



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:58 PM BST

PDB ID : 4K10
Title : Crystal Structure of Leshmaniasis major Farnesyl diphosphate synthase in complex with 3-FLUORO-1-(2-HYDROXY-2,2-DIPHOSPHONOETHYL)PYRIDINIUM and Mg²⁺
Authors : Aripirala, S.; Gabelli, S.; Amzel, L.M.
Deposited on : 2013-04-04
Resolution : 2.30 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

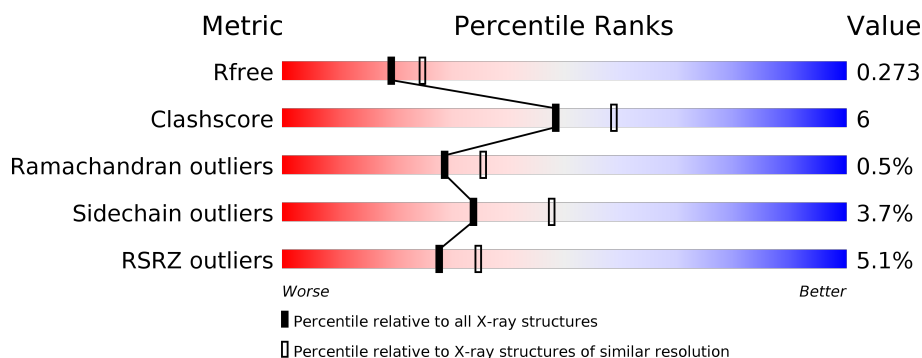
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	362	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	362	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	D	362	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11773 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	1	0
			2852	1824	472	532	24			
1	B	358	Total	C	N	O	S	0	0	0
			2835	1816	466	529	24			
1	D	360	Total	C	N	O	S	0	0	0
			2855	1828	472	531	24			
1	C	360	Total	C	N	O	S	0	0	0
			2856	1827	473	532	24			

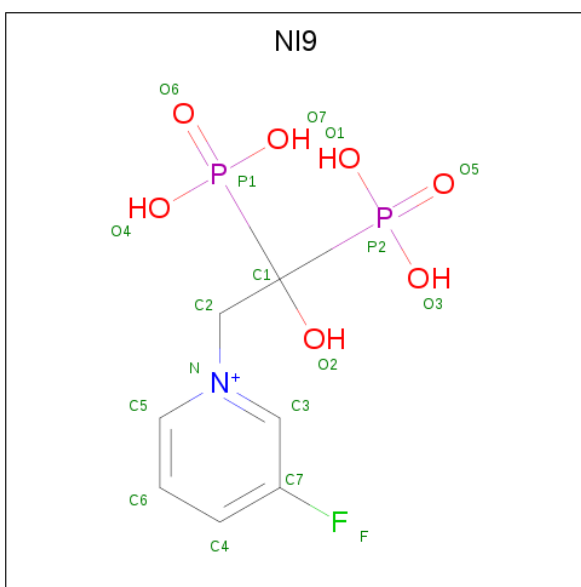
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	3	Total	Na	0	0
			3	3		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

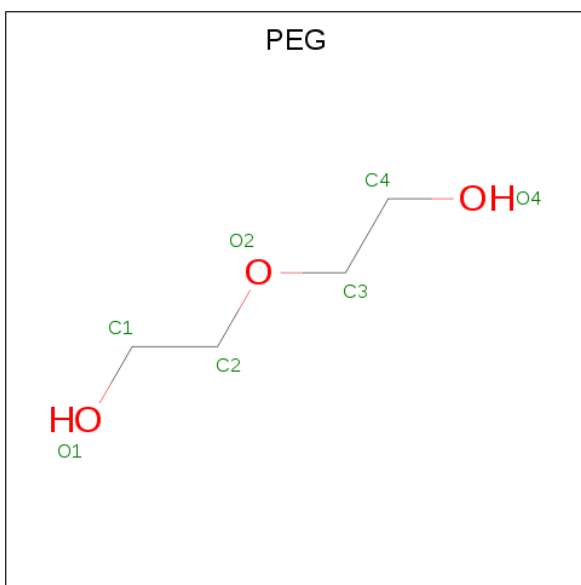
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is 3-FLUORO-1-(2-HYDROXY-2,2-DIPHOSPHONOETHYL)PYRIDINIUM (three-letter code: NI9) (formula: C₇H₁₁FNO₇P₂).



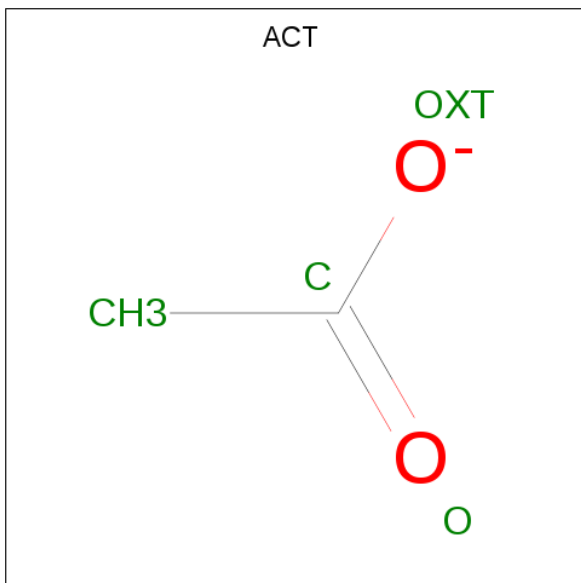
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 18	C 7	F 1	N 1	O 7	P 2	0	0
4	B	1	Total 18	C 7	F 1	N 1	O 7	P 2	0	0
4	D	1	Total 18	C 7	F 1	N 1	O 7	P 2	0	0
4	C	1	Total 18	C 7	F 1	N 1	O 7	P 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

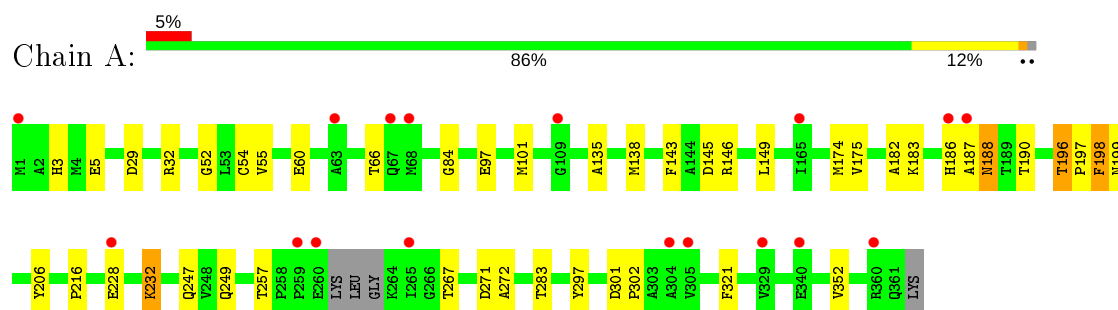
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	63	Total	O	0	0
			63	63		
8	B	70	Total	O	0	0
			70	70		
8	D	58	Total	O	0	0
			58	58		
8	C	71	Total	O	0	0
			71	71		

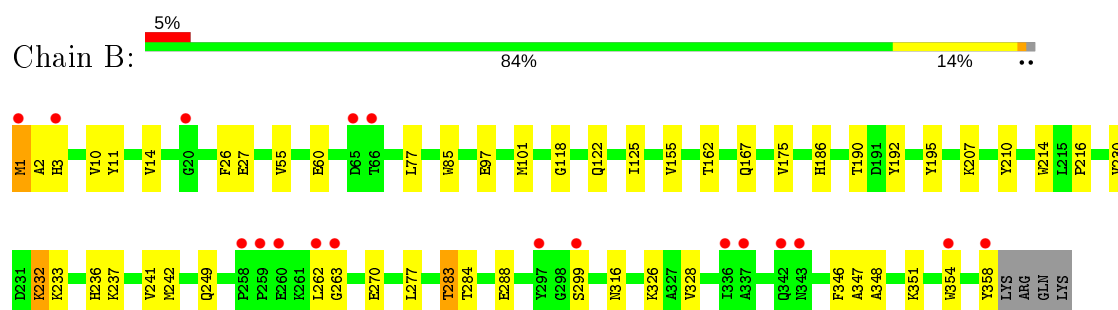
3 Residue-property plots [i](#)

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.

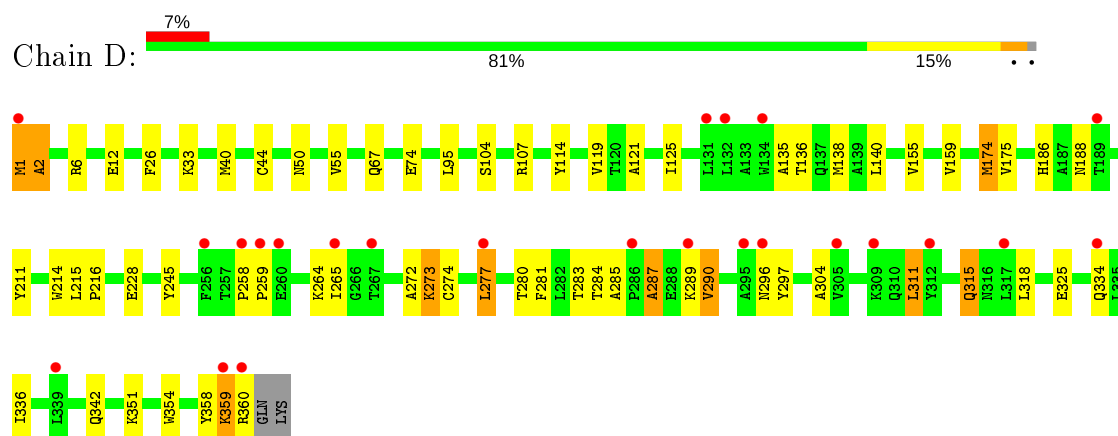
- Molecule 1: Farnesyl pyrophosphate synthase



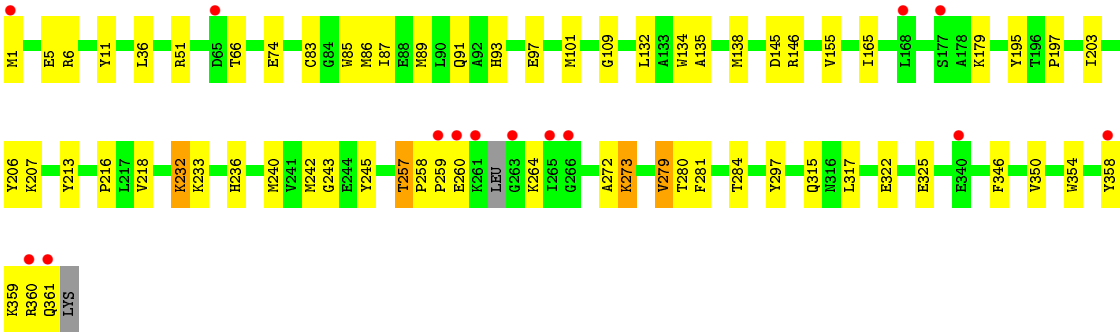
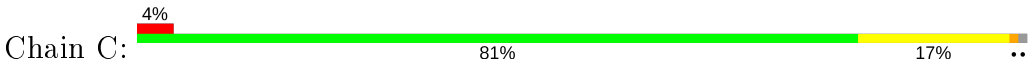
- Molecule 1: Farnesyl pyrophosphate synthase



- Molecule 1: Farnesyl pyrophosphate synthase



- Molecule 1: Farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.17Å 143.74Å 194.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 2.30 46.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.6 (115.47-2.30) 89.6 (46.14-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.276 0.231 , 0.273	Depositor DCC
R_{free} test set	3410 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.71$, $\langle L^2 \rangle = 0.60$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NA, NI9, MES, ACT, PEG

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	0.52	0/2913	0.58	0/3948
1	B	0.49	0/2897	0.56	0/3929
1	C	0.53	0/2917	0.61	0/3952
1	D	0.51	0/2917	0.58	0/3954
All	All	0.51	0/11644	0.58	0/15783

There are no bond length outliers.

There are no bond angle outliers.

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	2852	0	2815	32	0
1	B	2835	0	2802	34	0
1	C	2856	0	2824	39	0
1	D	2855	0	2828	42	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	18	0	7	0	0
4	B	18	0	7	0	0
4	C	18	0	7	0	0
4	D	18	0	7	1	0
5	A	7	0	10	1	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	D	12	0	12	0	0
8	A	63	0	0	2	0
8	B	70	0	0	1	0
8	C	71	0	0	2	0
8	D	58	0	0	3	0
All	All	11773	0	11325	138	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 6.

All (138) 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:264:LYS:HG2	1:D:265:ILE:H	1.31	0.95
1:C:273:LYS:HG2	8:C:562:HOH:O	1.78	0.83
1:D:175:VAL:HG21	1:D:186:HIS:HB2	1.62	0.81
1:B:232:LYS:HE3	1:B:233:LYS:HD3	1.64	0.78
1:A:187:ALA:HA	8:A:549:HOH:O	1.82	0.77
1:B:190:THR:HG22	1:B:192:TYR:H	1.48	0.77
1:A:267:THR:HG23	1:A:271:ASP:OD2	1.84	0.77
1:A:135:ALA:HA	1:A:138:MET:HE3	1.69	0.74
1:A:135:ALA:HA	1:A:138:MET:CE	2.21	0.71
1:A:206:TYR:OH	1:B:27:GLU:OE2	2.06	0.70
1:C:89:MET:HE3	1:C:134:TRP:HE3	1.56	0.70
1:C:245:TYR:HE2	1:C:325:GLU:HG2	1.60	0.67
1:A:5:GLU:HB2	8:A:529:HOH:O	1.96	0.66
1:B:55:VAL:HG22	1:B:216:PRO:HA	1.79	0.64
1:D:264:LYS:HG2	1:D:265:ILE:N	2.10	0.64
1:B:242:MET:HE1	1:B:354:TRP:HB2	1.82	0.62
1:A:101:MET:HE2	1:B:125:ILE:CG2	2.30	0.62
1:D:277:LEU:HD23	1:D:277:LEU:H	1.63	0.62
1:C:109:GLY:H	1:C:264:LYS:HE2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HG11	1:B:186:HIS:HB2	1.83	0.61
1:C:89:MET:HE1	1:C:134:TRP:HB2	1.82	0.60
1:C:6:ARG:NH1	1:C:74:GLU:OE2	2.22	0.60
1:A:145:ASP:OD1	1:A:146:ARG:NH1	2.33	0.60
1:B:348:ALA:HA	1:B:351:LYS:HD2	1.83	0.60
1:D:6:ARG:NH1	1:D:74:GLU:OE2	2.23	0.60
1:D:289:LYS:HZ3	1:D:315:GLN:HG3	1.68	0.59
1:D:273:LYS:HZ3	1:D:273:LYS:HA	1.67	0.59
1:D:296:ASN:HD22	1:D:304:ALA:HA	1.68	0.58
1:D:336:ILE:HD13	1:D:351:LYS:HG2	1.85	0.58
1:D:281:PHE:O	1:D:285:ALA:HB2	2.04	0.58
5:A:407:PEG:H21	1:D:33:LYS:HD3	1.86	0.57
1:D:2:ALA:O	8:D:510:HOH:O	2.17	0.57
1:A:196:THR:HG22	1:A:199:ASN:H	1.69	0.57
1:A:197:PRO:HD3	1:A:283:THR:HG21	1.86	0.57
1:D:287:ALA:O	1:D:290:VAL:HG13	2.06	0.55
1:D:283:THR:HG23	1:D:284:THR:HG23	1.88	0.55
1:C:51:ARG:CZ	1:C:91:GLN:HE22	2.20	0.54
1:A:101:MET:CE	1:B:125:ILE:HG22	2.38	0.54
1:C:272:ALA:HA	1:C:297:TYR:CE2	2.43	0.54
1:B:97:GLU:HB3	1:B:101:MET:HE2	1.89	0.53
1:D:1:MET:O	1:D:2:ALA:HB3	2.08	0.53
1:A:228:GLU:O	1:A:228:GLU:HG3	2.07	0.53
1:B:210:TYR:CE2	1:B:236:HIS:HE1	2.26	0.53
1:A:101:MET:HE2	1:B:125:ILE:HG21	1.91	0.53
1:D:354:TRP:CZ2	1:D:358:TYR:HB2	2.44	0.52
1:D:1:MET:O	1:D:2:ALA:CB	2.58	0.52
1:D:135:ALA:HA	1:D:138:MET:HE3	1.91	0.51
1:C:145:ASP:OD1	1:C:146:ARG:NH1	2.44	0.51
1:C:155:VAL:HG21	1:C:218:VAL:HG11	1.92	0.51
1:C:346:PHE:O	1:C:350:VAL:HG23	2.11	0.51
1:C:51:ARG:NH1	1:C:91:GLN:HE22	2.09	0.51
1:B:10:VAL:O	1:B:14:VAL:HG13	2.11	0.50
1:D:121:ALA:O	1:D:125:ILE:HG13	2.12	0.50
1:D:50:ASN:HB2	8:D:540:HOH:O	2.11	0.50
1:D:40:MET:O	1:D:44:CYS:HB2	2.12	0.50
1:D:135:ALA:HA	1:D:138:MET:CE	2.42	0.49
1:A:101:MET:O	1:B:122:GLN:HG3	2.11	0.49
1:C:203:ILE:O	1:C:207:LYS:HB3	2.13	0.49
1:D:174:MET:HE2	1:D:174:MET:HA	1.95	0.49
1:A:101:MET:HE2	1:B:125:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:TYR:O	1:D:359:LYS:HB3	2.12	0.49
1:A:175:VAL:HG21	1:A:186:HIS:HB3	1.94	0.49
1:C:87:ILE:HD13	1:C:216:PRO:HG3	1.95	0.49
1:C:232:LYS:HE2	1:C:232:LYS:O	2.13	0.48
1:D:245:TYR:HE2	1:D:325:GLU:HG3	1.78	0.48
1:C:236:HIS:O	1:C:240:MET:HG2	2.14	0.48
1:D:95:LEU:HD13	1:D:107:ARG:NH1	2.29	0.48
1:C:280:THR:O	1:C:284:THR:HG22	2.14	0.47
1:A:174:MET:O	1:A:190:THR:HA	2.15	0.47
1:D:273:LYS:HZ2	1:D:274:CYS:H	1.63	0.47
1:C:197:PRO:HA	1:C:279:VAL:HG11	1.96	0.47
1:D:215:LEU:HB3	1:D:216:PRO:HD3	1.97	0.47
1:B:155:VAL:HG23	1:B:214:TRP:CZ3	2.50	0.47
1:C:135:ALA:HA	1:C:138:MET:HE3	1.97	0.47
1:C:232:LYS:NZ	1:C:233:LYS:HD3	2.30	0.47
1:B:232:LYS:HE3	1:B:233:LYS:CD	2.39	0.46
1:B:60:GLU:HG3	1:B:77:LEU:HD21	1.97	0.46
1:B:242:MET:CE	1:B:354:TRP:HB2	2.44	0.46
1:D:289:LYS:HG2	1:D:311:LEU:HD13	1.97	0.46
1:A:182:ALA:O	1:B:118:GLY:N	2.42	0.46
1:B:11:TYR:HB2	1:B:85:TRP:CZ2	2.51	0.45
1:D:245:TYR:CE2	1:D:325:GLU:HG3	2.51	0.45
1:B:249:GLN:HE22	1:B:358:TYR:C	2.20	0.45
1:C:284:THR:HG23	1:C:315:GLN:HE21	1.80	0.45
1:B:190:THR:HG22	1:B:192:TYR:N	2.26	0.44
1:C:245:TYR:CE2	1:C:325:GLU:HG2	2.46	0.44
1:A:55:VAL:HG22	1:A:216:PRO:HA	1.99	0.44
1:A:232:LYS:C	1:A:232:LYS:HD3	2.38	0.44
1:C:358:TYR:O	1:C:359:LYS:HB2	2.17	0.44
1:A:97:GLU:O	1:A:101:MET:HG3	2.18	0.44
1:C:257:THR:HA	1:C:258:PRO:HD3	1.87	0.44
1:D:55:VAL:HG22	1:D:216:PRO:HA	2.00	0.44
1:B:1:MET:HA	1:B:2:ALA:HA	1.66	0.43
1:B:162:THR:HG21	1:B:210:TYR:CD1	2.52	0.43
1:A:3:HIS:NE2	1:A:60:GLU:OE1	2.45	0.43
1:D:136:THR:O	1:D:140:LEU:HG	2.17	0.43
1:A:143:PHE:HB2	1:A:149:LEU:HD13	1.99	0.43
1:B:230:VAL:HG11	1:B:346:PHE:CD2	2.53	0.43
1:D:359:LYS:O	1:D:360:ARG:C	2.56	0.43
8:D:531:HOH:O	1:C:101:MET:HE1	2.19	0.43
1:D:258:PRO:HA	1:D:259:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:HG23	1:A:198:PHE:H	1.83	0.43
1:A:249:GLN:HG3	1:A:321:PHE:CZ	2.53	0.43
1:A:54:CYS:SG	1:A:216:PRO:HB2	2.59	0.43
1:A:52:GLY:HA2	1:A:84:GLY:HA2	2.01	0.43
1:B:283:THR:HG22	1:B:284:THR:HG23	2.01	0.43
1:D:354:TRP:CE2	1:D:358:TYR:HB2	2.54	0.43
1:C:165:ILE:HA	1:C:165:ILE:HD13	1.89	0.43
1:B:347:ALA:O	1:B:351:LYS:HG3	2.20	0.42
4:D:405:NI9:C5	4:D:405:NI9:O2	2.66	0.42
1:B:167:GLN:OE1	1:B:207:LYS:HD2	2.20	0.42
1:C:83:CYS:O	1:C:86:MET:HB2	2.20	0.42
1:D:280:THR:HA	1:D:283:THR:HG22	2.02	0.42
1:C:89:MET:HE1	1:C:134:TRP:CB	2.49	0.42
1:C:213:TYR:CD1	1:C:243:GLY:HA2	2.55	0.42
1:C:11:TYR:HB2	1:C:85:TRP:CZ2	2.55	0.42
1:C:281:PHE:HB2	1:C:317:LEU:HD11	2.01	0.42
1:B:3:HIS:HA	8:B:513:HOH:O	2.19	0.42
1:C:233:LYS:HA	1:C:233:LYS:HD3	1.91	0.41
1:D:228:GLU:H	1:D:228:GLU:HG2	1.74	0.41
1:C:260:GLU:HB3	1:C:361:GLN:HE22	1.85	0.41
1:B:190:THR:HG21	1:B:195:TYR:CE1	2.55	0.41
1:D:155:VAL:HG23	1:D:214:TRP:CZ3	2.56	0.41
1:D:114:TYR:O	1:D:119:VAL:O	2.38	0.41
1:D:155:VAL:O	1:D:159:VAL:HG23	2.21	0.41
1:C:242:MET:HG2	1:C:354:TRP:CE3	2.55	0.41
1:A:29:ASP:OD2	1:A:32:ARG:HG3	2.20	0.41
1:B:237:LYS:O	1:B:241:VAL:HG23	2.20	0.41
1:D:26:PHE:HA	1:C:206:TYR:CZ	2.56	0.41
1:A:301:ASP:HA	1:A:302:PRO:HD3	1.96	0.41
1:C:132:LEU:HD23	8:C:559:HOH:O	2.21	0.41
1:C:179:LYS:HA	1:C:179:LYS:HD3	1.87	0.41
1:A:101:MET:HE1	1:B:125:ILE:HG22	2.03	0.40
1:C:195:TYR:C	1:C:279:VAL:HG22	2.41	0.40
1:A:206:TYR:CZ	1:B:26:PHE:HA	2.57	0.40
1:C:93:HIS:O	1:C:97:GLU:HG2	2.21	0.40
1:A:272:ALA:HA	1:A:297:TYR:CE2	2.57	0.40
1:D:272:ALA:HA	1:D:297:TYR:CE2	2.56	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	355/362 (98%)	341 (96%)	13 (4%)	1 (0%)	41	50
1	B	356/362 (98%)	346 (97%)	9 (2%)	1 (0%)	41	50
1	C	356/362 (98%)	347 (98%)	6 (2%)	3 (1%)	19	23
1	D	358/362 (99%)	349 (98%)	7 (2%)	2 (1%)	25	31
All	All	1425/1448 (98%)	1383 (97%)	35 (2%)	7 (0%)	29	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	B	263	GLY
1	D	2	ALA
1	D	287	ALA
1	C	360	ARG
1	C	66	THR
1	C	259	PRO

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	301/303 (99%)	292 (97%)	9 (3%)	41	57
1	B	299/303 (99%)	288 (96%)	11 (4%)	34	48
1	C	301/303 (99%)	293 (97%)	8 (3%)	44	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	301/303 (99%)	285 (95%)	16 (5%)	22	31
All	All	1202/1212 (99%)	1158 (96%)	44 (4%)	34	48

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	183	LYS
1	A	188	ASN
1	A	196	THR
1	A	198	PHE
1	A	232	LYS
1	A	247	GLN
1	A	257	THR
1	A	352	VAL
1	B	1	MET
1	B	232	LYS
1	B	262	LEU
1	B	270	GLU
1	B	277	LEU
1	B	283	THR
1	B	288	GLU
1	B	299	SER
1	B	316	ASN
1	B	326	LYS
1	B	328	VAL
1	D	1	MET
1	D	12	GLU
1	D	67	GLN
1	D	104	SER
1	D	174	MET
1	D	188	ASN
1	D	211	TYR
1	D	273	LYS
1	D	277	LEU
1	D	290	VAL
1	D	311	LEU
1	D	315	GLN
1	D	318	LEU
1	D	334	GLN
1	D	342	GLN
1	D	359	LYS

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Mol	Chain	Res	Type
1	C	1	MET
1	C	5	GLU
1	C	36	LEU
1	C	232	LYS
1	C	257	THR
1	C	273	LYS
1	C	279	VAL
1	C	322	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	236	HIS
1	B	3	HIS
1	B	236	HIS
1	B	249	GLN
1	B	296	ASN
1	D	67	GLN
1	D	188	ASN
1	D	236	HIS
1	D	247	GLN
1	D	296	ASN
1	C	67	GLN
1	C	91	GLN
1	C	236	HIS
1	C	249	GLN
1	C	361	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NI9	A	406	3	17,18,18	1.51	2 (11%)	25,29,29	0.91	0
7	MES	D	401	-	12,12,12	2.20	1 (8%)	14,16,16	7.72	11 (78%)
5	PEG	A	407	-	6,6,6	0.51	0	5,5,5	0.19	0
6	ACT	D	402	-	1,3,3	1.57	0	0,3,3	0.00	-
4	NI9	C	405	3	17,18,18	1.51	2 (11%)	25,29,29	1.12	3 (12%)
4	NI9	B	405	3	17,18,18	1.81	2 (11%)	25,29,29	0.92	0
4	NI9	D	405	-	17,18,18	1.72	3 (17%)	25,29,29	1.01	2 (8%)
6	ACT	B	402	-	1,3,3	1.59	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NI9	A	406	3	-	14/23/23/23	0/1/1/1
7	MES	D	401	-	-	4/6/14/14	0/1/1/1
5	PEG	A	407	-	-	2/4/4/4	-
4	NI9	C	405	3	-	14/23/23/23	0/1/1/1
4	NI9	B	405	3	-	5/23/23/23	0/1/1/1
4	NI9	D	405	-	-	5/23/23/23	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	401	MES	C8-S	-7.19	1.67	1.77
4	B	405	NI9	P2-C1	-4.41	1.82	1.85
4	B	405	NI9	P1-C1	-4.28	1.82	1.85
4	D	405	NI9	P2-C1	-4.21	1.82	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	405	NI9	P1-C1	-3.76	1.82	1.85
4	A	406	NI9	P1-C1	-3.52	1.82	1.85
4	C	405	NI9	P1-C1	-3.36	1.82	1.85
4	C	405	NI9	P2-C1	-3.22	1.82	1.85
4	A	406	NI9	P2-C1	-2.48	1.83	1.85
4	D	405	NI9	P1-O4	-2.01	1.51	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	MES	O1S-S-C8	-19.49	83.45	106.92
7	D	401	MES	O2S-S-C8	-15.18	88.64	106.92
7	D	401	MES	O3S-S-C8	-11.15	87.74	105.77
7	D	401	MES	C5-N4-C3	5.17	120.46	108.83
7	D	401	MES	C7-N4-C5	3.82	121.00	111.23
7	D	401	MES	O3S-S-O2S	3.60	120.08	111.27
7	D	401	MES	C2-C3-N4	-3.56	104.71	110.10
7	D	401	MES	C6-C5-N4	-2.97	105.61	110.10
7	D	401	MES	C7-N4-C3	2.85	118.53	111.23
4	C	405	NI9	O6-P1-C1	-2.79	102.55	109.86
7	D	401	MES	O3S-S-O1S	2.66	117.76	111.27
4	C	405	NI9	C2-N-C5	2.14	121.33	119.62
4	D	405	NI9	O3-P2-O1	2.08	113.85	107.99
7	D	401	MES	O2S-S-O1S	2.07	121.12	113.95
4	C	405	NI9	O3-P2-O1	2.04	113.75	107.99
4	D	405	NI9	C2-N-C5	2.02	121.23	119.62

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	401	MES	C7-C8-S-O1S
7	D	401	MES	C7-C8-S-O2S
7	D	401	MES	C7-C8-S-O3S
4	B	405	NI9	P1-C1-C2-N
4	B	405	NI9	P2-C1-C2-N
4	A	406	NI9	O2-C1-C2-N
4	A	406	NI9	P1-C1-C2-N
4	A	406	NI9	P2-C1-C2-N
4	A	406	NI9	O2-C1-P1-O4
4	A	406	NI9	O2-C1-P1-O6
4	A	406	NI9	O2-C1-P1-O7

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Mol	Chain	Res	Type	Atoms
4	A	406	NI9	C2-C1-P1-O4
4	A	406	NI9	C2-C1-P1-O6
4	A	406	NI9	C2-C1-P1-O7
4	A	406	NI9	P2-C1-P1-O4
4	A	406	NI9	P2-C1-P1-O6
4	A	406	NI9	P2-C1-P1-O7
4	C	405	NI9	O2-C1-C2-N
4	C	405	NI9	P1-C1-C2-N
4	C	405	NI9	P2-C1-C2-N
4	C	405	NI9	O2-C1-P1-O4
4	C	405	NI9	O2-C1-P1-O6
4	C	405	NI9	O2-C1-P1-O7
4	C	405	NI9	C2-C1-P1-O4
4	C	405	NI9	C2-C1-P1-O6
4	C	405	NI9	C2-C1-P1-O7
4	C	405	NI9	P2-C1-P1-O4
4	C	405	NI9	P2-C1-P1-O6
4	C	405	NI9	P2-C1-P1-O7
4	C	405	NI9	C1-C2-N-C3
4	C	405	NI9	C1-C2-N-C5
4	D	405	NI9	O2-C1-C2-N
4	D	405	NI9	P1-C1-C2-N
4	D	405	NI9	P2-C1-C2-N
5	A	407	PEG	O2-C3-C4-O4
5	A	407	PEG	O1-C1-C2-O2
4	A	406	NI9	C1-C2-N-C3
4	D	405	NI9	C1-C2-N-C3
4	D	405	NI9	C1-C2-N-C5
7	D	401	MES	C8-C7-N4-C3
4	B	405	NI9	P1-C1-P2-O5
4	B	405	NI9	O2-C1-C2-N
4	A	406	NI9	C1-C2-N-C5
4	B	405	NI9	O2-C1-P2-O5

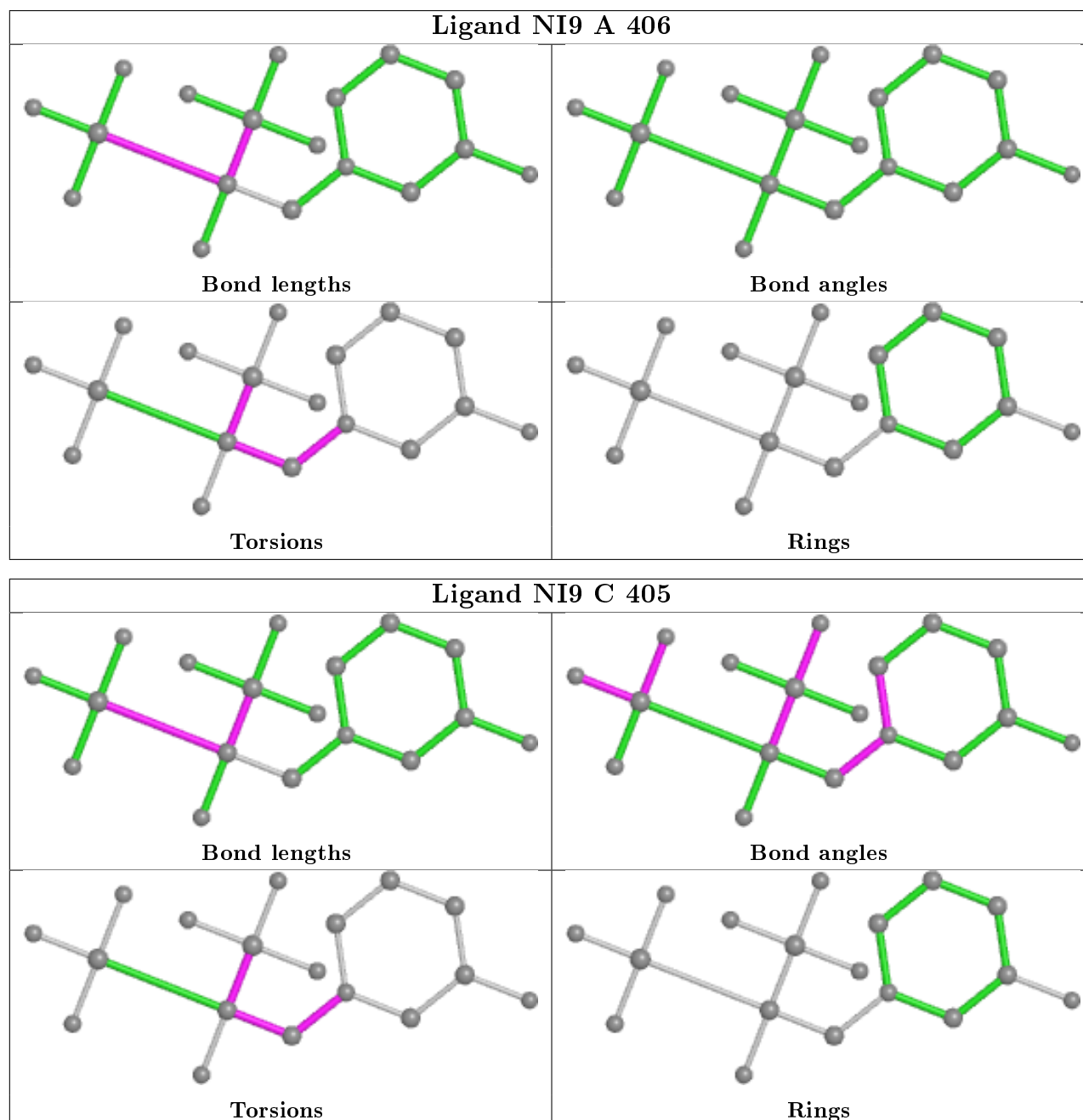
There are no ring outliers.

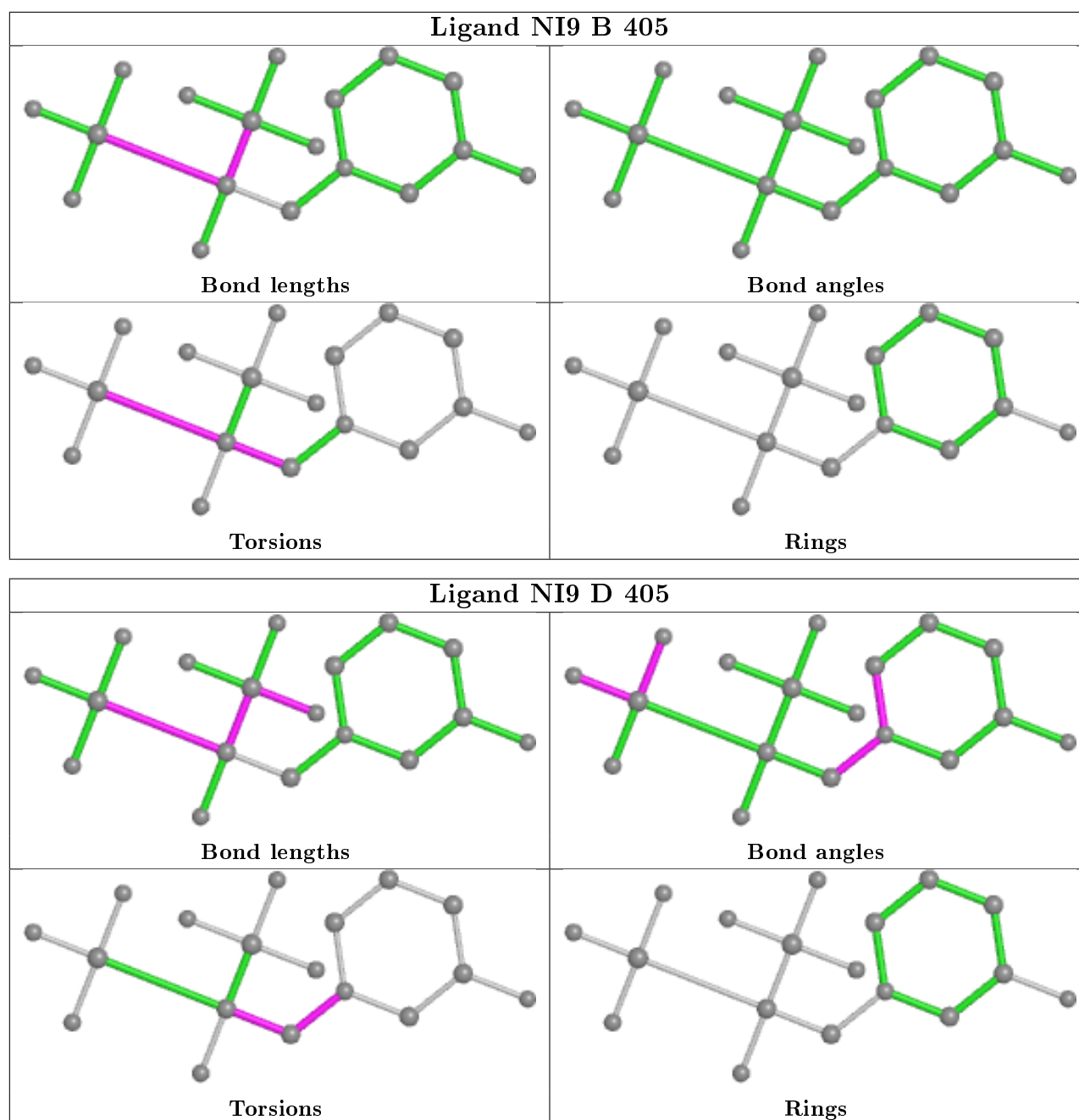
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	PEG	1	0
4	D	405	NI9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	358/362 (98%)	0.31	17 (4%) 31 38	31, 44, 65, 72	0
1	B	358/362 (98%)	0.40	18 (5%) 28 35	33, 50, 68, 82	0
1	C	360/362 (99%)	0.23	14 (3%) 39 46	32, 44, 65, 80	0
1	D	360/362 (99%)	0.54	24 (6%) 17 23	30, 49, 77, 84	0
All	All	1436/1448 (99%)	0.37	73 (5%) 28 35	30, 46, 72, 84	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	305	VAL	5.8
1	A	68	MET	5.6
1	C	263	GLY	5.3
1	B	262	LEU	5.1
1	D	265	ILE	4.7
1	C	265	ILE	4.7
1	C	261	LYS	4.4
1	A	1	MET	4.3
1	A	259	PRO	4.2
1	A	67	GLN	4.0
1	B	259	PRO	4.0
1	D	258	PRO	4.0
1	D	189	THR	4.0
1	D	317	LEU	4.0
1	D	259	PRO	3.9
1	B	65	ASP	3.9
1	D	296	ASN	3.8
1	C	1	MET	3.7
1	B	3	HIS	3.7
1	D	295	ALA	3.6
1	D	286	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	259	PRO	3.4
1	B	336	ILE	3.4
1	A	260	GLU	3.3
1	B	66	THR	3.3
1	B	358	TYR	3.3
1	C	266	GLY	3.1
1	B	354	TRP	3.1
1	D	1	MET	3.1
1	B	1	MET	3.0
1	D	260	GLU	2.9
1	A	63	ALA	2.9
1	B	260	GLU	2.7
1	D	277	LEU	2.7
1	A	360	ARG	2.7
1	B	258	PRO	2.7
1	B	297	TYR	2.7
1	C	65	ASP	2.7
1	A	265	ILE	2.7
1	D	256	PHE	2.6
1	C	360	ARG	2.6
1	B	263	GLY	2.6
1	C	177	SER	2.6
1	D	289	LYS	2.6
1	A	165	ILE	2.6
1	B	342	GLN	2.6
1	A	305	VAL	2.5
1	D	131	LEU	2.5
1	C	340	GLU	2.5
1	A	186	HIS	2.5
1	D	360	ARG	2.4
1	A	187	ALA	2.4
1	D	309	LYS	2.4
1	B	20	GLY	2.3
1	C	361	GLN	2.3
1	B	337	ALA	2.3
1	D	312	TYR	2.3
1	A	340	GLU	2.3
1	B	299	SER	2.3
1	D	132	LEU	2.2
1	B	343	ASN	2.2
1	C	260	GLU	2.2
1	A	304	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	228	GLU	2.2
1	D	334	GLN	2.2
1	C	168	LEU	2.2
1	D	267	THR	2.1
1	C	358	TYR	2.1
1	D	359	LYS	2.1
1	A	109	GLY	2.1
1	A	329	VAL	2.0
1	D	134	TRP	2.0
1	D	339	LEU	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	407	7/7	0.73	0.33	59,62,63,63	0
6	ACT	D	402	4/4	0.74	0.17	71,71,71,71	0
4	NI9	B	405	18/18	0.79	0.21	134,135,135,135	0
6	ACT	B	402	4/4	0.88	0.13	73,73,73,73	0
4	NI9	D	405	18/18	0.88	0.20	99,100,101,101	0
4	NI9	A	406	18/18	0.90	0.17	85,87,88,88	0
2	NA	A	403	1/1	0.91	0.24	41,41,41,41	0
4	NI9	C	405	18/18	0.91	0.20	83,83,84,85	0
7	MES	D	401	12/12	0.93	0.19	77,79,80,81	0
3	MG	C	404	1/1	0.94	0.23	35,35,35,35	0
3	MG	C	403	1/1	0.94	0.07	35,35,35,35	0
2	NA	C	401	1/1	0.95	0.13	43,43,43,43	0
2	NA	A	401	1/1	0.95	0.32	43,43,43,43	0

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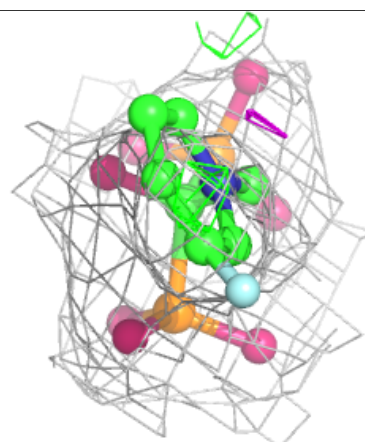
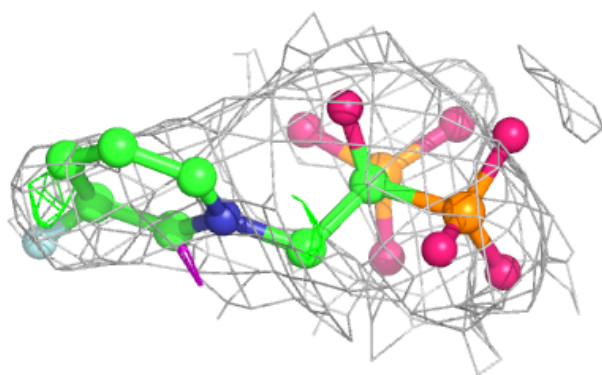
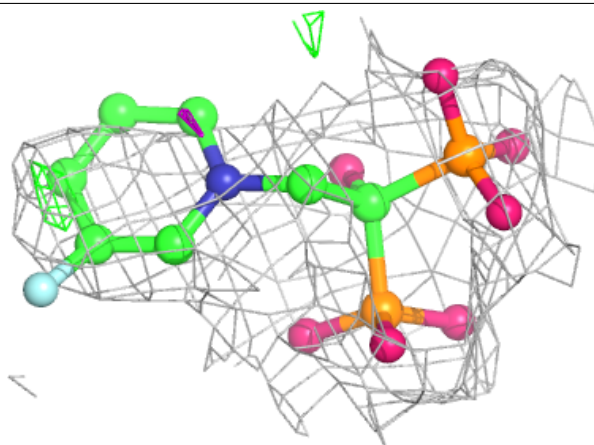
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	403	1/1	0.95	0.23	40,40,40,40	0
2	NA	B	401	1/1	0.96	0.22	50,50,50,50	0
2	NA	A	402	1/1	0.96	0.15	31,31,31,31	0
3	MG	A	404	1/1	0.97	0.08	32,32,32,32	0
3	MG	D	404	1/1	0.97	0.17	29,29,29,29	0
2	NA	C	402	1/1	0.97	0.23	39,39,39,39	0
3	MG	B	404	1/1	0.97	0.14	28,28,28,28	0
3	MG	D	403	1/1	0.99	0.18	50,50,50,50	0
3	MG	A	405	1/1	0.99	0.26	37,37,37,37	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.

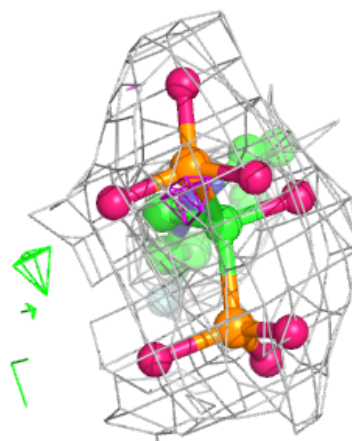
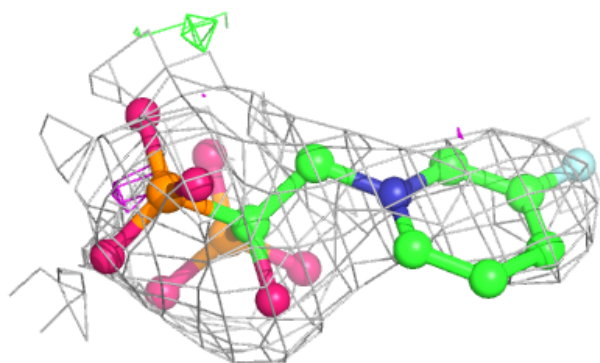
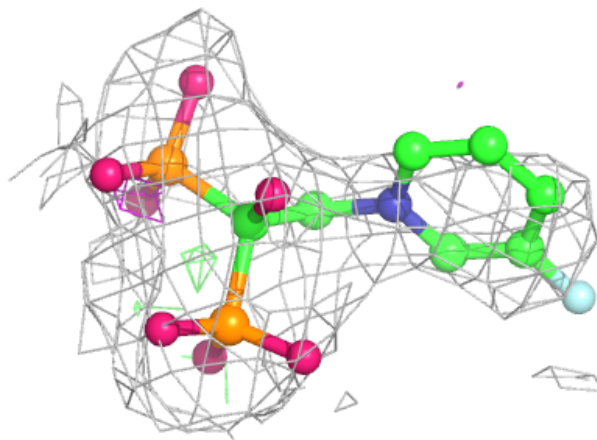
Electron density around NI9 B 405:

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



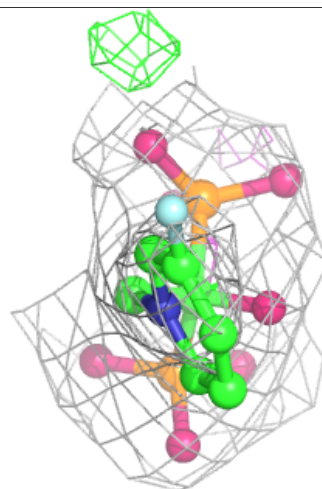
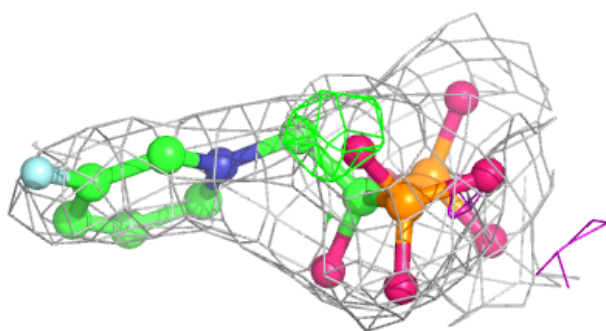
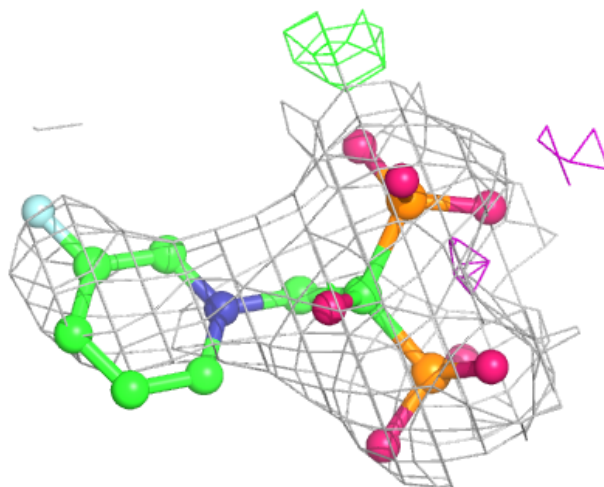
Electron density around NI9 D 405:

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



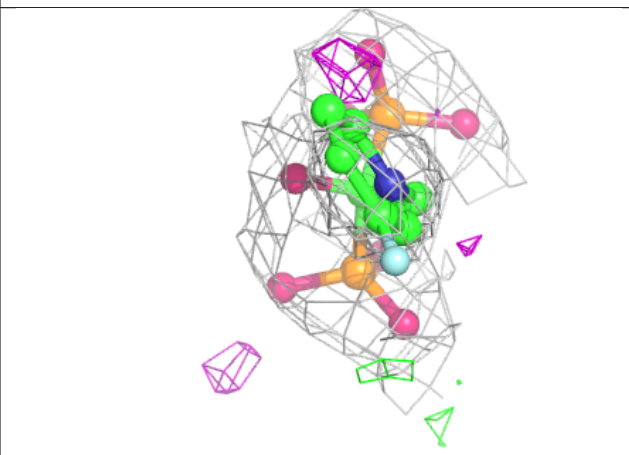
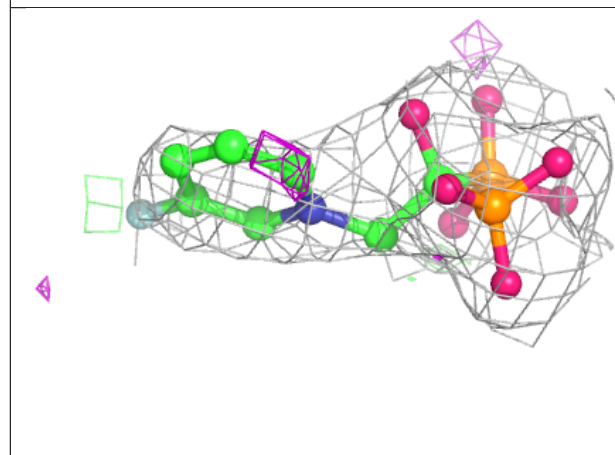
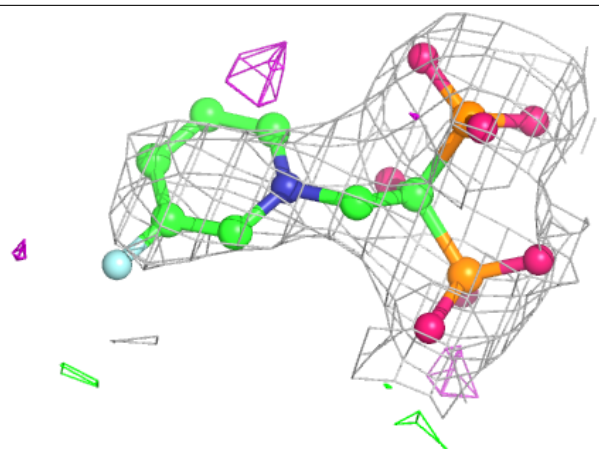
Electron density around NI9 A 406:

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



Electron density around NI9 C 405:

$2mF_o-DF_c$ (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.