG3	1:C:1106:LEU:HD21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:TRP:CD1	1:C:1117:ARG:HE	2.31	0.48
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.96	0.48
1:A:1236:VAL:O	1:A:1240:GLU:HB2	2.14	0.48
1:D:1005:ILE:HA	1:D:1008:ILE:HD12	1.95	0.48
1:A:1221:MET:HG3	1:D:1221:MET:SD	2.53	0.48
1:C:1002:TYR:HE1	1:C:1006:THR:HG1	1.52	0.48
1:D:1250:LEU:HA	1:D:1253:GLU:HG2	1.96	0.48
1:A:1041:PHE:O	1:A:1044:TYR:HB2	2.13	0.48
1:A:1101:LEU:HD22	1:A:1104:LEU:HD11	1.95	0.48
1:D:1079:PHE:O	1:D:1083:VAL:HG23	2.14	0.48
1:A:1251:ARG:HH12	1:D:1250:LEU:CD2	2.27	0.47
1:D:1076:TRP:HE3	1:D:1111:THR:HG22	1.79	0.47
1:B:1038:MET:HE2	1:B:1038:MET:HA	1.96	0.47
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.96	0.47
1:B:1221:MET:CE	1:C:1217:ILE:HG22	2.44	0.47
1:A:1251:ARG:HH11	1:A:1251:ARG:HA	1.80	0.47
1:B:1244:ASN:CA	1:B:1247:ILE:HG22	2.45	0.47
1:D:1087:SER:HB3	1:D:1105:ARG:HH21	1.80	0.47
1:A:1069:ILE:CD1	1:A:1073:LYS:CE	2.90	0.47
1:A:1241:ASP:OD1	1:A:1241:ASP:C	2.57	0.47
1:D:1201:PHE:O	1:D:1205:VAL:HB	2.14	0.47
1:D:1260:LEU:HD12	1:D:1260:LEU:N	2.30	0.47
1:D:1152:PHE:O	1:D:1156:PHE:HB2	2.15	0.47
1:B:1120:VAL:O	1:B:1124:ILE:HG13	2.15	0.47
1:C:1162:THR:HG21	2:C:1302:MC3:C4	2.44	0.47
1:C:1256:GLU:HB2	1:D:1258:LYS:HE3	1.96	0.47
1:C:1032:GLU:HA	1:C:1038:MET:HG3	1.97	0.46
1:C:1085:ALA:O	1:C:1088:LEU:HB2	2.16	0.46
1:A:1069:ILE:CG1	1:A:1070:SER:N	2.77	0.46
1:A:1227:LYS:HE3	1:A:1231:HIS:CE1	2.51	0.46
1:B:1236:VAL:O	1:B:1240:GLU:HB2	2.15	0.46
1:D:1249:LYS:O	1:D:1253:GLU:HG2	2.15	0.46
1:A:1009:VAL:HA	1:A:1014:PHE:CD2	2.50	0.46
1:A:1024:LEU:O	1:A:1028:THR:HG23	2.16	0.46
1:B:1038:MET:HE2	1:B:1042:GLY:HA2	1.97	0.46
1:B:1175:THR:HB	1:C:1176:LEU:HD13	1.98	0.46
1:C:1239:HIS:O	1:C:1242:ASN:CA	2.64	0.46
1:D:1024:LEU:O	1:D:1028:THR:HG23	2.16	0.46
1:D:1208:VAL:O	1:D:1212:LEU:HB2	2.16	0.46
1:A:1175:THR:HB	1:B:1176:LEU:HD13	1.98	0.46
1:A:1181:ASN:HA	1:A:1185:ARG:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:MET:CE	1:B:1221:MET:SD	3.04	0.46
1:C:1117:ARG:CG	1:C:1117:ARG:NH1	2.78	0.46
1:B:1033:THR:HG21	1:C:1163:LEU:HB2	1.98	0.46
1:B:1009:VAL:HG21	1:B:1066:VAL:HG21	1.97	0.46
1:C:1004:ARG:NE	1:C:1004:ARG:CA	2.76	0.46
1:C:1042:GLY:O	1:C:1046:THR:OG1	2.34	0.46
1:D:1181:ASN:O	1:D:1185:ARG:HB2	2.16	0.46
1:A:1240:GLU:HG2	1:B:1240:GLU:OE2	2.16	0.46
1:C:1240:GLU:OE1	1:C:1240:GLU:HA	2.15	0.46
1:A:1217:ILE:O	1:A:1221:MET:HG2	2.16	0.45
1:D:1024:LEU:HA	1:D:1027:ILE:HD12	1.98	0.45
1:D:1038:MET:HE2	1:D:1038:MET:HA	1.97	0.45
1:B:1118:LYS:HA	1:B:1121:SER:HB2	1.99	0.45
1:A:1133:VAL:HG22	1:D:1119:ILE:HD12	1.99	0.45
1:B:1258:LYS:C	1:B:1260:LEU:N	2.74	0.45
1:A:1091:THR:HG23	1:A:1102:ARG:NH1	2.31	0.45
1:B:1050:GLN:O	1:B:1053:ILE:HG22	2.17	0.45
1:D:1259:GLU:CD	1:D:1259:GLU:C	2.85	0.45
1:B:1030:GLY:O	1:B:1033:THR:HB	2.17	0.45
1:B:1142:TYR:CZ	1:B:1146:ILE:HD11	2.52	0.45
1:D:1122:ALA:O	1:D:1125:SER:OG	2.21	0.45
1:A:1051:ILE:O	1:A:1055:ILE:HG13	2.16	0.45
1:B:1064:ILE:O	1:B:1068:ARG:N	2.48	0.45
1:B:1252:GLU:O	1:B:1255:VAL:N	2.49	0.45
1:C:1060:ILE:O	1:C:1064:ILE:CG1	2.62	0.45
1:C:1115:GLN:H	1:C:1118:LYS:CG	2.29	0.45
1:C:1243:ILE:HD12	1:C:1243:ILE:HA	1.78	0.45
1:D:1079:PHE:CE2	1:D:1083:VAL:HG21	2.52	0.45
1:B:1137:MET:HE1	1:B:1205:VAL:HG22	1.98	0.45
1:B:1100:VAL:HG12	1:C:1147:MET:HG2	1.99	0.44
1:C:1088:LEU:HD23	1:C:1088:LEU:HA	1.78	0.44
1:D:1242:ASN:OD1	1:D:1242:ASN:C	2.60	0.44
1:C:1008:ILE:O	1:C:1014:PHE:HB2	2.17	0.44
1:D:1254:ILE:O	1:D:1258:LYS:NZ	2.46	0.44
1:A:1028:THR:O	1:A:1032:GLU:HG3	2.16	0.44
1:B:1023:VAL:O	1:B:1027:ILE:HG13	2.17	0.44
1:A:1050:GLN:HA	1:A:1053:ILE:HG22	2.00	0.44
1:A:1069:ILE:C	1:A:1071:PHE:N	2.70	0.44
1:B:1243:ILE:CD1	1:C:1243:ILE:HG21	2.47	0.44
1:C:1089:VAL:CG1	1:C:1090:PRO:HD2	2.47	0.44
1:C:1103:VAL:CG1	1:D:1147:MET:SD	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1230:GLN:NE2	1:C:1234:ASP:OD1	2.51	0.44
1:B:1098:LEU:HD23	1:B:1101:LEU:HD12	2.00	0.44
1:C:1255:VAL:HA	1:C:1258:LYS:HB3	1.99	0.44
1:D:1255:VAL:O	1:D:1258:LYS:HB2	2.18	0.44
1:A:1098:LEU:HD23	1:A:1101:LEU:HD12	2.00	0.44
1:C:1247:ILE:O	1:C:1251:ARG:HB2	2.18	0.44
1:D:1049:ASN:O	1:D:1053:ILE:HB	2.18	0.44
1:A:1136:LEU:HD23	1:D:1119:ILE:HD11	1.99	0.44
1:A:1240:GLU:H	1:A:1243:ILE:HG12	1.83	0.44
1:B:1021:LEU:HD22	1:B:1052:VAL:HG22	1.99	0.44
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.98	0.44
1:C:1253:GLU:CG	1:D:1254:ILE:HD13	2.48	0.44
1:B:1137:MET:HE1	1:B:1205:VAL:HA	2.00	0.44
1:D:1071:PHE:CE1	1:D:1077:SER:HB3	2.53	0.44
1:A:1048:PHE:O	1:A:1052:VAL:HG23	2.18	0.43
1:B:1114:PRO:HA	1:B:1117:ARG:HB2	1.98	0.43
1:B:1250:LEU:HD12	1:B:1250:LEU:HA	1.80	0.43
1:C:1035:LYS:H	1:C:1035:LYS:HG2	1.64	0.43
1:C:1114:PRO:C	1:C:1116:MET:N	2.72	0.43
1:A:1038:MET:HA	1:A:1038:MET:HE2	2.00	0.43
1:D:1255:VAL:HA	1:D:1258:LYS:CG	2.48	0.43
1:A:1239:HIS:HB3	1:B:1240:GLU:OE1	2.17	0.43
1:D:1088:LEU:HD23	1:D:1088:LEU:HA	1.82	0.43
1:A:1083:VAL:HG12	1:A:1105:ARG:HA	1.99	0.43
1:A:1178:ASP:O	1:A:1182:GLY:HA3	2.18	0.43
1:C:1080:ASP:OD2	1:C:1111:THR:HG21	2.19	0.43
1:D:1089:VAL:CG1	1:D:1090:PRO:HD2	2.44	0.43
1:A:1164:GLY:HA3	2:A:1301:MC3:O3P	2.19	0.43
1:C:1183:ILE:C	1:C:1186:PRO:HD2	2.44	0.43
1:D:1032:GLU:HG2	1:D:1045:THR:HG21	2.01	0.43
1:A:1147:MET:HB3	1:A:1197:PHE:HE2	1.84	0.43
1:A:1248:ILE:O	1:A:1252:GLU:HG2	2.18	0.43
1:B:1210:ILE:O	1:B:1213:VAL:HB	2.19	0.43
1:D:1067:HIS:HB2	1:D:1071:PHE:HB2	2.00	0.43
1:D:1133:VAL:HG21	1:D:1212:LEU:HD11	2.01	0.43
1:B:1108:ARG:HA	1:B:1111:THR:HB	2.00	0.42
1:B:1183:ILE:C	1:B:1186:PRO:HD2	2.44	0.42
1:C:1034:SER:OG	1:C:1036:THR:HB	2.19	0.42
1:C:1100:VAL:HG11	1:D:1151:LEU:HG	2.00	0.42
1:C:1101:LEU:O	1:C:1102:ARG:C	2.60	0.42
1:A:1018:ILE:HA	1:A:1018:ILE:HD13	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:VAL:HA	1:B:1014:PHE:CD2	2.54	0.42
1:B:1032:GLU:HG2	1:B:1038:MET:HE1	2.02	0.42
1:B:1258:LYS:O	1:B:1260:LEU:N	2.52	0.42
1:C:1191:TYR:HA	1:C:1192:PRO:HD2	1.88	0.42
1:D:1230:GLN:O	1:D:1234:ASP:N	2.45	0.42
1:A:1069:ILE:O	1:A:1072:PHE:N	2.51	0.42
1:C:1207:PHE:O	1:C:1211:ASN:ND2	2.49	0.42
1:D:1092:SER:O	1:D:1093:SER:CB	2.68	0.42
1:D:1110:VAL:HG11	1:D:1120:VAL:HG21	2.01	0.42
1:D:1023:VAL:O	1:D:1027:ILE:HG13	2.19	0.42
1:C:1094:GLY:O	1:C:1095:PHE:CD1	2.73	0.42
1:A:1030:GLY:O	1:A:1033:THR:HB	2.19	0.42
1:B:1245:ASN:O	1:B:1249:LYS:HD3	2.20	0.42
1:A:1169:THR:O	1:A:1173:VAL:HG23	2.20	0.41
1:C:1024:LEU:HD12	1:C:1024:LEU:HA	1.83	0.41
1:B:1099:ARG:HE	1:B:1099:ARG:HB2	1.59	0.41
1:B:1221:MET:HE3	1:C:1217:ILE:HG22	2.03	0.41
1:C:1002:TYR:O	1:C:1005:ILE:HG12	2.20	0.41
1:C:1004:ARG:C	1:C:1004:ARG:CD	2.93	0.41
1:C:1172:GLN:HG3	1:C:1177:ASP:HB3	2.01	0.41
1:C:1175:THR:HB	1:D:1176:LEU:HD13	2.02	0.41
1:A:1251:ARG:HH22	1:D:1253:GLU:HG3	1.86	0.41
1:B:1060:ILE:O	1:B:1064:ILE:HG13	2.20	0.41
1:B:1071:PHE:CE2	1:B:1077:SER:HB3	2.55	0.41
1:A:1123:LEU:O	1:A:1126:VAL:HG23	2.21	0.41
1:D:1162:THR:OG1	1:D:1165:GLU:HG3	2.20	0.41
1:D:1244:ASN:O	1:D:1248:ILE:HB	2.20	0.41
1:A:1100:VAL:O	1:A:1103:VAL:HG12	2.21	0.41
1:B:1018:ILE:O	1:B:1022:ILE:HG13	2.20	0.41
1:B:1032:GLU:HG2	1:B:1038:MET:CE	2.50	0.41
1:B:1260:LEU:C	1:B:1260:LEU:CD2	2.87	0.41
1:C:1047:LEU:O	1:C:1050:GLN:N	2.52	0.41
1:C:1048:PHE:O	1:C:1052:VAL:HG23	2.19	0.41
1:B:1080:ASP:CG	1:B:1111:THR:HG21	2.46	0.41
1:B:1113:VAL:HA	1:B:1114:PRO:HD3	1.84	0.41
1:C:1076:TRP:CH2	1:C:1117:ARG:CD	2.93	0.41
1:A:1060:ILE:HD11	1:A:1108:ARG:HH21	1.86	0.41
1:B:1050:GLN:O	1:B:1054:THR:OG1	2.37	0.41
1:B:1097:ILE:HG13	1:B:1098:LEU:N	2.31	0.41
1:B:1244:ASN:O	1:B:1247:ILE:HG22	2.21	0.41
1:C:1004:ARG:HD3	1:C:1004:ARG:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1236:VAL:O	1:C:1240:GLU:HB2	2.21	0.41
1:D:1221:MET:HE2	1:D:1221:MET:HB2	1.70	0.41
1:D:1239:HIS:O	1:D:1243:ILE:HG23	2.21	0.41
1:A:1228:GLU:HA	1:B:1229:GLU:OE1	2.21	0.41
1:B:1031:LEU:C	1:B:1033:THR:H	2.28	0.41
1:C:1115:GLN:H	1:C:1118:LYS:HG2	1.86	0.41
1:C:1257:LEU:O	1:C:1260:LEU:HB3	2.21	0.41
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.56	0.40
1:B:1131:LEU:HA	1:B:1131:LEU:HD23	1.92	0.40
1:C:1099:ARG:HA	1:C:1102:ARG:HD2	2.02	0.40
1:A:1017:PHE:CZ	1:A:1021:LEU:HD11	2.57	0.40
1:A:1069:ILE:HD12	1:A:1073:LYS:HE3	2.00	0.40
1:A:1089:VAL:HA	1:A:1090:PRO:HD3	1.93	0.40
1:A:1232:ILE:HA	1:B:1233:ILE:HD11	2.04	0.40
1:A:1248:ILE:CA	1:A:1251:ARG:HB3	2.51	0.40
1:C:1247:ILE:C	1:C:1247:ILE:CD1	2.90	0.40
1:D:1050:GLN:O	1:D:1053:ILE:HG22	2.21	0.40
1:A:1076:TRP:HB3	1:A:1111:THR:HG23	2.04	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	261/267 (98%)	237 (91%)	22 (8%)	2 (1%)	16	50
1	B	261/267 (98%)	239 (92%)	20 (8%)	2 (1%)	16	50
1	C	259/267 (97%)	234 (90%)	24 (9%)	1 (0%)	30	65
1	D	261/267 (98%)	230 (88%)	29 (11%)	2 (1%)	16	50
All	All	1042/1068 (98%)	940 (90%)	95 (9%)	7 (1%)	18	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1090	PRO
1	C	1090	PRO
1	A	1194	ALA
1	D	1093	SER
1	D	1182	GLY
1	B	1259	GLU
1	A	1093	SER

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	244/248 (98%)	214 (88%)	30 (12%)	4	21
1	B	244/248 (98%)	213 (87%)	31 (13%)	4	20
1	C	242/248 (98%)	199 (82%)	43 (18%)	2	10
1	D	244/248 (98%)	213 (87%)	31 (13%)	4	20
All	All	974/992 (98%)	839 (86%)	135 (14%)	3	17

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	GLU
1	A	1018	ILE
1	A	1028	THR
1	A	1029	MET
1	A	1035	LYS
1	A	1049	ASN
1	A	1050	GLN
1	A	1069	ILE
1	A	1070	SER
1	A	1091	THR
1	A	1095	PHE
1	A	1111	THR
1	A	1118	LYS
1	A	1125	SER
1	A	1126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1147	MET
1	A	1154	GLU
1	A	1155	ARG
1	A	1163	LEU
1	A	1165	GLU
1	A	1187	LEU
1	A	1217	ILE
1	A	1223	ILE
1	A	1233	ILE
1	A	1246	GLU
1	A	1249	LYS
1	A	1251	ARG
1	A	1253	GLU
1	A	1257	LEU
1	A	1258	LYS
1	B	1010	GLU
1	B	1033	THR
1	B	1036	THR
1	B	1046	THR
1	B	1053	ILE
1	B	1069	ILE
1	B	1083	VAL
1	B	1095	PHE
1	B	1096	GLU
1	B	1097	ILE
1	B	1111	THR
1	B	1126	VAL
1	B	1163	LEU
1	B	1165	GLU
1	B	1167	PHE
1	B	1187	LEU
1	B	1205	VAL
1	B	1209	MET
1	B	1218	VAL
1	B	1227	LYS
1	B	1230	GLN
1	B	1238	SER
1	B	1244	ASN
1	B	1249	LYS
1	B	1250	LEU
1	B	1251	ARG
1	B	1253	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1254	ILE
1	B	1259	GLU
1	B	1260	LEU
1	B	1261	ILE
1	C	1001	MET
1	C	1002	TYR
1	C	1005	ILE
1	C	1010	GLU
1	C	1024	LEU
1	C	1028	THR
1	C	1029	MET
1	C	1033	THR
1	C	1035	LYS
1	C	1038	MET
1	C	1043	VAL
1	C	1044	TYR
1	C	1045	THR
1	C	1053	ILE
1	C	1061	ILE
1	C	1068	ARG
1	C	1070	SER
1	C	1083	VAL
1	C	1084	VAL
1	C	1091	THR
1	C	1095	PHE
1	C	1117	ARG
1	C	1119	ILE
1	C	1126	VAL
1	C	1131	LEU
1	C	1133	VAL
1	C	1147	MET
1	C	1155	ARG
1	C	1162	THR
1	C	1163	LEU
1	C	1165	GLU
1	C	1187	LEU
1	C	1206	THR
1	C	1209	MET
1	C	1221	MET
1	C	1242	ASN
1	C	1243	ILE
1	C	1247	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1252	GLU
1	C	1254	ILE
1	C	1256	GLU
1	C	1257	LEU
1	C	1260	LEU
1	D	1010	GLU
1	D	1021	LEU
1	D	1022	ILE
1	D	1033	THR
1	D	1046	THR
1	D	1049	ASN
1	D	1053	ILE
1	D	1057	THR
1	D	1093	SER
1	D	1097	ILE
1	D	1115	GLN
1	D	1119	ILE
1	D	1147	MET
1	D	1163	LEU
1	D	1183	ILE
1	D	1185	ARG
1	D	1189	GLU
1	D	1200	PRO
1	D	1205	VAL
1	D	1209	MET
1	D	1221	MET
1	D	1233	ILE
1	D	1235	GLU
1	D	1237	GLN
1	D	1242	ASN
1	D	1247	ILE
1	D	1249	LYS
1	D	1250	LEU
1	D	1253	GLU
1	D	1259	GLU
1	D	1261	ILE

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

Mol	Chain	Res	Type
1	B	1049	ASN
1	B	1226	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1239	HIS
1	B	1242	ASN
1	C	1007	ASN
1	D	1049	ASN
1	D	1237	GLN
1	D	1239	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	PX4	C	1304	-	9,9,45	1.13	1 (11%)	10,12,53	1.10	1 (10%)
4	G3P	C	1306	-	9,9,9	1.01	1 (11%)	10,12,12	1.03	1 (10%)
2	MC3	C	1302	-	20,20,45	1.79	3 (15%)	22,24,53	1.67	3 (13%)
3	PX4	C	1303	-	9,9,45	0.97	1 (11%)	10,12,53	1.03	1 (10%)
3	PX4	B	1303	-	9,9,45	0.98	0	10,12,53	1.10	1 (10%)
2	MC3	B	1302	-	20,20,45	1.68	3 (15%)	22,24,53	1.80	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	G3P	A	1303	-	9,9,9	1.00	1 (11%)	10,12,12	1.20	2 (20%)
4	G3P	D	1303	-	9,9,9	0.92	1 (11%)	10,12,12	1.21	1 (10%)
2	MC3	D	1302	-	20,20,45	1.79	2 (10%)	22,24,53	1.85	2 (9%)
6	C9X	D	1301	-	48,49,49	4.91	32 (66%)	63,71,71	4.02	31 (49%)
4	G3P	C	1305	-	9,9,9	0.94	0	10,12,12	0.75	0
3	PX4	A	1302	-	9,9,45	1.08	1 (11%)	10,12,53	1.27	1 (10%)
2	MC3	A	1301	-	20,20,45	1.90	4 (20%)	22,24,53	1.57	3 (13%)

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	PX4	C	1304	-	-	7/8/8/49	-
4	G3P	C	1306	-	-	6/8/8/8	-
2	MC3	C	1302	-	-	11/22/22/49	-
3	PX4	C	1303	-	-	5/8/8/49	-
3	PX4	B	1303	-	-	5/8/8/49	-
2	MC3	B	1302	-	-	11/22/22/49	-
4	G3P	A	1303	-	-	7/8/8/8	-
4	G3P	D	1303	-	-	2/8/8/8	-
2	MC3	D	1302	-	-	9/22/22/49	-
6	C9X	D	1301	-	-	5/26/66/66	0/5/5/5
4	G3P	C	1305	-	-	4/8/8/8	-
3	PX4	A	1302	-	-	7/8/8/49	-
2	MC3	A	1301	-	-	7/22/22/49	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1301	C9X	C04-N03	13.59	1.56	1.38
6	D	1301	C9X	P09-O11	12.87	1.68	1.57
6	D	1301	C9X	C07-C08	12.52	1.66	1.54
6	D	1301	C9X	C33-N32	8.57	1.58	1.46
6	D	1301	C9X	C33-C34	8.33	1.66	1.51
6	D	1301	C9X	C40-N32	7.75	1.60	1.38
6	D	1301	C9X	P09-O17	7.40	1.64	1.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1301	C9X	C27-C06	7.24	1.60	1.47
2	A	1301	MC3	O11-C11	6.12	1.40	1.22
2	D	1302	MC3	O11-C11	5.91	1.40	1.22
2	C	1302	MC3	O11-C11	5.73	1.39	1.22
6	D	1301	C9X	C01-C02	5.46	1.59	1.49
2	B	1302	MC3	O11-C11	5.31	1.38	1.22
6	D	1301	C9X	C23-C18	5.25	1.46	1.39
6	D	1301	C9X	C04-C06	5.19	1.41	1.35
6	D	1301	C9X	C45-C40	4.90	1.48	1.39
6	D	1301	C9X	C22-N24	4.84	1.56	1.45
6	D	1301	C9X	C12-C13	4.33	1.59	1.52
6	D	1301	C9X	P09-C08	4.02	1.85	1.78
6	D	1301	C9X	C02-N03	-3.89	1.33	1.38
6	D	1301	C9X	O11-C12	-3.86	1.39	1.46
6	D	1301	C9X	C05-C04	3.46	1.55	1.49
6	D	1301	C9X	C42-C41	3.43	1.44	1.38
6	D	1301	C9X	C20-C21	3.37	1.44	1.38
6	D	1301	C9X	C31-C30	3.33	1.60	1.50
2	A	1301	MC3	O3-C11	3.21	1.42	1.33
6	D	1301	C9X	P09-O10	3.19	1.50	1.46
6	D	1301	C9X	C44-C45	3.12	1.44	1.38
2	C	1302	MC3	O3-C11	3.12	1.42	1.33
6	D	1301	C9X	C16-C13	3.04	1.57	1.52
2	A	1301	MC3	P-O4P	2.90	1.68	1.58
6	D	1301	C9X	O29-C27	2.83	1.39	1.33
2	B	1302	MC3	O3-C11	2.81	1.41	1.33
6	D	1301	C9X	C41-C40	2.80	1.44	1.39
2	D	1302	MC3	O3-C11	2.74	1.41	1.33
3	C	1304	PX4	P1-O4	2.65	1.68	1.60
3	A	1302	PX4	P1-O4	2.56	1.68	1.60
6	D	1301	C9X	C21-C22	2.47	1.43	1.38
2	B	1302	MC3	O3-C3	-2.42	1.39	1.45
6	D	1301	C9X	C07-C06	2.38	1.55	1.52
4	A	1303	G3P	P-O1P	2.34	1.67	1.60
4	C	1306	G3P	P-O1P	2.32	1.67	1.60
6	D	1301	C9X	C36-C35	2.21	1.42	1.38
2	A	1301	MC3	O3-C3	-2.17	1.40	1.45
3	C	1303	PX4	P1-O4	2.17	1.67	1.60
6	D	1301	C9X	C35-C34	2.15	1.43	1.38
4	D	1303	G3P	P-O1P	2.14	1.67	1.60
6	D	1301	C9X	O26-N24	-2.13	1.21	1.35
2	C	1302	MC3	P-O4P	2.11	1.65	1.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1301	C9X	C20-C19	2.04	1.42	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1301	C9X	C01-C02-C08	-16.03	111.69	127.61
6	D	1301	C9X	C01-C02-N03	15.61	131.58	113.42
2	D	1302	MC3	O3-C11-O11	-7.70	104.37	123.63
6	D	1301	C9X	C34-C33-N32	6.51	124.67	114.13
6	D	1301	C9X	O29-C27-C06	6.08	123.23	112.28
6	D	1301	C9X	O17-P09-O11	-5.77	98.35	104.80
2	B	1302	MC3	O3-C11-O11	-5.64	109.52	123.63
6	D	1301	C9X	C05-C04-C06	-5.55	122.10	127.61
6	D	1301	C9X	C18-C07-C08	-5.48	101.74	111.48
2	C	1302	MC3	O3-C11-O11	-5.43	110.04	123.63
6	D	1301	C9X	C27-C06-C04	5.43	134.63	122.35
2	B	1302	MC3	O11-C11-C12	-5.16	103.61	123.78
6	D	1301	C9X	O29-C27-O28	-5.16	114.10	123.37
6	D	1301	C9X	C23-C18-C07	-5.13	113.93	120.42
6	D	1301	C9X	C21-C22-N24	4.73	123.47	119.34
6	D	1301	C9X	C08-C02-N03	-4.53	115.49	119.30
6	D	1301	C9X	C07-C06-C04	-4.20	116.08	120.86
2	A	1301	MC3	O3-C11-O11	-4.18	113.16	123.63
2	A	1301	MC3	O11-C11-C12	-4.11	107.72	123.78
2	C	1302	MC3	O11-C11-C12	-3.81	108.86	123.78
6	D	1301	C9X	C20-C19-C18	-3.81	116.08	120.65
6	D	1301	C9X	C44-C45-C40	3.54	123.89	119.68
6	D	1301	C9X	C06-C07-C08	3.34	117.21	108.73
6	D	1301	C9X	C45-C40-C41	-3.32	112.85	119.18
6	D	1301	C9X	C33-C34-C39	3.21	126.66	120.75
6	D	1301	C9X	C07-C06-C27	-3.18	109.28	117.09
6	D	1301	C9X	C30-O29-C27	3.15	122.97	116.55
6	D	1301	C9X	C39-C34-C35	-2.96	113.84	118.23
6	D	1301	C9X	C04-N03-C02	-2.89	120.75	123.44
6	D	1301	C9X	C05-C04-N03	2.86	116.74	113.42
4	D	1303	G3P	O4P-P-O1P	2.83	114.05	106.67
2	D	1302	MC3	O11-C11-C12	-2.83	112.73	123.78
6	D	1301	C9X	C36-C35-C34	2.80	124.55	120.61
6	D	1301	C9X	C19-C18-C07	2.70	124.41	120.95
6	D	1301	C9X	C22-C23-C18	2.59	121.44	119.06
4	A	1303	G3P	O4P-P-O1P	2.52	113.25	106.67
6	D	1301	C9X	C19-C18-C23	2.52	121.65	118.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1301	C9X	C18-C07-C06	-2.38	108.19	111.61
2	C	1302	MC3	O2-C2-C3	2.37	117.90	109.70
6	D	1301	C9X	O11-P09-O10	2.37	115.70	112.32
4	A	1303	G3P	O1P-P-O2P	2.33	112.73	106.44
6	D	1301	C9X	C42-C41-C40	2.28	122.39	119.68
6	D	1301	C9X	C06-C04-N03	2.21	121.15	119.29
3	B	1303	PX4	O4-P1-O2	2.19	112.37	106.44
3	A	1302	PX4	O1-P1-O2	-2.10	102.66	110.83
3	C	1304	PX4	O3-P1-O4	2.07	112.06	106.67
2	A	1301	MC3	O2P-P-O3P	2.06	116.92	107.57
3	C	1303	PX4	O3-P1-O4	2.06	112.04	106.67
4	C	1306	G3P	O1P-P-O2P	2.03	111.94	106.44

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	MC3	C1-O3P-P-O4P
2	B	1302	MC3	C1-C2-C3-O3
2	B	1302	MC3	C1-O3P-P-O1P
2	B	1302	MC3	C1-O3P-P-O2P
2	B	1302	MC3	C1-O3P-P-O4P
2	C	1302	MC3	C1-O3P-P-O1P
2	C	1302	MC3	C1-O3P-P-O2P
2	C	1302	MC3	C1-O3P-P-O4P
2	D	1302	MC3	C4-O4P-P-O2P
3	A	1302	PX4	C6-O4-P1-O1
3	A	1302	PX4	C6-O4-P1-O2
3	A	1302	PX4	C6-O4-P1-O3
3	A	1302	PX4	O4-C6-C7-O7
3	A	1302	PX4	C6-C7-C8-O5
3	B	1303	PX4	C6-O4-P1-O1
3	B	1303	PX4	C6-O4-P1-O2
3	C	1303	PX4	O4-C6-C7-C8
3	C	1304	PX4	C6-O4-P1-O1
3	C	1304	PX4	C6-O4-P1-O3
3	C	1304	PX4	C6-C7-C8-O5
4	A	1303	G3P	O1-C1-C2-C3
4	A	1303	G3P	C3-O1P-P-O3P
4	C	1305	G3P	C3-O1P-P-O4P
4	C	1305	G3P	C3-O1P-P-O2P
4	C	1305	G3P	C3-O1P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1306	G3P	O1-C1-C2-C3
4	D	1303	G3P	O1-C1-C2-O2
4	D	1303	G3P	O1-C1-C2-C3
6	D	1301	C9X	C02-C08-P09-O11
6	D	1301	C9X	C02-C08-P09-O17
6	D	1301	C9X	O28-C27-O29-C30
6	D	1301	C9X	C06-C27-O29-C30
2	B	1302	MC3	O11-C11-O3-C3
2	C	1302	MC3	O3P-C1-C2-O2
3	C	1303	PX4	O4-C6-C7-O7
2	D	1302	MC3	O3P-C1-C2-C3
2	C	1302	MC3	C12-C11-O3-C3
3	C	1304	PX4	O4-C6-C7-O7
2	B	1302	MC3	O2-C2-C3-O3
2	B	1302	MC3	C12-C11-O3-C3
3	A	1302	PX4	O7-C7-C8-O5
3	C	1303	PX4	O7-C7-C8-O5
2	C	1302	MC3	C11-C12-C13-C14
2	D	1302	MC3	O3P-C1-C2-O2
4	A	1303	G3P	O2-C2-C3-O1P
3	A	1302	PX4	O4-C6-C7-C8
3	B	1303	PX4	C6-C7-C8-O5
3	C	1303	PX4	C6-C7-C8-O5
2	D	1302	MC3	O11-C11-O3-C3
3	B	1303	PX4	O7-C7-C8-O5
4	A	1303	G3P	O1-C1-C2-O2
2	B	1302	MC3	C12-C13-C14-C15
6	D	1301	C9X	C34-C33-N32-C31
2	D	1302	MC3	C15-C16-C17-C18
2	C	1302	MC3	C15-C16-C17-C18
2	B	1302	MC3	C15-C16-C17-C18
4	A	1303	G3P	C1-C2-C3-O1P
4	C	1306	G3P	O1-C1-C2-O2
2	A	1301	MC3	O11-C11-O3-C3
2	A	1301	MC3	C15-C16-C17-C18
3	C	1304	PX4	C6-O4-P1-O2
2	D	1302	MC3	C13-C14-C15-C16
2	B	1302	MC3	C14-C15-C16-C17
2	D	1302	MC3	C16-C17-C18-C19
2	B	1302	MC3	C13-C14-C15-C16
4	A	1303	G3P	C3-O1P-P-O4P
3	C	1303	PX4	C7-C6-O4-P1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1303	G3P	C3-O1P-P-O2P
2	C	1302	MC3	C12-C13-C14-C15
2	D	1302	MC3	C14-C15-C16-C17
4	C	1306	G3P	O2-C2-C3-O1P
2	A	1301	MC3	C4-O4P-P-O1P
2	A	1301	MC3	C16-C17-C18-C19
3	C	1304	PX4	C7-C6-O4-P1
3	C	1304	PX4	O7-C7-C8-O5
2	C	1302	MC3	O3P-C1-C2-C3
2	A	1301	MC3	C11-C12-C13-C14
4	C	1305	G3P	C2-C3-O1P-P
3	B	1303	PX4	C6-O4-P1-O3
4	C	1306	G3P	C3-O1P-P-O2P
4	C	1306	G3P	C3-O1P-P-O3P
4	C	1306	G3P	C1-C2-C3-O1P
2	C	1302	MC3	O2-C2-C3-O3
2	A	1301	MC3	C12-C13-C14-C15
2	C	1302	MC3	C4-O4P-P-O1P
2	D	1302	MC3	O3-C11-C12-C13

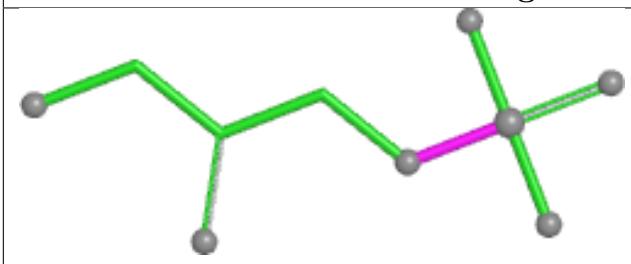
There are no ring outliers.

3 monomers are involved in 3 short contacts:

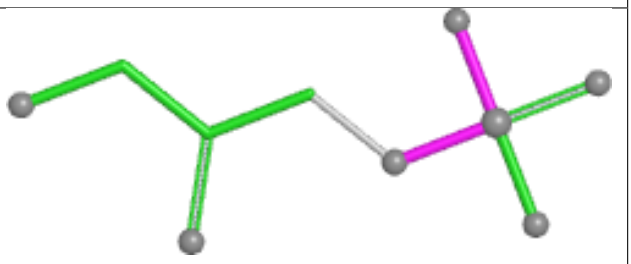
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1302	MC3	1	0
3	A	1302	PX4	1	0
2	A	1301	MC3	1	0

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 PX4 C 1304



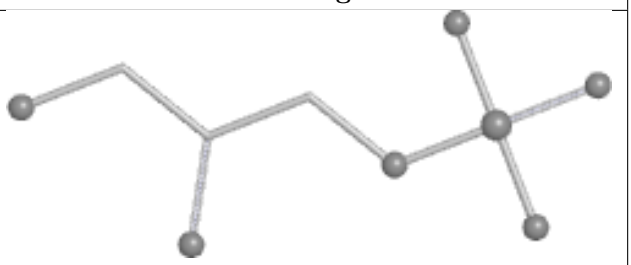
Bond lengths



Bond angles

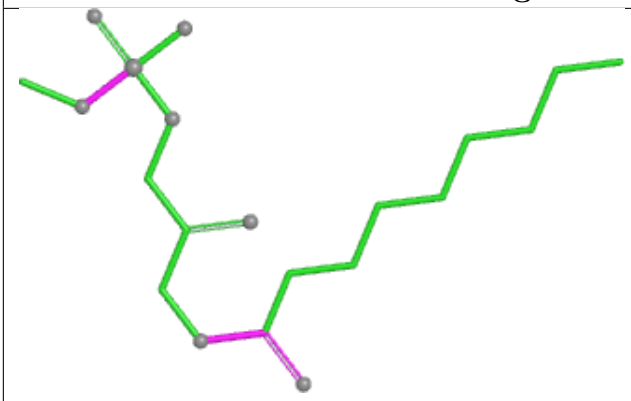


Torsions

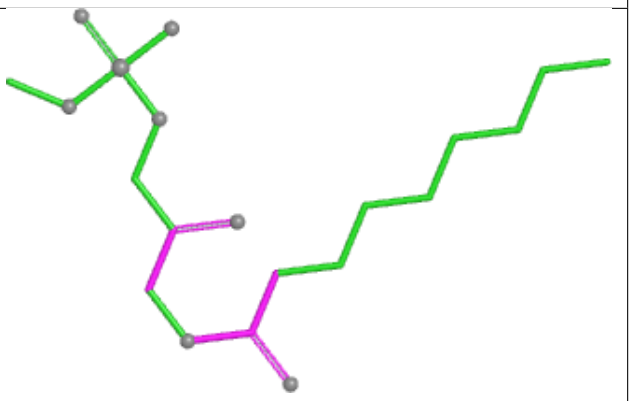


Rings

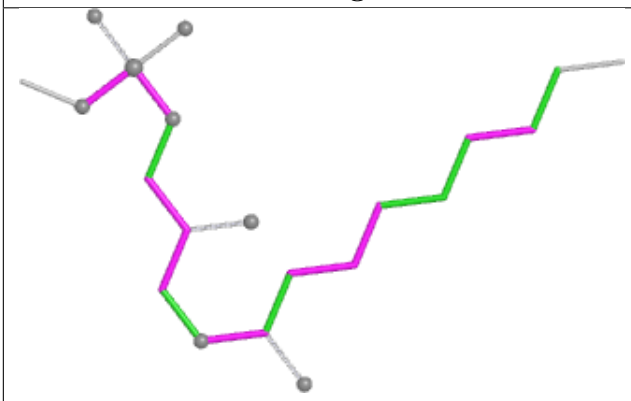
Ligand MC3 C 1302



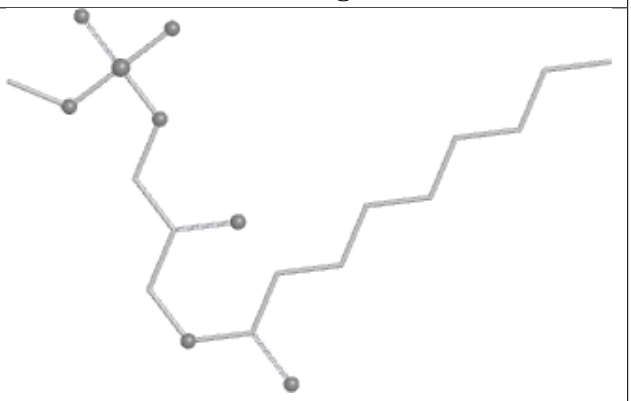
Bond lengths



Bond angles

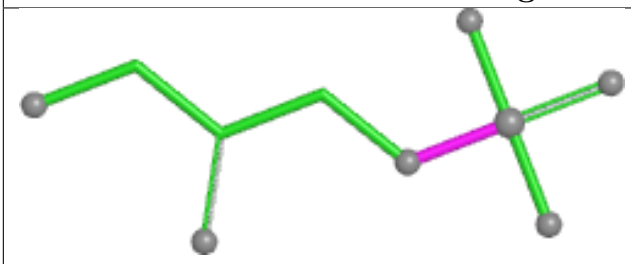


Torsions

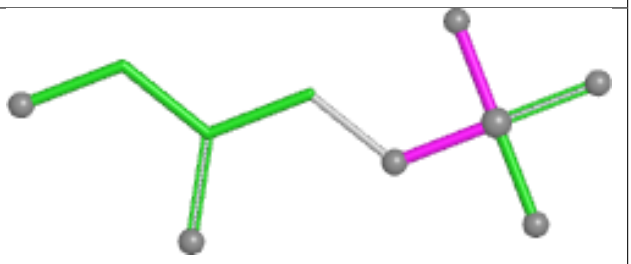


Rings

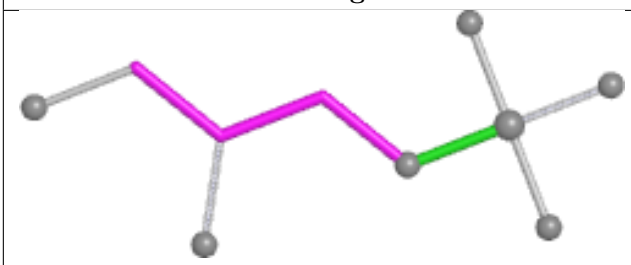
Ligand PX4 C 1303



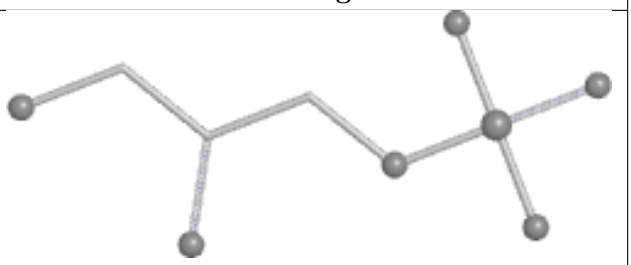
Bond lengths



Bond angles

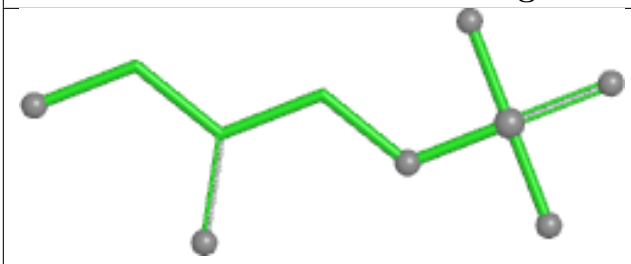


Torsions

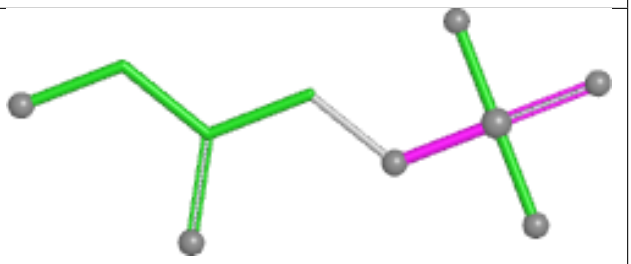


Rings

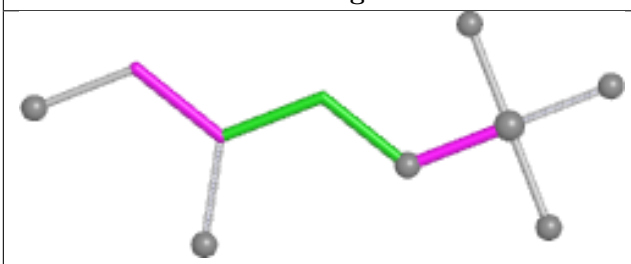
Ligand PX4 B 1303



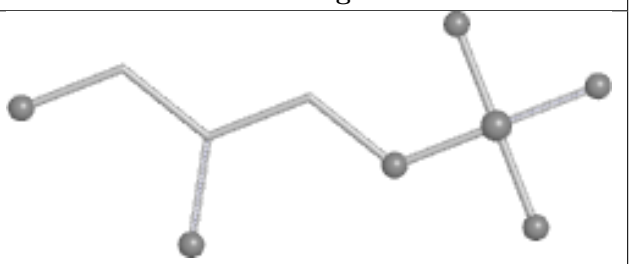
Bond lengths



Bond angles

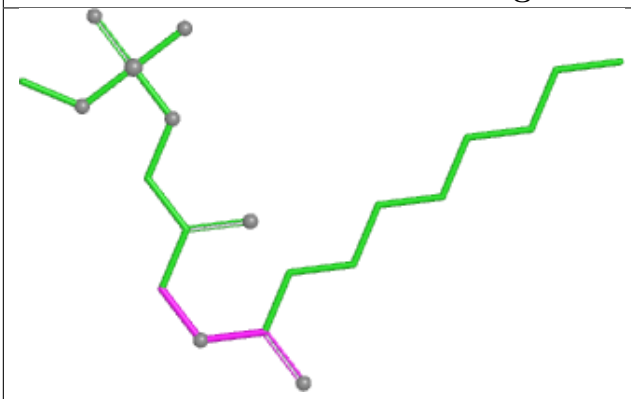


Torsions

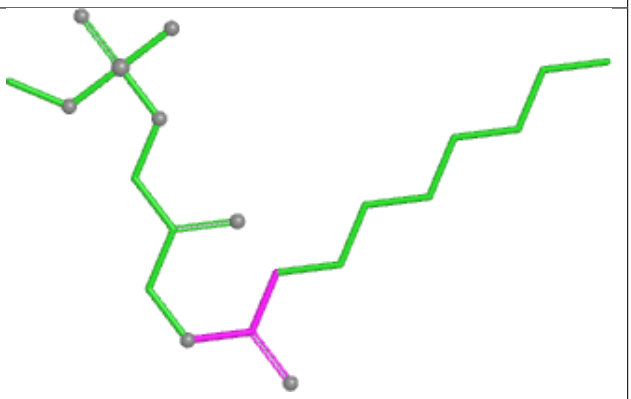


Rings

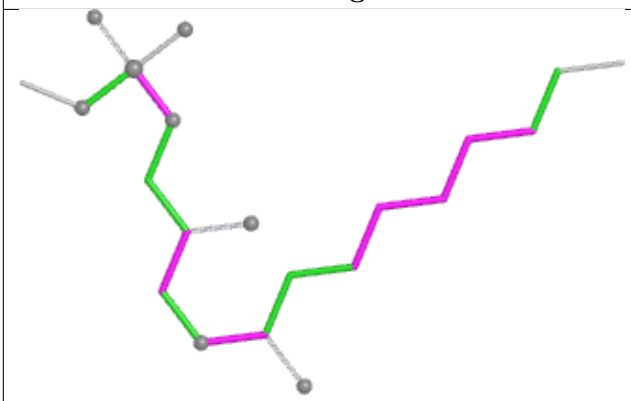
Ligand MC3 B 1302



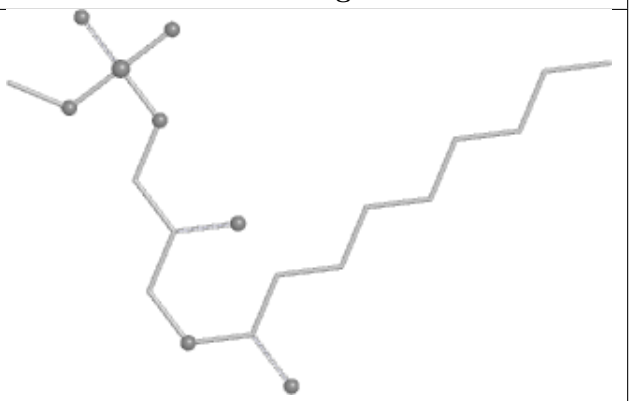
Bond lengths



Bond angles

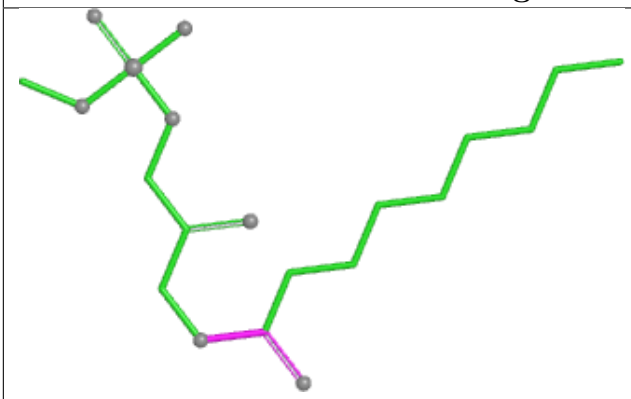


Torsions

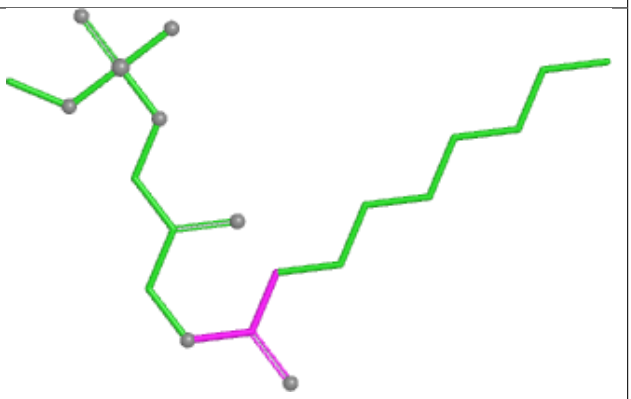


Rings

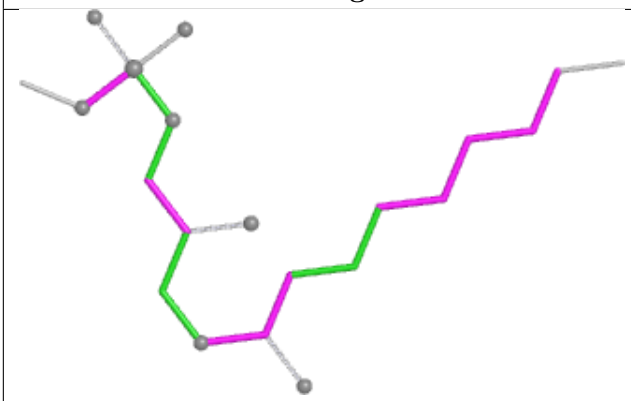
Ligand MC3 D 1302



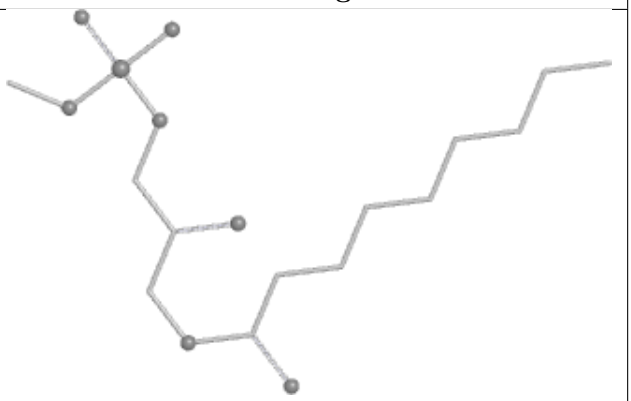
Bond lengths



Bond angles

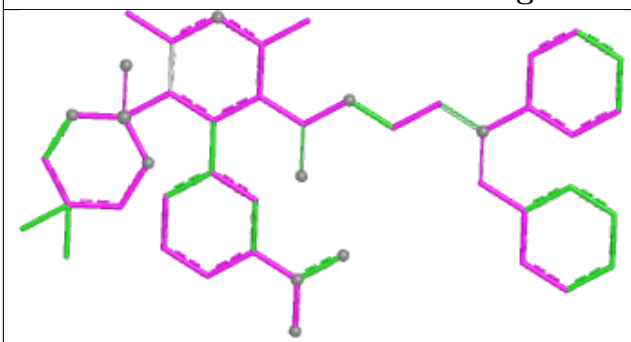


Torsions

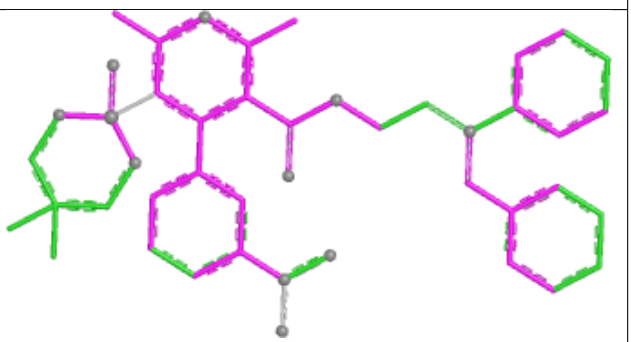


Rings

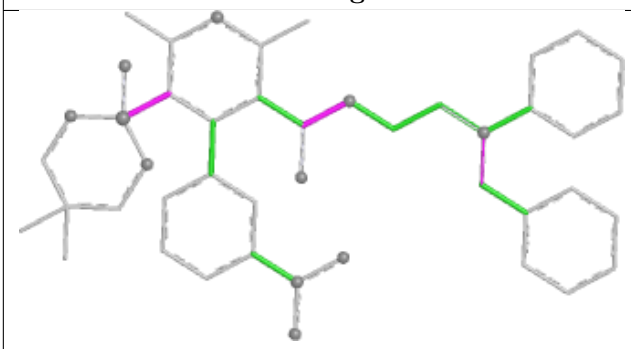
Ligand C9X D 1301



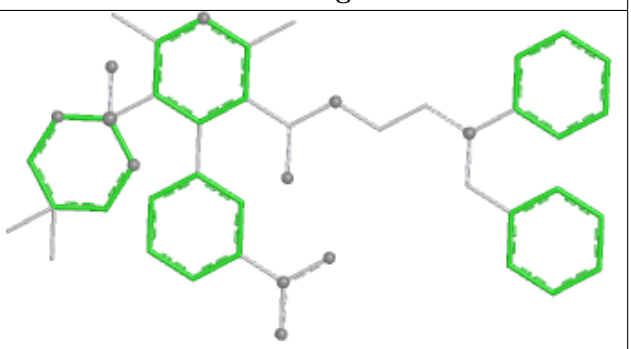
Bond lengths



Bond angles

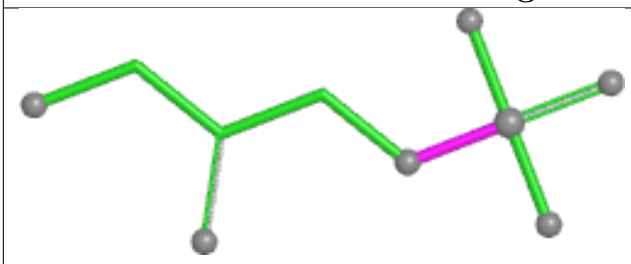


Torsions

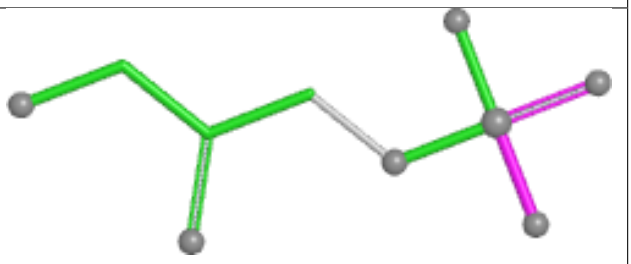


Rings

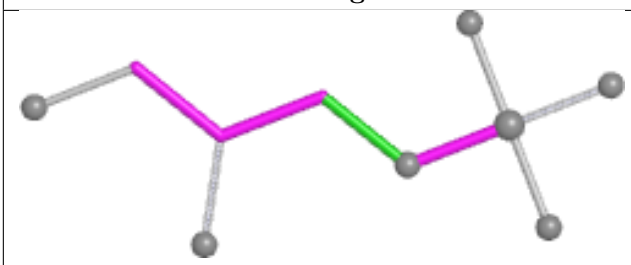
Ligand PX4 A 1302



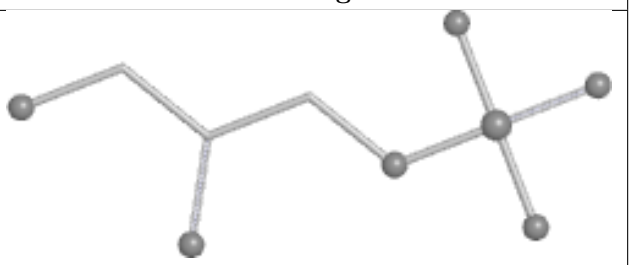
Bond lengths



Bond angles

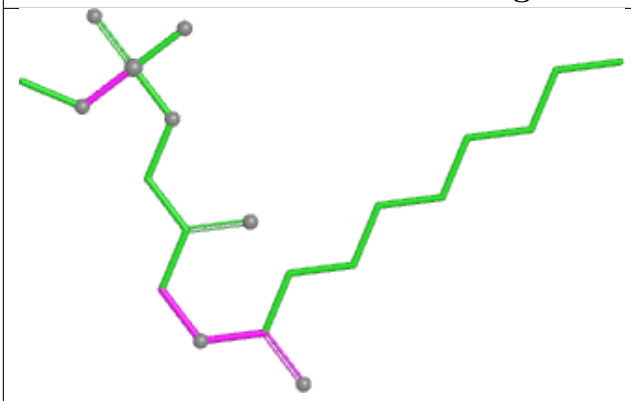


Torsions

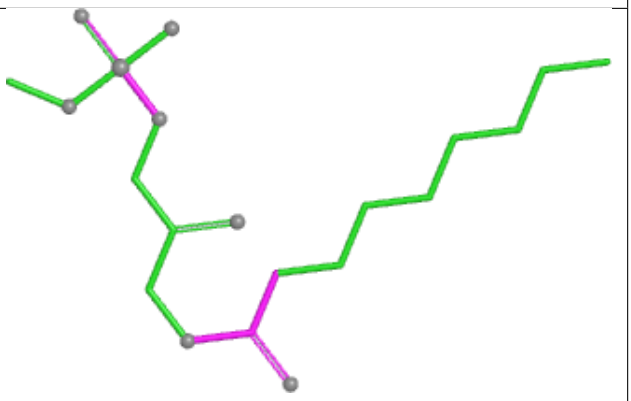


Rings

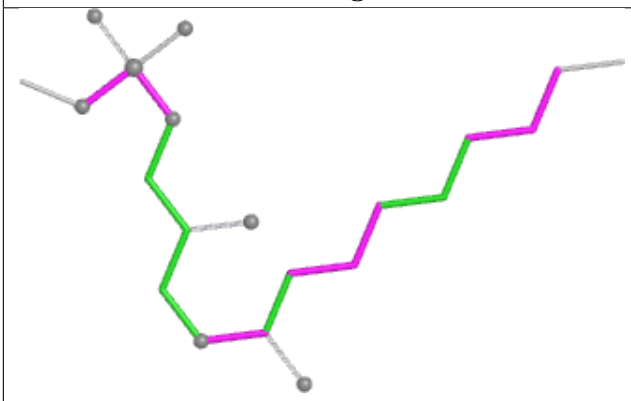
Ligand MC3 A 1301



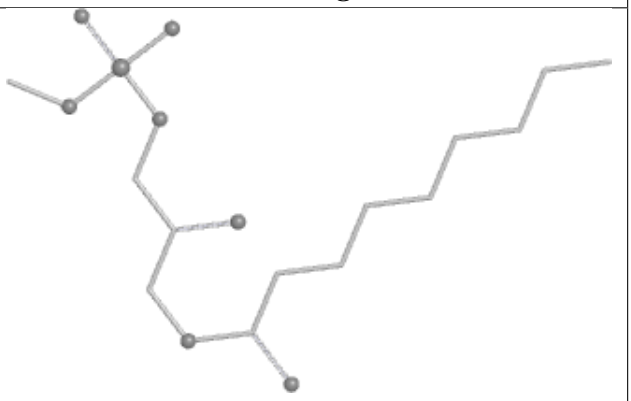
Bond lengths



Bond angles



Torsions



Rings

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	263/267 (98%)	0.21	13 (4%)	35	18	39, 79, 171, 199	0
1	B	263/267 (98%)	0.22	18 (6%)	23	12	35, 78, 162, 218	0
1	C	261/267 (97%)	0.24	22 (8%)	17	9	37, 81, 171, 198	0
1	D	263/267 (98%)	0.19	18 (6%)	23	12	39, 80, 189, 234	0
All	All	1050/1068 (98%)	0.21	71 (6%)	23	12	35, 80, 176, 234	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1260	LEU	5.9
1	C	1261	ILE	5.5
1	B	1242	ASN	5.2
1	A	1244	ASN	4.3
1	C	1239	HIS	4.1
1	C	1001	MET	4.0
1	B	1259	GLU	4.0
1	D	1240	GLU	4.0
1	D	1247	ILE	3.9
1	C	1245	ASN	3.8
1	C	1246	GLU	3.7
1	D	1182	GLY	3.7
1	A	1095	PHE	3.6
1	B	1263	THR	3.5
1	B	1095	PHE	3.5
1	A	1263	THR	3.5
1	B	1091	THR	3.4
1	D	1257	LEU	3.4
1	B	1246	GLU	3.4
1	A	1260	LEU	3.2
1	C	1096	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1090	PRO	3.2
1	C	1043	VAL	3.1
1	B	1245	ASN	3.1
1	D	1095	PHE	3.1
1	C	1244	ASN	3.0
1	B	1256	GLU	3.0
1	D	1261	ILE	3.0
1	A	1261	ILE	2.9
1	D	1099	ARG	2.9
1	D	1244	ASN	2.8
1	D	1226	GLN	2.8
1	D	1248	ILE	2.7
1	B	1040	SER	2.7
1	B	1089	VAL	2.7
1	A	1065	TYR	2.6
1	C	1243	ILE	2.6
1	A	1258	LYS	2.6
1	B	1249	LYS	2.6
1	D	1235	GLU	2.6
1	C	1254	ILE	2.6
1	A	1242	ASN	2.5
1	C	1248	ILE	2.5
1	D	1246	GLU	2.4
1	A	1043	VAL	2.4
1	D	1249	LYS	2.4
1	D	1239	HIS	2.4
1	C	1240	GLU	2.4
1	B	1261	ILE	2.3
1	C	1225	ASN	2.3
1	D	1007	ASN	2.3
1	C	1003	LEU	2.3
1	B	1252	GLU	2.3
1	B	1244	ASN	2.3
1	B	1238	SER	2.3
1	C	1095	PHE	2.3
1	A	1254	ILE	2.2
1	C	1221	MET	2.2
1	D	1253	GLU	2.2
1	B	1086	ILE	2.2
1	C	1092	SER	2.2
1	B	1044	TYR	2.1
1	C	1260	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1070	SER	2.1
1	A	1259	GLU	2.1
1	A	1262	LYS	2.1
1	D	1258	LYS	2.1
1	D	1256	GLU	2.1
1	C	1065	TYR	2.1
1	A	1002	TYR	2.1
1	C	1247	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

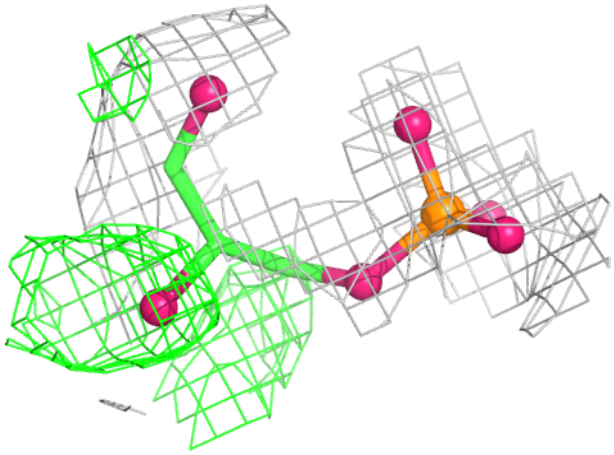
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

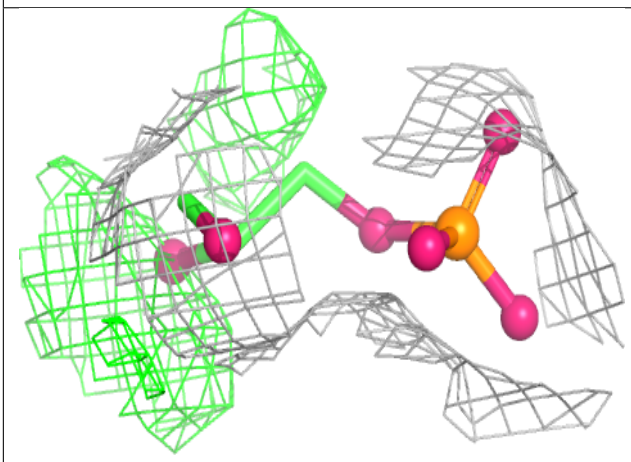
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PX4	C	1303	10/46	0.60	0.20	99,139,178,181	0
4	G3P	C	1305	10/10	0.70	0.20	116,134,149,154	0
3	PX4	A	1302	10/46	0.77	0.13	68,83,116,116	0
4	G3P	A	1303	10/10	0.84	0.15	89,102,134,135	0
3	PX4	B	1303	10/46	0.84	0.11	50,80,111,126	0
6	C9X	D	1301	45/45	0.84	0.19	56,95,114,115	0
4	G3P	D	1303	10/10	0.86	0.17	75,96,128,139	0
3	PX4	C	1304	10/46	0.86	0.12	58,81,118,124	0
4	G3P	C	1306	10/10	0.87	0.18	100,115,123,128	0
2	MC3	C	1302	21/46	0.90	0.16	55,80,88,88	0
2	MC3	D	1302	21/46	0.91	0.15	41,83,95,96	0
2	MC3	A	1301	21/46	0.92	0.15	61,74,88,93	0
2	MC3	B	1302	21/46	0.94	0.12	56,68,87,95	0
5	CA	B	1301	1/1	0.95	0.22	97,97,97,97	0
5	CA	C	1301	1/1	1.00	0.02	56,56,56,56	0

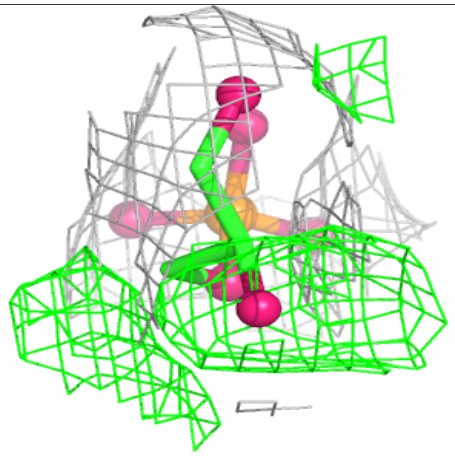
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PX4 C 1303:

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

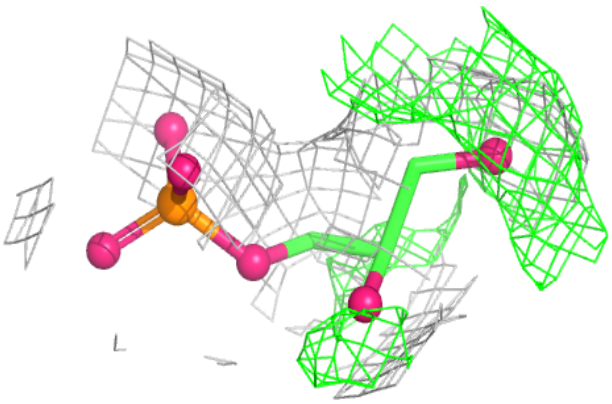


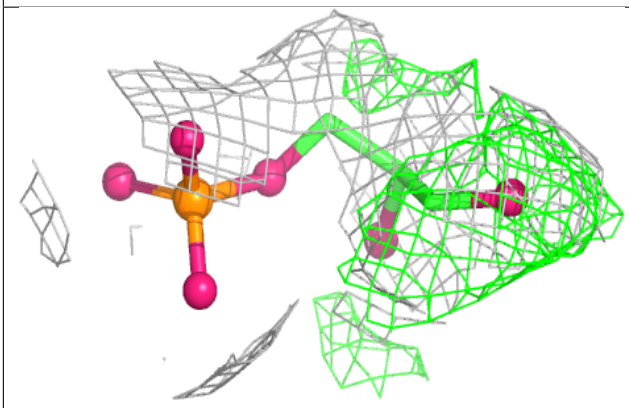


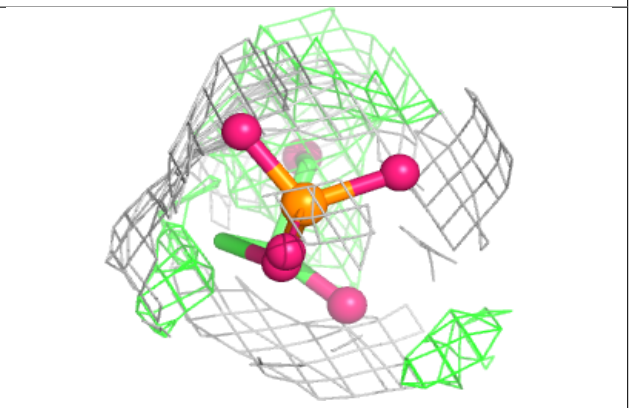


Electron density around PX4 A 1302:

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

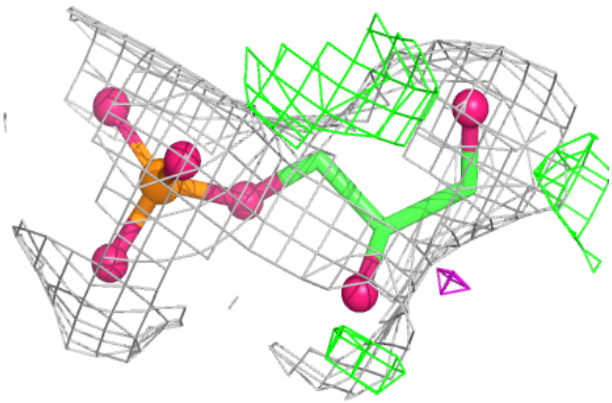


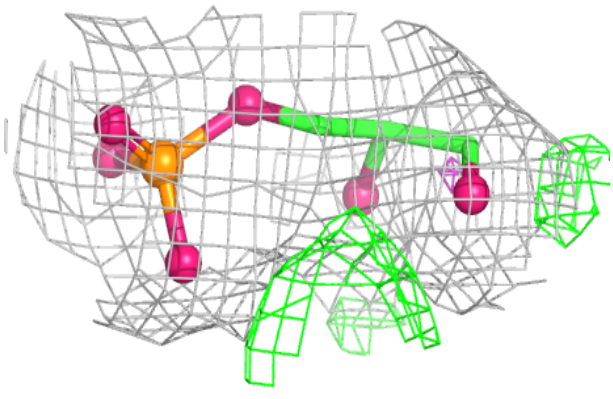


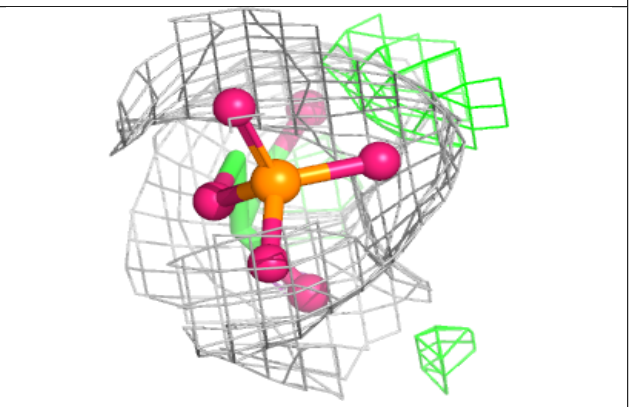


Electron density around PX4 B 1303:

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

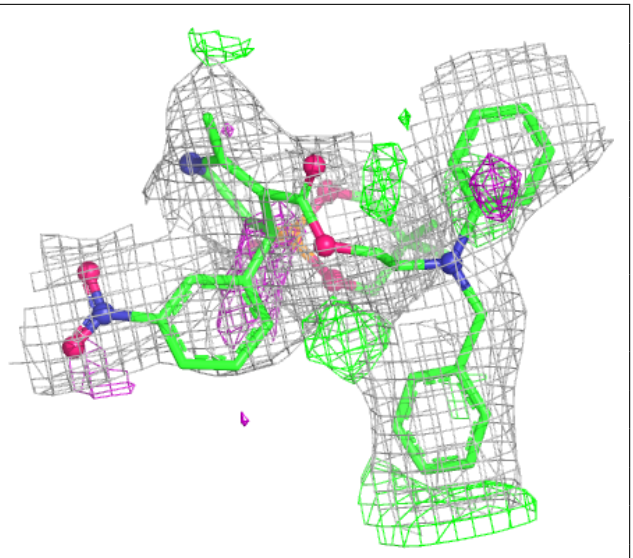


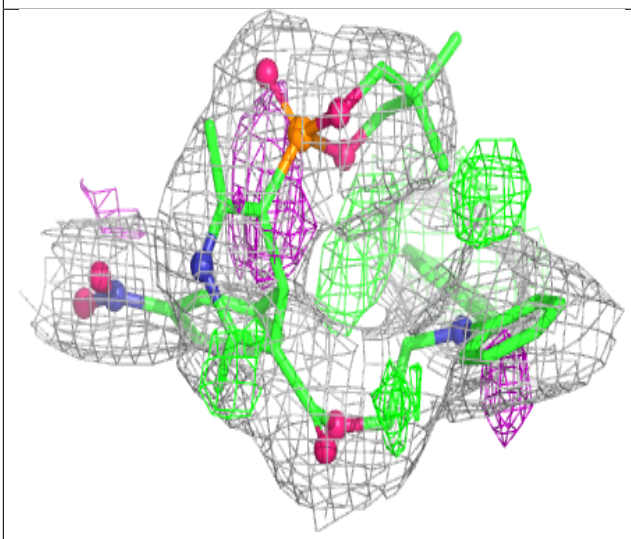


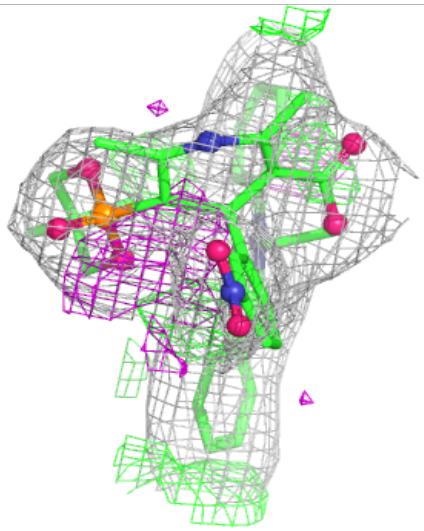


Electron density around C9X D 1301:

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

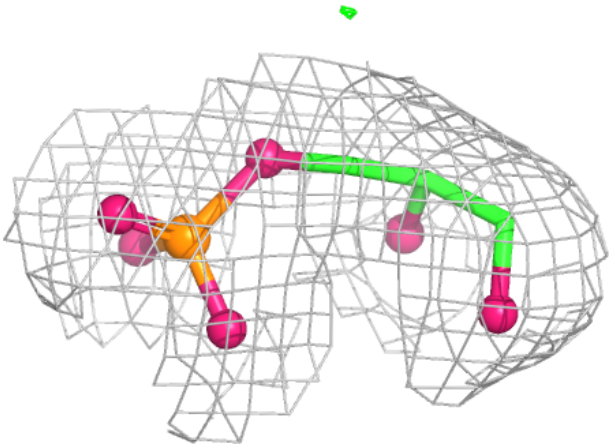


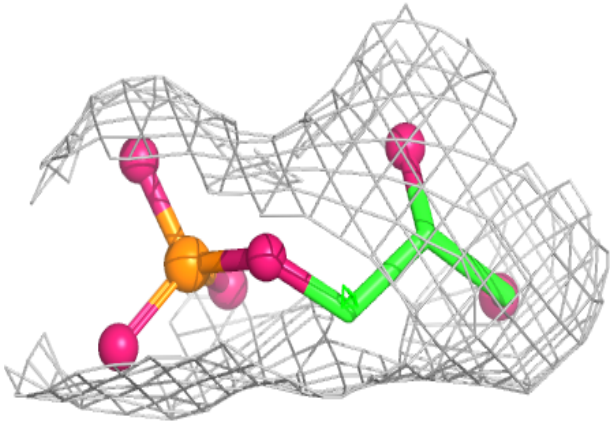


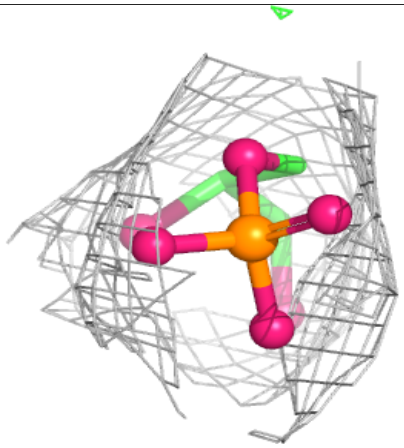


Electron density around PX4 C 1304:

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

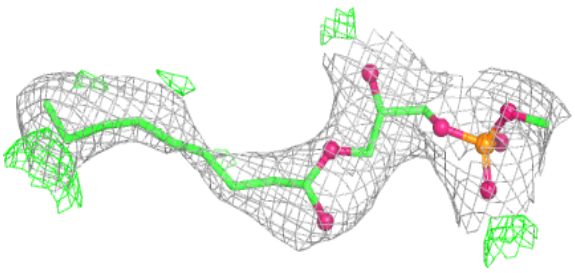


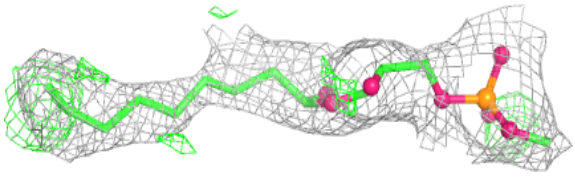


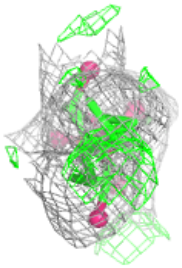


Electron density around MC3 C 1302:

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

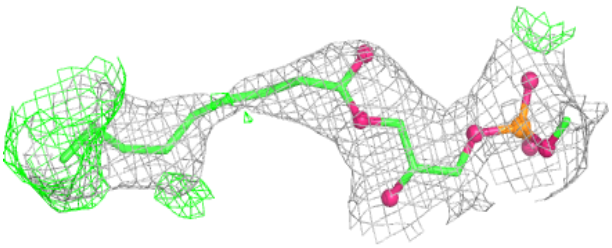


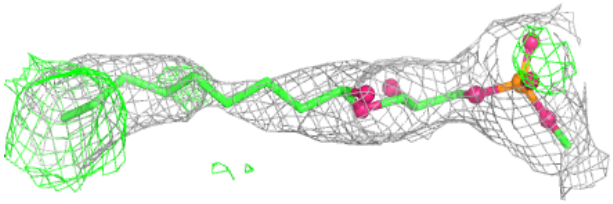


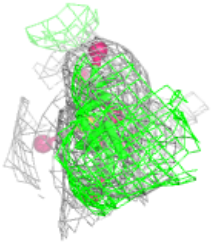


Electron density around MC3 D 1302:

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

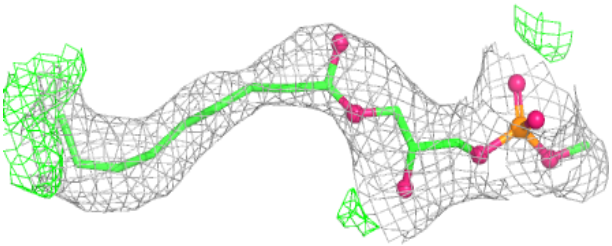


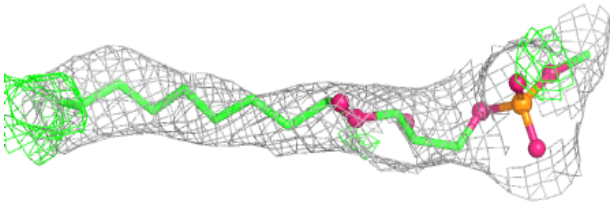


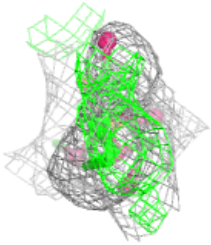


Electron density around MC3 A 1301:

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

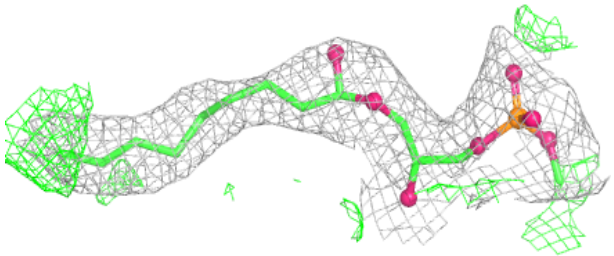


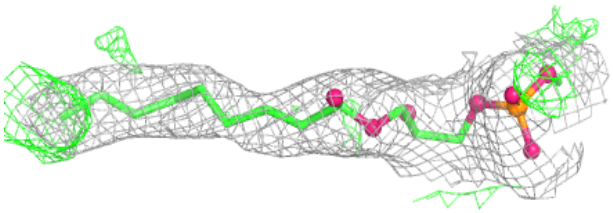


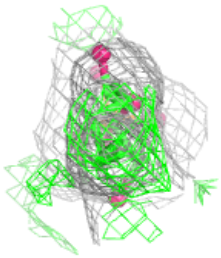


Electron density around MC3 B 1302:

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







6.5 Other polymers

There are no such residues in this entry.